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MATHEMATICAL MODELING OF EXPERIMENTS WITH THE HELP OF INVERSE PROBLEMS

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The problem of interpreting observations under conditions when the properties of the object of interest depend on the state of the object is studied. A procedure that permits studying an experiment from the viewpoint of achieving maximum information from it is proposed and justified on the basis of linear abstract models.

In the last few years the theory of the analysis of measurements based on the use of solutions of inverse problems has been developing rapidly. In thermal physics the well-known works [1-4] as well as many other investigations are devoted to this subject.

We shall analyze, based on the approach proposed by the theory of inverse problems, the information content of an experiment as a problem of determining the conditions under which the maximum information about an object can be obtained with a limited number of tests on the object and finite sampling of observations of the state of the object. In this connection we shall pose and study the following questions.

First, we shall determine the maximum volume of information that can be extracted from observations of a single function of state of the object. Second, we shall establish the nature of the experiment as well as where and how observations which will permit determining simultaneously a number of parameters characterizing the sought properties of the object should be performed. Finally, third, we shall determine how an experiment should be planned so that the required values can be determined with minimum error of identification taking into account the effect of a wide class of measurement noise and modeling errors.

We shall define the relation between the observed state u, the action on the object f, and the sought properties of the object $a = \{a_k\}_{k = 1,\ p}$ in the form of the following equation:

$$L_a u = f. \tag{1}$$

It is assumed everywhere below that Eq. (1) has a unique and stable solution u for fixed values of a and f, and it is also assumed that the domain D of the operator L_a does not depend on the values of a sought.

We shall obtain the answer to the first question assuming that the model (1) is given in the form of a superposition of commuting operators. In this case the following theorem holds.

Theorem 1. To determine all properties of an object described by the model (1), where $L_a \equiv \sum_{k=1}^{p} a_k L_k$, a_k = const, it is necessary and sufficient to perform a single experiment in which observations of the state $u \notin U_* = \left\{u_*: \sum_{k=1}^{p} \lambda_k L_k u_* = 0\right\}$, where $\lambda_k = \text{const}, \exists\, i,\ j \in [1,\ p] : \lambda_i,\ \lambda_j \neq 0.$ can be performed.

Proof. Necessity. Assume that among the states $u \in D$ of the model (1) there exists a state u_* to which on a set of coefficients A there correspond nonunique values $a' \neq a''$. Subtracting from one another Eqs. (1) with these values of the coefficients we obtain

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$$\sum_{k=1}^{p}(a_k' - a_k'')L_k u_* = 0.$$

From here we obtain the following condition for the linear dependence of the terms in the equation of interest:

$$\sum_{k=1}^{p}\lambda_k L_k u_* = 0, \ \lambda_k \in \Lambda, \tag{2}$$

where Λ is a set that contains at least two elements different from zero.

The condition (2) shows that all states of the object can be divided into two groups. The one-to-one correspondence between its state and the properties breaks down in one group and is preserved in the other group.

The breakdown of the one-to-one correspondence means that among the observations there can be states u_* which are invariants relative to transformations of the quantity sought. When the one-to-one correspondence is preserved there is no invariance and to each function of state there corresponds a unique element in the set A.

Thus we find that observations of a unique state u, which does not belong to the subspace $U_* = \left\{u_* : \sum_{k=1}^{p}\lambda_k L_k u_* = 0\right\}$, permit finding simultaneously all values $\{a_k\}_{k=\overline{1,p}}$ but if $u \in U_*$ then no further observations of the state can eliminate the breakdown of the uniqueness of the identification of the coefficients $\{a_k\}_{k=\overline{1,p}}$.

Sufficiency. To the given function $u_* \in D$ we associate the following functional:

$$J(a) = \int_Q \left(\sum_{k=1}^{p} a_k L_k u_* - f\right)^2 dQ.$$

With respect to the coefficients $\{a_k\}$ the functional J(a) is quadratic and positive-definite. For this reason, under variations of u_* it will have a unique minimum, in which the given function u_* satisfies Eq. (1). The condition for J(a) to have a minimum leads to the system

$$Sa = g, \tag{3}$$

where

$$s_{ij} = \int_Q L_i u_* L_j u_* dQ, \ g_i = \int_Q f L_i u_* dQ, \ i, \ j = \overline{1, p}.$$

From the assumption that there exists a solution $u \in D$ of Eq. (1) for all $a \in A$ it follows that the problem (3) can be solved. The condition for its solution to be nonunique is that both the principal and additional determinants of the system (3) must vanish; this is expressed in the form of a linear dependence of the terms of the equation under study. Then specifying a state that does not satisfy the condition (2) means that it is possible to determine uniquely all values of $\{a_k\}_{k=\overline{1,p}}$ from observations $u \notin U_*$. This is what we were required to prove.

The foregoing analysis answers the question posed above regarding the amount of information that can be extracted from observations of a single function of state. It turns out that a single experiment in which the appearance of the states u_*, satisfying the condition that the terms in the given equation are linearly independent, is excluded permits finding simultaneously all phenomenological properties of the object. This result shows that it is in principle possible to obtain maximum information from an experiment under conditions when the total number of tests is limited.

We shall now establish the form of the subset of nonuniqueness A_* and we shall determine the properties of the free term f_* with which the existence of the invariance of Eq. (1) with respect to the coefficients as noted above is related.

If the operators in Eq. (1) commute, i.e., $\forall i, j \in [1, p] : L_i L_j = L_j L_i$ then operating with them on both sides of the equation under study and adding the terms multiplied by the coefficients $\lambda_k \in \Lambda$ we obtain an analogous condition of linear dependence for the elements of the image space of Eq. (1). Therefore the condition (2) determines the subspace whose elements under the mapping (1) with mutually commuting operators retain the property of linear dependence.

Next, by expressing from the condition (2) any term in Eq. (1) it is posible to find the form of the families of the subset of nonuniqueness A_* as well as the form of the equation whose solution is a function that satisfies the condition of linear dependence (2). As a result we obtain the following corollary.

COROLLARY 1. If the solution of Eq. (1) with mutually commuting operators satisfies the condition (2), then the coefficients in the equation belong to the family

$$\lambda_p a_i - \lambda_i a_p = \rho_i, \ i = \overline{1, p-1}, \tag{4}$$

the free term f_* also satisfies the condition of linear dependence

$$\sum_{k=1}^{p} \lambda_k L_k f_* = 0, \ \lambda_k \in \Lambda, \tag{5}$$

and the state u^* is determined as the solution of the equation

$$\sum_{k=1}^{p-1} \rho_k L_k u_* = \lambda_p f_*. \tag{6}$$

In this case the highest-order operator L_p is singled out, so that the family (4) found above establishes a one-parameter dependence of the coefficients of Eq. (1) relative to a_p. Expressing the latter in terms of the coefficients of the family (4) it is possible to prove that other representations of the one-parameter dependence with the same composition of nonzero parameters $\lambda_k \in \Lambda$, but obtained with the help of other terms in Eq. (2) are equivalent.

If the number of coefficients p > 2, then new linearly dependent terms which will lead to a two-parameter family and will reduce the order of the equation found can be singled out in Eq. (6). Therefore the subset of nonuniqueness of Eq. (1) contains different families of coefficients from one-parameter up to (p − 1)-parameter families.

We note that the condition (5) holds for any λ_k, when $f \equiv 0$, i.e., in the case that the model (1) is homogeneous. Then the one-parameter family from the subset of nonuniqueness A_* has the form $a_k/a_p = \lambda_k$. It shows that all coefficients of the homogeneous equation with independent boundary conditions can be found only to within the ratio λ_k. This well-known property is supplemented by the results obtained above. It turns out that aside from the one-parameter family the homogeneous equation (1) admits the existence of other families ranging from two-parameter up to (p − 1)-parameter to within which the coefficients of the model can be determined given the observations u_*.

Thus the nonuniqueness of the mapping from the space of states into the space of coefficients of Eq. (1) is expressed in the existence of a family of the type (4), all terms of which correspond to one and the same solution u_* satisfying (6). The one-to-one correspondence breaks down only for certain f_*, which must satisfy the condition (5). For thermophysical processes the results obtained show that among the temperature fields there exist fields u_* which are preserved, if the actions on the object are chosen according to (5), while the thermophysical properties and the conditions of heat transfer change, as in (4).

Having studied the information content from the viewpoint of the number of experiments performed on an object in order to determine all of its properties we shall now determine the conditions that must be imposed on the observations in order to ensure that the indicated set of properties is found at the same time. The answer to this question is given by the following theorem on the basis of the determinate formulation under study and under the same assumptions about the form of the model representation of the object.

THEOREM 2. The model (1) is identifiable relative to the parameters $\{a_k\}_{k=\overline{1, p}}$ according to the sample $\{u|_{x_i}\}_{i=\overline{1, m}}$ when the observations and the actions on the object exclude satisfaction of the conditions

$$\sum_{i=1}^{p} \lambda_i L_k u|_{x_i} = 0, \ \ k = \overline{1, p}, \tag{7}$$

$$\sum_{i=1}^{p} \lambda_i f|_{x_i} = 0, \tag{8}$$

where $\lambda_i = \text{const}, \exists\, i,\ j \in [1,\ p] : \lambda_i,\ \lambda_j \neq 0.$

Proof. If the set $\{u|_{x_i}\}_{i=\overline{1,\ m}}$ is a discrete sampling of observations of the solution of Eq. (1) under the assumption that there is not noise in the measurements, then the values of the coefficients sought must satisfy the following system of equations:

$$\sum_{k=1}^{p} a_k L_k u|_{x_i} = f|_{x_i},\quad i = \overline{1,\ m}. \tag{9}$$

In order for this system to have a solution the condition m = p must hold; this condition shows the minimum size of the sample of observations required for finding all coefficients $(a_k)_{k=\overline{1,\ p}}$. This number of observations is predicated on the possibility of calculating the values of $L_k u|_{x_i}$. Since we are talking about the solution of practical problems, when the measurements are performed on a discrete set for all independent variables, we note that to determine p unknown properties of the object we must add to the number of observations m = p on which an approximation of the values $L_k u|_{x_i}$ cannot be constructed observations that ensure that the function u from (1) is determined uniquely for given values of a. Such observations are the starting and boundary conditions.

The system (9) has a nonunique solution if its principal and auxiliary determinants vanish. Therefore the impossibility of determining all coefficients of the model (1) from $\{u|_{x_i}\{_{i=\overline{1,\ m}}\}$ is expressed by the conditions of linear dependence (7) and (8) and, conversely, linear independence of the terms of the equation means that the parameters $\{a_k\}_{k=\overline{1,\ p}}$ can be identified from the observations $\{u|_{x_i}\}_{i=\overline{1,\ m}}$. This is what we were required to prove.

Thus performing a single experiment and carrying out observations of a state which excludes satisfaction of the conditions of linear dependence found above both as a whole for the entire function of state and in particular for a sample of observations of the state permits finding immediately all coefficients of the mathematical model. This result shows in the general case that when multiple physical modeling of the object is impossible and also when the technical means of the experiment are limited the information content of the experiment can still reach a maximum if the observations are appropriately planned.

For a thermophysical experiment this conclusion means in particular, that in determining the coefficients of heat capacity and thermal conductivity it is generally speaking, not necessary to find beforehand the conditions of heat transfer for the sample. The results obtained show that data from one experiment contain all information about the process occurring. Because of this condition of heat transfer for the sample the thermophysical properties of the sample can be found at the same time, and in so doing it is not necessary to perform additional experiments, but the conditions for maintaining a one-to-one correspondence should be satisfied. For example, for a thermal model of the form

$$a_1 \frac{\partial u}{\partial t} = a_2 \sum_{l=1}^{r} \frac{\partial^2 u}{\partial x_l^2} + a_3 u + f(x,\ t)$$

these conditions are expressed by the linear independence of the terms $\partial \mu/\partial t$, $\partial^2 u/\partial x_\ell^2$, 6}, with whose help the form of the temperature fields and the coordinates of the measurement points, making it possible to determine simultaneously the heat capacity, thermal conductivity, and coefficient of heat transfer can be determined simultaneously.

We note that the question of the maximum number of thermal parameters sought was first posed and solved in [5]. Since under the conditions examined above no restrictions are placed on the form of the operators L_k the conclusion that it is possible to determine simultaneously quantities which do not belong to the subset of nonuniqueness can also be generalized and extended to the widest class of processes and phenomena described by linear equations.

The results obtained reflect the general functional properties of mathematical models for which there is no unique correspondence between the coefficients in the equation and the solution of the equation. The manifestation of these properties is determined by specifying the boundary conditions and external actions. We shall study their determination for the example of the equation

$$a_1L_1u + a_2L_2u = f, \tag{10}$$

which is assumed to be given in a region Q with the boundary $\partial Q = G_1 \cup G_2$, on which the solution u satisfies the boundary conditions

$$K_iu|_{G_i} = \varphi_i, \ i = 1,\ 2, \tag{11}$$

where $L_{1,2}$ are given linear operators; $K_{1,2}$ are the corresponding linear operators of the boundary conditions, one of which, for example K_1, determines the Cauchy conditions on the boundary G_1; and, f and $\varphi_{1,2}$ are known functions.

It is assumed that there exists a unique function u satisfying (10) and (11) while the functions f and $\varphi_{1,2}$ are smooth enough so that the values of $L_{1\ 2}f$, $K_1f|G_1$, $K_2f|G_2$, $L_1\varphi_2$, $L_2\varphi_1$. can be determined. In this case the following theorem holds.

THEOREM 3. The one-to-one correspondence in the problem (10) and (11) breaks down when and only when its solution is the function $u_* = \rho^{-1}L_1^{-1}f$, for the existence of which it is necessary and sufficient that the boundary conditions

$$K_1\varphi_2|_{G_1} = K_2\varphi_1|_{G_2}, \tag{12}$$

be satisfied, the free term f_* must satisfy the equation

$$\lambda L_1f_* = L_2f_*,\ \lambda \neq 0 \tag{13}$$

with the conditions

$$\lambda K_1f_*|_{G_1} = \rho L_2\varphi_1, \tag{14}$$

$$K_2f_*|_{G_2} = \rho L_1\varphi_2 \tag{15}$$

and the coefficients are given from the single family

$$a_1 + \lambda a_2 = \rho. \tag{16}$$

The theorem is proved analogously to the proof given in [5].

For applications the following corollary is important.

COROLLARY 2. If the conditions (12) and (13) hold, then the one-to-one correspondence in (10) and (11) is ensured by the homogeneous conditions $L_1\varphi_2=0$ u $L_2\varphi_1=0$ $K_1f|_{G_1}=0$ u $K_2f|_{G_2}=0$.

Analysis of the cases in which the conditions under which the one-to-one correspondence (13)-(15) breaks down have terms that vanish identically gives the following corollary.

COROLLARY 3. All solutions of the problem (10) and (11) are described by the function

$$u_* = \frac{K_1f|_{G_1} - a_2L_2\varphi_1}{a_1K_1f|_{G_1}} L_1^{-1}f, \tag{17}$$

if the boundary conditions $K_1\varphi_2|_{G_1} = K_2\varphi_1|_{G_2}$, are consistent, and the requirements $K_2f|_{G_2} = 0$, $L_{1,2}f = 0$, $L_1\varphi_2 = 0$, $K_1f|_{G_1}/L_2\varphi_1 = \text{const.}$ are satisfied.

The existence of solutions of the form (17) means that for any $a \in A$ the formulation of the problem (10) and (11) has linearly dependent terms. In this case the subset of non-uniqueness is the entire starting set of coefficients, $A^* \equiv A$, and for this reason it contains an infinite number of families of the type (16). This does not contradict theorem 3, since the infinity of families is associated with different solutions of the problem (10) and (11), to each of which their corresponds a unique family (16). An example of such a formulation is presented in [5].

The results obtained permit giving the following final answers to the questions posed above.

First, to find the maximum volume of information about the properties of an object it is necessary and sufficient to perform a single experiment. In the case of the class of linear abstract models studied above the corresponding observations must satisfy both on the whole and in particular the conditions of linear independence of the terms in the starting equation. In order for the latter conditions to hold in practical problems a number of simple requirements must be met.

Second, strictly defined boundary conditions and external action on the object are necessary in order for the one-to-one correspondence between the function of state and its coefficients to break down. The difference from them can serve as a criterion of identifiability of the properties sought. In addition it should be kept in mind that there exist models all of whose states are unidentifiable on the whole.

Thus, summarizing, we can say that if a preliminary analysis of the experiment is performed from the viewpoint of ensuring that the conditions for preserving one-to-one correspondence are satisfied then the sample of observations obtained in this case not only contains complete information about the properties of the object but it also permits determining them uniquely.

In conclusion we note that the study of the properties of an experiment taking into account noise in the measurements and errors in modeling is a subject for further study, the results of which will be presented in a following paper.

NOTATION

L_a, starting mathematical model; Q, range of variation of the independent variables; ∂Q — ee boundary of the region Q; A, region of admissible solutions; A_*, subset of nonuniqueness; λ and ρ, parameters of the subset of nonuniqueness; U_*, subset of unidentifiable states; u_*, unidentifiable states; and, x_i, points of observation.

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