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IDENTIFICATION OF PHYSICAL PROCESSES AND INVERSE PROBLEMS

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General procedures of parametric and structural identification are considered as are inverse problems as their methodological basis.

The progress of physical processes in different media (gases, liquids, solids) can be assessed according to some external phenomena that are recorded by special devices. Relying on the results of observations (measurements) as well as on general physical laws and regularities, the process being studied can be compared to some mathematical model. The development and founding of the mathematical models are often called identification.

A mathematical model (MM) as an abstract means of the approximate representation (mapping) of a real process in order to investigate it is the mathematical description of substantial factors of the process and its interconnections. A certain set of models, distinguished particularly by the number of factors being taken into account and by the completeness and accuracy of description of the process, respectively, on the one hand and by the complexity of the model on the other, can ordinarily be compared to the identical process. One of the main requirements on a MM is the need to take account of all fundamental factors and interconnections of the process under consideration and the elimination of the secondaries. The selection of a model is dictated primarily by the purpose of the investigation being performed, here the tendency is always ultimately to simplify the model so as to make its practical application possible and convenient.

Therefore, the first step in the mathematical formulation of a problem in the general case is reasonable construction of the model structure, i.e., a qualitative description of the process under investigation by using some operators. This procedure is called structural identification.

Differential operators most often comprise the basis of mathematical models of physical processes. Models with lumped parameters described by ordinary differential equations and models with distributed parameters described by partial differential equation are differentiated.

The second step in the mathematical formulation of a problem is the "allotment" of the model of quantitative information, i.e., the determination (estimation) of the unknown characteristics (model parameters) in the structural MM. This stage is called parametric identification.

Structure and parametric identification of physical processes are closely related to the solution of inverse problems for differential equations. The formulations of direct problems, each of which can be compared with a certain set of inverse problems within the framework of the model being identified are assumed known in the formalization of the general formulations and extractions of the fundamental classes of inverse problems. Characteristic examples of inverse problems are presented below.

SYSTEMS WITH LUMPED PARAMETERS

Let the process being investigated be characterized by n dependences of the scalar argument t (variables of coordinates of the process): $y(t) = [y_1(t), \ldots, y_n(t)]^T$, and in conformity with a certain mathematical model this vector will satisfy a system of ordinary differential equations of the form

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$$\frac{dy}{dt} = A(t)y + g(t),\ y(0) = 0, \tag{1}$$

where $g(t) = [g_1(t), \ldots, g_n(t)]^T$, and T is the symobl for the transpose

$$A(t) = \begin{bmatrix} a_{11}(t) & a_{12}(t) & \ldots & a_{1n}(t) \\ a_{21}(t) & a_{22}(t) & \ldots & a_{2n}(t) \\ \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ a_{n1}(t) & a_{n2}(t) & \ldots & a_{nn}(t) \end{bmatrix}.$$

Unknown quantities are contained among the components of the vector g(t) and the matrix A(T), and they must be determined by means of the known vector $z(t) = [z_1(t), z_2(t), \ldots, z_l(t)]^T$, $l \leqslant n$, (from the measurement results) that is linearly related to the vector y(t): z(t) = C(t)y(t), where C(t) is a given matrix.

This formulation of the inverse problem corresponds to identification of the vector equation (1) with known initial data. A particular case is a problem with matrix A and vector g constant in time.

The inverse problem formulation considered must be relied upon in many applications, particularly in the investigation of the thermal regimes of engineering objects. If the method of partitioning the object into n isothermal elements is used and it is assumed that the heat-transfer process is realized by heat conduction and convection, then the heat balance equation written for each element will form the following system

$$C_k \frac{dT_k}{d\tau} = \sum_{j=1}^{n} \lambda_{kj}(T_j - T_k) + Q_k,\ k = \overline{1, n},\ \tau \in (0, \tau_m],$$
$$T_k(0) = T_{0k},\ k = \overline{1, n}, \tag{2}$$

where $T_k(\tau)$ is the temperature of the k-th element, C_k is its bulk specific heat, λ_{kj} are the heat transfer coefficients (thermal conductivities) between elements with numbers k and j, and Q_k is the quantity of heat acting on the k-th element, and τ is the time.

The inverse problem for the system (2) consists of finding some causal characteristics C_k, λ_{kj}, Q_k by means of certain information about the temperature state of the object.

SYSTEM WITH DISTRIBUTED PARAMETERS

As an illustration, let us consider the problem of heat conductivity in two solids, with different thermophysical characteristics that are in contact. Let the domains of the three-dimensional space $E_3(xOyz)$, occupied by these bodies be Ω_1 and Ω_2 and their common boundary surface (the contact surface) S_{12}. The external boundary surfaces of these bodies (the body surfaces with the exception of S_{12}) will be S_1 and S_2, respectively. We assume that a change in the geometric characteristics of the surface mentioned can occur with the lapse of time in the general case (for instance, because of material departure from the body surface, linear expansion, or thermal contractions). Let the time segment $[0, \tau_m]$, $\tau_m < +\infty$ be considered.

We write the heat-conduction equations in these bodies by assuming that heat sources of intensity Q_1 and Q_2, respectively, act within them:

$$C_1 \frac{\partial T_1(P, \tau)}{\partial \tau} = \operatorname{div}[\lambda_1 \operatorname{grad} T_1(P, \tau)] + Q_1,\ P \in \Omega_1,\ \tau \in (0, \tau_m];$$
$$C_2 \frac{\partial T_2(P, \tau)}{\partial \tau} = \operatorname{div}[\lambda_2 \operatorname{grad} T_2(P, \tau)] + Q_2,\ P \in \Omega_2,\ \tau \in (0, \tau_m],$$

where T_1 and T_2 are the temperature fields of the mentioned bodies, and C_i, λ_i are their bulk specific heats and heat-conduction coefficients (i = 1, 2).

We append the initial temperature distribution

$$T_1(P,\ 0) = \psi_1(P),\ P \in \Omega_1;\ T_2(P,\ 0) = \psi_2(P),\ P \in \Omega_2,$$

and the adjoint conditions on the contact surface that take account of the equality of the thermal flux densities and the temperature discontinuity of the first kind

$$\lambda_1 \frac{\partial T_1}{\partial n_{12}}\bigg|_{S_{12}} = \lambda_2 \frac{\partial T_2}{\partial n_{12}}\bigg|_{S_{12}},\ (T_2 - T_1)|_{S_{12}} = R\lambda_1 \frac{\partial T_1}{\partial n_{12}}\bigg|_{S_{12}}.$$

to these equations. Here n_{12} is the direction of the interior normal to S_{12} and R is the thermal contact resistance.

We can give as conditions on the external surface ($s \in S_i$, $\tau \in (0, \tau_m]$, $i=1, 2$):

Boundary conditions of the first kind $T_i(s, \tau) = \varphi_i(s, \tau)$;

Of the second kind — $\lambda_i \dfrac{\partial T_i(s,\ \tau)}{\partial n_i} = f_i(s,\ \tau)$, where n_i is the direction of the interior normal to ths surface S_i;

Of the third kind $-\lambda_i \dfrac{\partial T_i(s,\ \tau)}{\partial n_i} = \alpha_i(T_i(s,\ \tau) - T^*(\tau))$, where α_i are convective heat-elimination coefficients between solids and the environment; T* is the temperature of the temperature of the environment, or if we take $h_i = \alpha_i/\lambda_i$, $\xi_i = h_i T^*$, $\partial T_i(s,\ \tau)/\partial n_i + h_i T_i(s,\ \tau) = \xi_i(s,\ \tau)$;

Boundary conditions taking account of heat transfer from the body to the environment by convection and radiation from its surface, as well as the thermal effect q*(T(s, τ)) due to other physicochemical processes (melting, evaporation, atom recombination, etc.):

$$-\lambda_i \frac{\partial T_i(s,\ \tau)}{\partial n_i} = \alpha_i(T_i(s,\ \tau) - T^*(\tau)) + \varepsilon_i \sigma T_i^4(s,\ \tau) + q^*,$$

where ε_i is the radiation coefficient of the surface S_i and σ is the Stefan—Boltzmann constant.

The coefficients C_i, λ_i, Q_i, i = 1, 2, as well as the quantities R, α_i, h_i, ε_i, i = 1, 2, can be assumed constants, functions of the spatial coordinates x, y, z and (or) the time τ, functions of the temperature, and in the general case, functions of the variables T, x, y, z, τ.

If any quantities from the set of causal characteristics $\{C_i,\ \lambda_i,\ Q_i,\ \psi_i,\ R,\ \varphi_i,\ f_i,\ \alpha_i,\ T^*,\ h_i,\ \xi_i,\ \varepsilon_i\}$, $i = 1, 2$, are unknown and they and the temperature field T(x, y, z, τ) must be found in the domain $\bar{\Omega}_1(\tau) \cup \Omega_2(\tau)$ in a known time segment $[0, \tau_m]$ by means of the known remaining causal characteristics and the additional conditions $T(M_j, \tau) = f_j(\tau)$, $j = \overline{1,\ m}$, where $M_j \in \bar{\Omega}_1 + \bar{\Omega}_2$ are neither fixed points or those that change position with the lapse of time, then we have an inverse problem for the heat-conduction equation.

Let us choose the formulation of the inverse problem when quantities averaged over a certain volume v_j

$$\bar{T}_j(\tau) = \frac{1}{v_j} \int_{v_j} T(x,\ y,\ z,\ \tau)\, dv.$$

are known rather than values of the temperatures at the points M_j. Such a case must be considered if it is impossible to consider the dimensions of the thermal sensors used to measure the temperature in the body as negligibly small.

Let us also note that in certain cases (usually sufficiently scarce) the need may occur for averaging the measurements not only with respect to space but also with respect to time, i.e., the finiteness of the interval during which the value of the temperature is determined must be taken into account.

Strictly speaking, it would be more correct to consider the formulation of the inverse problem with the inclusion of the measuring apparatus, the thermocouples, say, in the body since they cause distortion of the temperature field in a certain neighborhood of their placement. However, such problems are awkward and difficult to realize in computational respects. Consequently, the tendency is ordinarily to set up the experiment in such a manner as to eliminate the distorting influence of the sensors from the considerations (for instance, to diminish their dimensions maximally, to derive the thermocouple electrodes along isotherms, etc.) or to take this influence into account by inserting a correction into the measurement results.

Inverse problems for other equations of parabolic, elliptic, and hyperbolic type, to which gasdynamics, heat and mass transfer, radiation transport, elasticity theory, quantum mechanics, etc., problems reduce, can also be formulated analogously.

Remark. The inverse problem formulations are considered above as physical process identification problems. Other formulations are also possible, among which inverse problems of the technical object design type and the systems control type should be extracted.

In designing an object on the basis of the mathematical model taken the design characteristics entering into this model are selected by starting from the requisite technico-economic and exploitational indices. The desired characteristics are causal with respect to the quality indices of the object, i.e., the the design problem can be formulated as an inverse problem.

In the case of systems control (physical, mechanical, etc.), the role of the causal characteristics is performed by the control actions (the input variables) whose change realizes some kind of control effect that is expressed in terms of the variable states of the system (output variables). Determination of the input in terms of the output variables can also be treated as an inverse problem of the control type.

It must be noted that one distinction in principle exists between inverse problems of the identification type and inverse problems of the design or control type. Extension of the class of allowable solutions for the latter usually improves the situation since any technically realizable solution assuring an extremum of the quality criterion with a given accuracy must be found in these problems. At the same time, the broader the class of the possible solutions for identification problems, the greater can the error be in determining the causal characteristics, which requires certain utilization of regular methods of solution.

PARAMETRIC IDENTIFICATION

We shall later understand the mathematical model of a certain physical process to be a set of equations and relationships characterizing this process, including the initial and boundary conditions for the differential equations.

We assume that the structure of the MM of the process is given but certain model characteristics require quantitative definition, i.e., the parametric identification problem must be solved. Let us write it in operator form. We introduce the following notation: u is the desired quantity (a constant, vector, function, or vector-function), considered as an element of a certain normed space U; y is a variable state of the process that belongs to the normed space Y (for the MM described by partial differential equations of elliptic type, y is the function $x = (x_1, x_2, \ldots, x_p)$, $x \in \Omega$, where Ω is the domain of spatial variables, therefore, in this case $y = y(x, u)$; if nonstationary problems described by parabolic or hyperbolic equations are considered, then $y = y(x, \tau, u)$, where $\tau \in (0, \tau_m)$ is the time variable), G is a given operator generated by the structural mathematical model taken for the process ($G:U \to Y$); is connects the elements u and y: $Gu = y$, $u \in U$, $y \in Y$; f is a known quantity (input data) considered as an element of the normed space F related to the variable state of the process by means of the operator B: $f = By$, $B:Y \to F$.

In an exact formulation, the inverse problem has the form

$$Au = f \tag{3}$$

with exactly assigned initial data $A = BG$ and f. Here values of the variable state of the process at certain points of the domain of spatial variables under consideration are most often taken as f. These points can be fixed or can change position with the lapse of time.

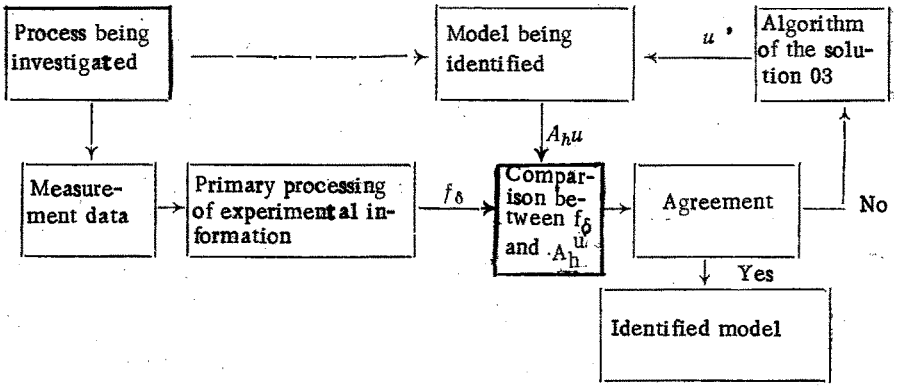

Fig. 1. Block diagram of parametric identification.

A variational approach to the solution of the problem (3) is to minimize the functional $J(u)=\|Au-f\|_F^2$ in a certain set $D \subseteq U$, containing the exact solution u: $\inf J(u)$, $u \in D$.

However, such a method of solving the parametric identification problem cannot possibly be applied directly because the problem (3) is usually unstable (the inverse operator A^{-1} turns out to be unbounded) and in practice just certain approximations A_h and f_δ are known instead of the exact data A and f.

The inaccuracy in giving the initial data can be due, in particular, to the approximate quantitative description of the known causal characteristics in the operator A and to the presence of random and systematic errors in the right side of f. In addition the passage to approximate initial data is associated with the fact that an appropriate computational algorithm is constructed for the numerical solution of (3) in which the operator A is usually approximated by a certain finite-dimensional operator while the vector-functions u and f are parametrized.

Taking account of the remarks made, the identification problem is reduced to the determination of a certain approximation in the given $\{A_h, f_\delta\}$ to the desired solution $u_{h\delta} = F_A(A_h, f_\delta)$, which would assure all the better approximation to the exact solution of the problem (3) in a certain sense, as the errors in giving the operator and the right side tend to zero.

The parametric identification process is displayed schematically in the figure. Comparing the characteristic of the response f_δ from the real object of investigation with the results of solving the direct problem $A_h u$ for a given approximation to the quantity being variated u permits making a conclusion about the correctness of "adjusting" the mathematical model for numerical values of the vector u, i.e., about the quantitative adequacy of the MM for the physical process.

In application to heat-conduction and heat-transfer processes in engineering systems, the computational model can be represented in the following abstract form:

$$A_h[\alpha_{TPC}, T_0, \Phi, \Gamma, T, g, x, \tau] = f_\delta, \tag{4}$$

where A_h is an operator approximating the operator A of the differential model and giving the structure of the computational model, it governs the relationship between the thermophysical characteristics (given by using the vector α_{TPC}), the initial temperature distribution (the vector T_0), the geometric characteristics Φ conditions, or their parameters Γ discretized by the temperature field T, the loading action g, and certain information about the temperature field f.

The vector f_δ is ordinarily comprised of time series corresponding to the discrete representation of the temperature dependence on the time for the selected points of the space.

In the formulation (4), some of the quantities from the numbers α_{TPC}, T_0, Φ, Γ are the desired characteristics. The process of selecting their approximations is organized in such a manner as to match the residual to the accuracy of the initial data, which is defined by the measurement errors, the recording and decoding of the experimental information, and also the errors in linearization and approximation in solving the problem.

Let us note that in many cases the need to use results of measuring the temperature at a larger number of points than is required for a unique determination of the desired charac-

teristics occurs in the identification of the MM parameters. The passage to overdefined formulations of inverse problems ordinarily permits more confident data to be obtained.

CRITERION FOR THE ADEQUACY OF THE MATHEMATICAL MODEL

Assuming that sufficiently complete information can be obtained about the field of physical quantities (for example, the temperature field) in the form of given f, we introduce a criterion for adequacy of the MM of the actual process

$$\eta = \eta(A) = \sup_{f \in F_0} \inf_{u \in U} \| Au - f \|_F ,$$

where $F_0 \subseteq F$ is a certain set of possible states of the process under investigation that should be described by the given MM.

Since the state of the process is a result of some loading actions, these actions, thermal loads, say, are variated in such a manner in calculating η as to include the domain of possible utilization of the model being developed, which is characterized by the operator A.

In practice, in place of η a certain approximation $\eta_{h\delta}$ is available which is calculated for inaccurately given A_h and f_δ. However, in the majority of cases a "good" approximation can be obtained for the operator A and only the error in the experimental data is taken into account. Then the decision about the degree of adequacy of the MM is made by starting from the quantity $\varepsilon(\eta, \max_{f \in F_0} \delta_f)$ in the inequality $\eta_\delta(A) \leqslant \varepsilon$. Here $\delta_f = \|f_\delta - f\|_F$ is the error in giving a certain realization f from F_0.

The residual $\Delta = \|Au - f_\delta\|_F$ can be taken as the distance between two elements in the functional space L_2. Assuming that f is a n-dimensional vector function (n dependences on the spatial coordinates and the time), we write

$$\Delta = \left\{ \int_0^{\tau_m} \int_\Omega [z(x, \tau) - f_\delta(x, \tau)]^T [z(x, \tau) - f_\delta(x, \tau)] \, d\Omega d\tau \right\}^{1/2}, \quad (5)$$

where $z(x, \tau) = Au$ is the "reaction" of the model corresponding to a certain approximation to u.

If f is a scalar (for instance, one measurement was performed at each point of space at each time), the expression (5) takes the form

$$\Delta = \left\{ \int_0^{\tau_m} \int_\Omega [z(x, \tau) - f_\delta(x, \tau)]^2 \, d\Omega d\tau \right\}^{1/2} .$$

In practice the case is extent when measurements are realized at individual points of space and the function $f(x, \tau)$ cannot be restored with acceptable accuracy. Then the residual is taken in the form

$$\Delta = \left\{ \int_0^{\tau_m} [z - f_\delta]^T \, W [z - f_\delta] \, d\tau \right\}^{1/2} ,$$

where $W = W(z, f_\delta, \tau)$ is a weight function whose selection is determined by the conditions of conducting the experiment and the measurements.

Residuals written in an uniform metric, $\Delta = \max_{x, \tau} |z - f_\delta|$, say, can also be used.

STRUCTURAL IDENTIFICATION

It is ordinarily assumed in solving structural identification problems that there is *a priori* information about the process being investigated that permits postulation of some set of possible MM, and it is then necessary to solve the questions of whether the process "belongs" to one of them on the basis of a determination of its most important singularities.

Let us represent the "learning" MM of the process in the provisional operator-vector form

$$A_k [\alpha_k, \ \beta_k, \ \vartheta_k^1, \vartheta_k^2, \ldots, \vartheta_k^{m_k}, \ g_k, \ x_k, \ \tau] = f_k^j, \ k = 0, \ 1, \ldots, \ j = \overline{1, m_k} , \quad (6)$$

where in the general case A_k are nonlinear operators governing the correspondence between the vectors (vector-functions) of the known structural characteristics of the model α_k, the fields of the physical quantities $\vartheta_k^j(\alpha_k, \beta_k, g_k, x_k, \tau)$, the loading actions g_k, and the initial data f_k^j which are certain information about the fields of the physical quantities, x_k is the spatial variable in the coordinate system taken in the k-th iteration, τ is the time, and m_k is the number of physical quantities being considered in the k-th iteration. The subscript k denotes the number of the approximation to the desired operator A and the vector β for which acceptable adequacy of the MM to the physical process under investigation (a completely learned model) is observed.

Therefore, in this formulation the structure of the operator is not determined to the end, it is unknown whether to include some terms in the model, to take into account the nonlinearity, etc. All these indeterminacies are gradually exposed, i.e., the A_k and β_k are formed from the condition of exposure of some qualitative features of the model in each approximation to the desired MM. The strategy of successive refinement is often used. Initially the simplest model is formulated from the number of predictables, and its adequacy to the process is verified within the limits of previously stipulated accuracy. If this condition is not satisfied the model is made complicated (for instance, the vector of the desired structural singularities is extended) and its adequacy is again verified. And so on until the desired result has been obtained. Let us note that the iterative process of sorting the model is heuristic to a great extent.

In many cases the structural identification includes parametric identification and can be realized in the following form.

Let us assume there is a certain approximation to the structural features of the model characterized by the vector β_ζ. For a given loading action g_l^I, to which the fields ϑ_l^{jI}, $j=\overline{1, m_l}$, correspond, let experimental information be obtained about these fields in the form of a certain vector quantity f_l^{jI}, $j=\overline{1, m_l}$. Usually this is continuous or discrete measurements in time at fixed or moving points of space.

Considering the data f_l^{jI} or part of them as input information, inverse problems are solved in order to restore numerical values of components of the vector β_ζ from experiment. The residual

$$\Delta_l^I = \| A_l[\alpha_l, \beta_l, \vartheta_l^{1I}, \vartheta_l^{2I}, \ldots, \vartheta_l^{m_lI}, g_l^I, x_l, \tau] - f_l^{jI} \|_F .$$

is computed from these data.

If $\Delta_l^I > \delta_l^I$, where δ_l^I is the error in the input data f_l^{jI} in the metric of the space F, then a deduction can at once be made about the unsatisfactory selection of the approximation β_ζ and the necessity of going over to another structure of the model.

If $\Delta_l^I \leqslant \delta_l^I$, then this MM is not excluded from the number of "doubtful" models, however, its adequacy must be verified in application to other loading actions g_l^i, $i=\overline{2, I}$, which should include all practical situations of subsequent utilization of the model to a sufficient degree. For all g_ζ^i the residuals Δ_ζ^i are computed. The model is usually considered adequate to the real process if the residual agrees with the errors in the input data as follows:

$$\Delta_l^i \leqslant \delta_l^i, \quad i = \overline{1, I} . \tag{7}$$

If the residual for certain g_ζ exceeds the error in the input data, a decision is made about the correction of the numerical values of the components of the vector β_ζ. The correction can be made by using the solution of inverse problems for other data f_l^{ji}, $i=\overline{2, I}$, with a subsequent verification of the adequacy by means of conditions of the type (7). If it turns out here that such quantitative data as satisfy the accuracy required do not exist for the vector β_ζ, the model is converted to another structure determined by a new operator $A_{\zeta+1}$ and the procedure described is repeated. And so on until a consistent mathematical model is found for the domain under consideration for its practical application.

Only the loading actions were variated in this analysis, however, the numerical values of the components of the vector α can also be variated.

The procedures elucidated above for parametric and structural identification are the modern approach to the development of MM for physical processes. This approach which is based on a mathematical description in the system states space and on inverse problem methodology often turns out to be the only one possible for the construction of mathematical models of complex nonlinear heat and mass transfer processes.