BINARY CORRESPONDENCES
AND THE INVERSE PROBLEM OF CHEMICAL KINETICS[♯]

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Abstract. We show how binary correspondences can be used for simple formalization of the notion of problem, definition of the basic components of problems, their properties, and constructions. In particular, formalization of the following notions is presented: condition, data, unknowns, and solutions of a problem, solvability and unique solvability, inverse problem, composition and restriction of problems, isomorphism between problems. We also consider topological problems and the related notions of stability and correctness. A connection is indicated between the stability and continuity of a uniquely solvable topological problem. The definition of parametrized set is given. The notions are introduced of parametrized problem, the problem of reconstruction of an object by the values of parameters, as well as the notions of locally free set of parameters and stability with respect to a set of parameters.

As an illustration, we consider a singularly perturbed system of ordinary differential equations which describe a process in chemical kinetics and burning. Direct and inverse problems are stated for such a system. We extend the class of problems under study by considering polynomials of arbitrary degree as the right-hand sides of the differential equations. It is shown how the inverse problem of chemical kinetics can be corrected and made more practical by means of the composition with a simple auxiliary problem which represents the relation between functions and finite sets of numerical characteristics being measured. For the corrected inverse problem, formulas for the solution are presented and the conditions of unique solvability are indicated. Within the study of solvability, a criterion is established for linear independence of functions in terms of finite sets of their values. With the help of the criterion, realizability is clarified of the condition for unique solvability of the inverse problem of chemical kinetics.

Key words: binary correspondence, inverse problem, solvability, composition, stability, correctness, differential equation, chemical kinetics, linear independence.

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We continue the study started in [1, 2] which is devoted to formalization of the notion of problem and solution of the inverse problem of chemical kinetics. In particular, we extend the class of problems under study by considering polynomials of arbitrary degree as the right-hand sides of the differential equations.

1. Formalization of the notion of problem

In this section, we employ binary correspondences for formalizing the notion of problem, basic components of problems, their properties, and constructions: the condition of a problem, data and unknowns, solvability and unique solvability, inverse problem, composition and rest-

riction of problems. We also consider topological problems, the related notions of stability and correctness, and problems with parameters.

1.1. By a *problem* we mean an arbitrary correspondence between the elements of two sets, i. e., a triple $P = (A, B, C)$, where A and B are any sets and $C \subseteq A \times B$. The sets A, B, and C (i. e., the set of departure, the set of destination, and the graph of the correspondence P) are denoted by $\operatorname{Dom} P$, $\operatorname{Im} P$, and $\operatorname{Gr} P$ and called the *domain of data*, the *domain of unknowns*, and the *condition* of the problem P. The containment $(a, b) \in \operatorname{Gr} P$ is written as $P(a, b)$ and is treated as the condition expressing the fact that the unknown b corresponds to the data a. Therefore, the problem P assumes the following informal interpretation:

Given data $a \in \operatorname{Dom} P$, find unknowns $b \in \operatorname{Im} P$ which meet the condition $P(a, b)$.

The *image* $P[X]$ and *preimage* $P^{-1}[Y]$ of subsets $X \subseteq \operatorname{Dom} P$ and $Y \subseteq \operatorname{Im} P$ with respect to the correspondence P are defined by the traditional formulas

$$P[X] = \{b \in \operatorname{Im} P : \ (\exists\, x \in X) \ P(x, b)\},$$
$$P^{-1}[Y] = \{a \in \operatorname{Dom} P : \ (\exists\, y \in Y) \ P(a, y)\}.$$

1.2. A *solution* to a problem P for a data instance $a \in \operatorname{Dom} P$ is an arbitrary unknown $b \in \operatorname{Im} P$ which meets the condition $P(a, b)$. The set of solutions to P for a is denoted by $P[a]$. Therefore,

$$P[a] = P[\{a\}] = \{b \in \operatorname{Im} P : \ P(a, b)\}, \quad a \in \operatorname{Dom} P.$$

A problem P is *solvable* for $a \in \operatorname{Dom} P$ whenever $P[a] \neq \varnothing$, i. e., given a, the problem P has at least one solution. The domain of definition of the correspondence P

$$\operatorname{dom} P := \{a \in \operatorname{Dom} P : \ P[a] \neq \varnothing\}$$

is called the *domain of solvability* of the problem P. If $\operatorname{dom} P = \operatorname{Dom} P$, the problem P is called *solvable* or, more precisely, *everywhere solvable*.

1.3. A problem P is said to be *uniquely solvable for $a \in \operatorname{Dom} P$* if, given a, the problem P has a unique solution, i. e., $P[a] = \{b\}$ for some $b \in \operatorname{Im} P$. The corresponding solution b is denoted by $P^{\mathrm{s}}(a)$. Therefore, if P is uniquely solvable for a then

$$P[a] = \{P^{\mathrm{s}}(a)\}.$$

The set

$$\operatorname{dom} P^{\mathrm{s}} := \{a \in \operatorname{Dom} P : \ P \text{ is uniquely solvable for } a\}$$

is called the *domain of unique solvability* of the problem P, and the function

$$P^{\mathrm{s}} \colon \operatorname{dom} P^{\mathrm{s}} \to \operatorname{Im} P, \quad a \mapsto P^{\mathrm{s}}(a)$$

is called the *solution function* of the problem P. Obviously, $\operatorname{dom} P^{\mathrm{s}} \subseteq \operatorname{dom} P \subseteq \operatorname{Dom} P$. The problem P is *uniquely solvable on a set $D \subseteq \operatorname{Dom} P$* if $D \subseteq \operatorname{dom} P^{\mathrm{s}}$. The problem P is called *uniquely solvable* or, more precisely, *everywhere uniquely solvable* if it is uniquely solvable on $\operatorname{Dom} P$, i. e., $\operatorname{dom} P^{\mathrm{s}} = \operatorname{Dom} P$. In this case, the correspondence P is an everywhere defined function and thus coincides with P^{s}.

1.4. Given a problem $P = (\operatorname{Dom} P, \operatorname{Im} P, \operatorname{Gr} P)$, the *inverse problem* is the inverse correspondence

$$P^{-1} := \big(\operatorname{Im} P, \operatorname{Dom} P, (\operatorname{Gr} P)^{-1}\big), \quad \text{where } (\operatorname{Gr} P)^{-1} = \{(b, a) : \ (a, b) \in \operatorname{Gr} P\}.$$

REMARK. If a problem P models a real physical process, consideration of the inverse problem P^{-1} is motivated by the search of a relatively simple formal law which describes the process with adequate accuracy. The data of the inverse problem are experimentally measurable characteristics of the process, while the unknowns are, for instance, the coefficients of a differential equation describing the process under observation.

In the case when the problem P is based on a functional equation, the formal data of the inverse problem P^{-1} are functions of the corresponding class, while, in practice, the role of data of the inverse problem is not played by the functions themselves but rather by some of their characteristics which can be measured, i. e., by certain finite sets of numbers.

The inverse problem can be suitably corrected by means of the composition (see 1.5) of the problem P^{-1} and a simple auxiliary problem which represents the relation between functions and their characteristics being measured. (An example of such correction is presented in 2.3.)

1.5. The *composition* of problems P and Q is the composition of the correspondences, which is the problem

$$Q \circ P := (\operatorname{Dom} P, \operatorname{Im} Q, \operatorname{Gr} Q \circ \operatorname{Gr} P)$$

with condition

$$\operatorname{Gr} Q \circ \operatorname{Gr} P = \big\{(a,c) \in \operatorname{Dom} P \times \operatorname{Im} Q : \ (\exists\, b \in \operatorname{Im} P \cap \operatorname{Dom} Q) \ P(a,b) \ \& \ Q(b,c)\big\}.$$

The composition $Q \circ P$ is usually considered in the case when $\operatorname{Im} P = \operatorname{Dom} Q$.

1.6. The *restriction* of a problem P onto subsets $A \subseteq \operatorname{Dom} P$ and $B \subseteq \operatorname{Im} P$ is the problem

$$P\big|_A^B := \big(A,\, B,\, \operatorname{Gr} P \cap (A \times B)\big).$$

The restrictions $P|_A := P\big|_A^{\operatorname{Im} P}$ and $P|^B := P\big|_{\operatorname{Dom} P}^B$ are particular cases.

The restriction of a problem can be defined by means of composition with the corresponding embedding problems. Given arbitrary sets X and Y, consider the problem $\operatorname{Id}_X^Y := (X, Y, I_X^Y)$, where

$$I_X^Y = \{(z,z): \ z \in X \cap Y\} = \{(x,y) \in X \times Y: \ x = y\}.$$

Then, for every problem P and any subsets $A \subseteq \operatorname{Dom} P$ and $B \subseteq \operatorname{Im} P$, the following hold:

$$P|_A = P \circ \operatorname{Id}_A^{\operatorname{Dom} P}, \quad P|^B = \operatorname{Id}_{\operatorname{Im} P}^B \circ P, \quad P\big|_A^B = \operatorname{Id}_{\operatorname{Im} P}^B \circ P \circ \operatorname{Id}_A^{\operatorname{Dom} P}.$$

1.7. An *isomorphism* between problems P and Q is a pair (f,g) of bijective mappings $f \colon \operatorname{Dom} P \to \operatorname{Dom} Q$, $g \colon \operatorname{Im} P \to \operatorname{Im} Q$ such that

$$\operatorname{Gr} Q = \big\{\big(f(a), g(b)\big) : (a,b) \in \operatorname{Gr} P\big\}.$$

Two problems are called *isomorphic* if there is an isomorphism between them.

1.8. Call P a *topological problem* if the domain of data $\operatorname{Dom} P$ and the domain of unknowns $\operatorname{Im} P$ are endowed with any topologies, i. e., the domains are topological spaces. An isomorphism (f,g) between topological problems is a *topological isomorphism* if each of the mappings f and g is a topological isomorphism (i. e., a homeomorphism).

All the notions introduced here, which are related to topologies or continuity, admit natural analogs for the case of uniformities and uniform continuity. (Metric and, in particular, normed spaces are examples of uniform spaces.) We will not present the corresponding clarified definitions, which are rather obvious.

1.9. A topological problem P is called *stable at a point* $a \in \operatorname{dom} P$ if the correspondence P is upper semi-continuous at the point, i. e., for every neighborhood V of the set $P[a]$ in $\operatorname{Im} P$, the preimage $P^{-1}[V]$ is a neighborhood of the point a in $\operatorname{dom} P$. The problem P is *stable on a set* $D \subseteq \operatorname{dom} P$ if P is stable at each point $a \in D$. The problem P is called *stable* or, more precisely, *everywhere stable* if P is stable on $\operatorname{dom} P$.

In the case when a is an interior point of $\operatorname{dom} P^{\mathrm{s}}$ relative to $\operatorname{dom} P$ (i. e., there exists an open set $G \subseteq \operatorname{Dom} P$ such that $a \in G \cap \operatorname{dom} P \subseteq \operatorname{dom} P^{\mathrm{s}}$), the stability of the problem P at a is equivalent to the continuity of the function P^{s} at a. Analogously, if a set D is included in the interior of $\operatorname{dom} P^{\mathrm{s}}$ relative to $\operatorname{dom} P$ (i. e., there exists an open set $G \subseteq \operatorname{Dom} P$ such that $D \subseteq G \cap \operatorname{dom} P \subseteq \operatorname{dom} P^{\mathrm{s}}$), then the stability of the problem P on D is equivalent to the continuity of the function P^{s} on D. In particular, the stability of a uniquely solvable problem is equivalent to its continuity.

1.10. A topological problem P is called *correct* (or, more precisely, *locally correct*) *at a point* $a \in \operatorname{Dom} P$ if a is an interior point of $\operatorname{dom} P^{\mathrm{s}}$ and the problem P is stable at a. In other words, a problem is correct at a if, for data sufficiently close to a, the problem has a unique solution, and the solution continuously depends on the data as it tends to a. A problem P is said to be *correct* (or, more precisely, *conditionally correct*) *on a set* $D \subseteq \operatorname{Dom} P$ if P is correct at each point $a \in D$. A problem P is called *correct* if P is correct on $\operatorname{Dom} P$. Therefore, the correctness of a problem means its unique solvability and stability (or, which is the same, continuity).

1.11. By a family $(v_i)_{i \in I}$ we traditionally mean a function defined on I, and the term v_i denotes the value of the function at a point $i \in I$. Given an arbitrary family $(V_i)_{i \in I}$, the symbol $\prod_{i \in I} V_i$ stands for the corresponding Cartesian product, which is the set of families $(v_i)_{i \in I}$ such that $v_i \in V_i$ for all $i \in I$. If $\pi \colon X \to \prod_{i \in I} V_i$, $i \in I$, and $J \subseteq I$, the functions

$$\pi_i \colon X \to V_i, \quad \pi_J \colon X \to \prod_{j \in J} V_j$$

are defined by the formulas

$$\pi_i(x) := \pi(x)_i \in V_i, \quad \pi_J(x) := \pi(x)|_J \in \prod_{j \in J} V_j, \quad x \in X.$$

1.12. A *parametrization* of a set X is an arbitrary injective mapping π defined on $\operatorname{Dom} \pi := \operatorname{dom} \pi = X$ and acting into the Cartesian product $\operatorname{Im} \pi := \prod_{i \in I} V_i$ of some family $(V_i)_{i \in I}$. In this case, I is called the *set of parameters* and denoted by $\operatorname{Par} \pi$, the elements $i \in \operatorname{Par} \pi$ are called *parameters*, the set $\operatorname{Im} \pi_i := V_i$ is called the *range of the parameter* i, and $\pi_i(x) \in \operatorname{Im} \pi_i$ is the *value of the parameter* i for an object $x \in X$. The product $\prod_{j \in J} V_j$ is called the *range of the set of parameters* $J \subseteq \operatorname{Par} \pi$ and denoted by $\operatorname{Im} \pi_J$.

Note that the range $\operatorname{Im} \pi_i$ of a parameter i need not coincide with the set $\operatorname{im} \pi_i = \pi_i[X]$ of the values of the parameter, i. e., the inclusion $\operatorname{im} \pi_i \subseteq \operatorname{Im} \pi_i$ can be strict. In the case of equality $\operatorname{im} \pi_i = \operatorname{Im} \pi_i$, the range of the parameter i is called *exact*.

A set endowed with a parametrization is called a *parametrized set*. By default, the parametrization of X is denoted by π or, more explicitely, by π^X.

1.13. When considering a parametrization π of a topological space X, it is natural to endow the set $\operatorname{Im} \pi_J$, where $J \subseteq \operatorname{Par} \pi$, with the image of the topology of X with respect to π_J, i. e., to assume open those subsets $U \subseteq \operatorname{Im} \pi_J$ whose preimage $\pi_J^{-1}[U]$ is open in X. In this case, π occurs a continuous mapping from X into $\operatorname{Im} \pi$ and a topological isomorphism between X and $\operatorname{im} \pi$.

The ranges $\operatorname{Im} \pi_i$ of the parameters $i \in \operatorname{Par} \pi$ usually have their own natural topologies which make the mappings π_i continuous. Otherwise, $\operatorname{Im} \pi_i$ can be endowed with the image of the topology of X with respect to π_i or with the topology induced from $\operatorname{Im} \pi$ in which the open subsets of $\operatorname{Im} \pi_i$ are the sets of the form $\{u_i : u \in U\}$, where U is open in $\operatorname{Im} \pi$.

The ranges of parameters are often Banach spaces. In this case, parametrized topological spaces are close analogs of Banach bundles (see, for instance, [3]), where the domain I of a bundle V plays the role of the set of parameters, and the stalks $V(i)$ are the ranges of parameters $i \in I$.

1.14. A problem P is called *parametrized* (or a problem *with parameters*) if its domain of data $\operatorname{Dom} P$ and domain of unknowns $\operatorname{Im} P$ are parametrized sets. Every problem can be regarded parametrized if we assume that non-parametrized domains X are endowed with trivial parametrizations having single parameter: $\pi_1(x) = x$ for all $x \in X$.

As is easily seen, the pair (π^A, π^B) is an isomorphism between a parametrized problem (A, B, C) and the problem (A', B', C'), where $A' = \operatorname{im} \pi^A$, $B' = \operatorname{im} \pi^B$, and $C' = \left\{ \left(\pi^A(a), \pi^B(b) \right) : (a, b) \in C \right\}$. Furthermore, if the problem (A, B, C) is topological then so are the problem (A', B', C') and the isomorphism (π^A, π^B).

1.15. Let π be a parametrization of a set A, $a \in A$, $J \subseteq \operatorname{Par} \pi$, $J' := \operatorname{Par} \pi \backslash J$. Denote by $\operatorname{Res}_J^a(A)$ the problem $(\operatorname{Im} \pi_J, A, R_J^a)$, where

$$R_J^a = \{ (v, b) : \ v \in \operatorname{Im} \pi_J, \ b \in A, \ \pi_J(b) = v, \ \pi_{J'}(b) = \pi_{J'}(a) \},$$

which is the problem of reconstruction of an element of A by the values of the parameters J on assuming fixed the values of the rest parameters. In the case $J = \{i\}$, we write $\operatorname{Res}_i^a(A)$ instead of $\operatorname{Res}_{\{i\}}^a(A)$.

Since π is injective, the problem $\operatorname{Res}_J^a(A)$ is uniquely solvable on the set

$$\operatorname{dom} \operatorname{Res}_J^a(A) = \{ \pi_{J'}(b) : b \in A, \ \pi_{J'}(b) = \pi_{J'}(a) \}$$

and its solution for every $v \in \operatorname{dom} \operatorname{Res}_J^a(A)$ is determined by the formula

$$\operatorname{Res}_J^a(A)^{\mathrm{s}}(v) = \pi^{-1}\left(v \otimes \pi_{J'}(a) \right), \quad \text{where} \quad (v \otimes w)_i = \begin{cases} v_i, & \text{if } i \in J; \\ w_i, & \text{if } i \notin J. \end{cases}$$

1.16. Let π be a parametrization of a topological space A, $a \in A$, $J \subseteq \operatorname{Par} \pi$. A set of parameters J is *locally free* at the point a, if the domain of solvability $\operatorname{dom} \operatorname{Res}_J^a(A)$ of the problem $\operatorname{Res}_J^a(A)$ is a neighborhood of the point $\pi_J(a)$ in the topological space $\operatorname{Im} \pi_J$. Therefore, a locally free set of parameters realizes all sufficiently small changes of values with the values of the rest parameters fixed. A parameter i is *locally free* at a if so is the set $\{i\}$.

1.17. Let P be a parametrized topological problem, $a \in \operatorname{dom} P$, and let $J \subseteq \operatorname{Par} \pi$, where $\pi := \pi^{\operatorname{dom} P}$. The problem P is *stable at the point a with respect to J*, if the problem $P \circ \operatorname{Res}_J^a(\operatorname{dom} P)$ is stable at the point $\pi_J(a)$. Stability of a problem at a with respect to J is usually considered in the case when the set of parameters J is locally free at the point a.

The problem P is *stable on a set $D \subseteq \operatorname{dom} P$ with respect to J*, if P is stable at each point $a \in D$ with respect to J. The problem P is *stable with respect to J* if P is stable on $\operatorname{dom} P$ with respect to J. In the case $J = \{i\}$, the term *stability with respect to the parameter i* is used.

If the natural topology on $\operatorname{im} \pi_J$ is considered and a is an interior point of $\operatorname{dom} P^{\mathrm{s}}$ relative to $\operatorname{dom} P$, the stability of a uniquely solvable problem P at the point a with respect to J is equivalent to the continuity at a of the function

$$v \in \pi_J[\operatorname{dom} R] \;\mapsto\; P^{\mathrm{s}}\left(R^{\mathrm{s}}(v)\right), \quad \text{where} \quad R := \operatorname{Res}_J^a(\operatorname{Dom} P).$$

The latter, in its turn, means that the solution $P^{\mathrm{s}}(b)$ continuously depends on the values $\pi_J(b)$ of the parameters J as $\pi_J(b)$ tend to $\pi_J(a)$ with the equality $\pi_{J'}(b) = \pi_{J'}(a)$ preserved.

1.18. Let P be a parametrized topological problem, $i \in \operatorname{Par} \pi$. The problem P is called a "problem with small parameter i" if $\operatorname{Im} \pi_i \subseteq \mathbb{R}$, the number 0 is a limit point of $\operatorname{Im} \pi_i$, and a question is under consideration about any asymptotic behavior of P for the values of i close to 0, for instance, about the stability of P with respect to i at a point a with $\pi_i(a) = 0$.

2. The inverse problem of chemical kinetics

As an illustration, we consider a singularly perturbed system of ordinary differential equations which arises in modeling certain processes of chemical kinetics and burning (see, for instance, [4,5]). Within the study of the corresponding inverse problem, a criterion will be established for linear independence of functions in terms of finite sets of their values (see 2.5).

2.1. Suppose that $m, n \in \mathbb{N}$, $X := \mathbb{R}^m$, Y is a domain in $\mathbb{R}^n$, $T := \mathbb{R}$, $0 < \varepsilon_0 \in \mathbb{R}$. Put $E := \{\varepsilon \in \mathbb{R} : 0 \leqslant \varepsilon \leqslant \varepsilon_0\}$, $F := C(X \times Y \times T \times E, \mathbb{R}^m)$, $G := C(X \times Y \times T \times E, \mathbb{R}^n)$.

Consider the problem P with domain of data $\operatorname{Dom} P = F \times G \times E$, domain of unknowns $\operatorname{Im} P = C^1(T, X) \times C^1(T, Y)$, and condition

$$P((f, g, \varepsilon), (x, y)) \;\Leftrightarrow\; \begin{cases} \dot{x}(t) = f(x(t), y(t), t, \varepsilon), \\ \varepsilon\, \dot{y}(t) = g(x(t), y(t), t, \varepsilon) \end{cases} \quad \text{for all } t \in T,$$

where $f \in F$, $g \in G$, $\varepsilon \in E$, $x \in C^1(T, X)$, $y \in C^1(T, Y)$.

Solution of the problem P is based on the method of integral manifolds (see [6–8]), a convenient tool for studying multidimensional singularly perturbed systems of differential equations which makes it possible to lower the dimension of the system under study.

In the problem P, the number ε plays the role of "small parameter" thus splitting the system into "slow" and "fast" subsystems:

$$\dot{x}(t) = f(x(t), y(t), t, \varepsilon) \quad \text{and} \quad \varepsilon\, \dot{y}(t) = g(x(t), y(t), t, \varepsilon).$$

Solution of P in a sense reduces to solving the so called *degenerate system* which is obtained from the initial system by putting the parameter ε equal to zero. This is justified by the results of A. N. Tikhonov (see, for instance, [9]) on passing to a solution to the degenerate problem as a small parameter tends to zero.

2.2. The inverse problem to P consists in finding the unknown functions on the right-hand side of the system, given some data on the solution to the direct problem P. The close connection of the initial problem with the degenerate system motivates the study of the case $\varepsilon = 0$. We additionally assume that the "slow surface" defined by the equation

$$g\big(x, y, t, 0\big) = 0$$

consists of a single sheet (with respect to the dependence of y on x) and that the function $g \in G$ meets the condition of the implicit function theorem, which fact allows us to replace the equation

$$g(x(t), y(t), t, 0) = 0$$

by the equivalent equation of the form

$$y(t) = h(x(t), t).$$

We also assume that the right-hand side f of the main differential equation is a polynomial (which is natural for problems of chemical kinetics).

So, consider the partial case of the problem P in which $m = n = 1$, $E = \{0\}$, and the functions $f \in F$ are polynomials in two variables of degree at most $p \in \mathbb{N}$:

$$f(x, y, t, \varepsilon) \;=\; \sum_{(i,j)\in K(p)} \gamma_{ij}\, x^i y^j,$$

where $\gamma_{ij} \in \mathbb{R}$, $(i, j) \in K(p)$,

$$K(p) := \{(i, j) : \; 0 \leqslant i, j \in \mathbb{Z}, \, i + j \leqslant p\}.$$

Introduce the notation

$$\kappa(p) \; := \; \frac{(p + 1)(p + 2)}{2}$$

for the number of elements of the set $K(p)$ and fix an arbitrary enumeration

$$K(p) = \big\{(i_1, j_1), (i_2, j_2), \ldots, \big(i_{\kappa(p)}, j_{\kappa(p)}\big)\big\}.$$

Therefore, the expression $\sum_{k=1}^{\kappa(p)} \gamma_k\, x^{i_k} y^{j_k}$ is the general form of a polynomial in two variables x, y of degree at most p.

As a result of the above agreements, we arrive at the problem Q with domain of data $\mathrm{Dom}\, Q = \mathbb{R}^{\kappa(p)}$, domain of unknowns $\mathrm{Im}\, Q = C^1(\mathbb{R})^2$, and condition

$$Q\big(\gamma, (x, y)\big) \; \Leftrightarrow \; \begin{cases} \dot{x}(t) = \sum\limits_{k=1}^{\kappa(p)} \gamma_k\, x(t)^{i_k}\, y(t)^{j_k}, \\ y(t) = h(x(t), t) \end{cases} \quad \text{for all} \;\; t \in \mathbb{R},$$

where $\gamma_1, \gamma_2, \ldots, \gamma_{\kappa(p)} \in \mathbb{R}$, $x, y \in C^1(\mathbb{R})$, $h \in C^1(\mathbb{R}^2)$.

2.3. The formal inverse problem Q^{-1}, which has pairs of functions $(x, y) \in C^1(\mathbb{R})^2$ as data, is very simple and impractical. For representing the domain of data, finite collections of the values of functions or their derivatives are more adequate than everywhere defined functions. The corresponding correction of the inverse problem is realized by composition of

the problem Q^{-1} and the auxiliary problem R with domain of data $\operatorname{Dom} R = (\mathbb{R}^{\kappa(p)})^3$, domain of unknowns $\operatorname{Im} R = C^1(\mathbb{R})^2$, and condition

$$R\left((\tau,\alpha,\beta),(x,y)\right) \;\Leftrightarrow\; \begin{cases} x(\tau_1) = \alpha_1,\; x(\tau_2) = \alpha_2,\; \ldots,\; x(\tau_{\kappa(p)}) = \alpha_{\kappa(p)}, \\ \dot{x}(\tau_1) = \beta_1,\; \dot{x}(\tau_2) = \beta_2,\; \ldots,\; \dot{x}(\tau_{\kappa(p)}) = \beta_{\kappa(p)}, \end{cases}$$

where $\tau,\alpha,\beta \in \mathbb{R}^{\kappa(p)}$, $x,y \in C^1(\mathbb{R})$.

As compared to the formal inverse Q^{-1}, the composition $Q^{-1} \circ R$ is more practical and amounts to the following problem: Given $\tau,\alpha,\beta \in \mathbb{R}^{\kappa(p)}$, find the coefficients $\gamma \in \mathbb{R}^{\kappa(p)}$ for which there exist functions $x,y \in C^1(\mathbb{R})$ subject to the condition

$$\begin{cases} x(\tau_1) = \alpha_1,\; x(\tau_2) = \alpha_2,\; \ldots,\; x(\tau_{\kappa(p)}) = \alpha_{\kappa(p)}, \\ \dot{x}(\tau_1) = \beta_1,\; \dot{x}(\tau_2) = \beta_2,\; \ldots,\; \dot{x}(\tau_{\kappa(p)}) = \beta_{\kappa(p)}, \\ \dot{x}(t) = \displaystyle\sum_{k=1}^{\kappa(p)} \gamma_k\, x(t)^{i_k}\, y(t)^{j_k} \;\text{ for all }\; t \in \mathbb{R}, \\ y(t) = h\bigl(x(t),t\bigr) \;\text{ for all }\; t \in \mathbb{R}. \end{cases}$$

2.4. The following assertion can be proven for arbitrary $p \in \mathbb{N}$ in the same way as the case $p = 1$ which is considered in [10, 11].

Theorem. *If $\tau,\alpha \in \mathbb{R}^{\kappa(p)}$ meet the condition*

$$\Delta(\tau,\alpha) := \begin{vmatrix} \alpha_1^{i_1}\, h(\alpha_1,\tau_1)^{j_1} & \alpha_1^{i_2}\, h(\alpha_1,\tau_1)^{j_2} & \ldots & \alpha_1^{i_{\kappa(p)}}\, h(\alpha_1,\tau_1)^{j_{\kappa(p)}} \\ \alpha_2^{i_1}\, h(\alpha_2,\tau_2)^{j_1} & \alpha_2^{i_2}\, h(\alpha_2,\tau_2)^{j_2} & \ldots & \alpha_2^{i_{\kappa(p)}}\, h(\alpha_2,\tau_2)^{j_{\kappa(p)}} \\ \ldots & \ldots & \ldots & \ldots \\ \alpha_{\kappa(p)}^{i_1}\, h(\alpha_{\kappa(p)},\tau_{\kappa(p)})^{j_1} & \alpha_{\kappa(p)}^{i_2}\, h(\alpha_{\kappa(p)},\tau_{\kappa(p)})^{j_2} & \ldots & \alpha_{\kappa(p)}^{i_{\kappa(p)}}\, h(\alpha_{\kappa(p)},\tau_{\kappa(p)})^{j_{\kappa(p)}} \end{vmatrix} \neq 0,$$

then, given arbitrary $\beta \in \mathbb{R}^{\kappa(p)}$, the problem $Q^{-1}\circ R$ is uniquely solvable for the data (τ,α,β), and its solution $(\gamma_1,\gamma_2,\ldots,\gamma_{\kappa(p)}) = (Q^{-1}\circ R)^{\mathrm{s}}(\tau,\alpha,\beta)$ can be calculated by Cramer's formulas

$$\gamma_k = \frac{\Delta_k(\tau,\alpha,\beta)}{\Delta(\tau,\alpha)}, \quad k = 1,2,\ldots,\kappa(p),$$

where $\Delta_k(\tau,\alpha,\beta)$ is the determinant of the matrix formed from the above matrix by replacing the kth column $\bigl(\alpha_1^{i_k}\, h(\alpha_1,\tau_1)^{j_k},\, \alpha_2^{i_k}\, h(\alpha_2,\tau_2)^{j_k},\, \ldots,\, \alpha_{\kappa(p)}^{i_k}\, h(\alpha_{\kappa(p)},\tau_{\kappa(p)})^{j_k}\bigr)$ with the column $\beta = (\beta_1,\beta_2,\ldots,\beta_{\kappa(p)})$.

2.5. The following criterion clarifies the case in which there exist numbers $\tau_1,\ldots,\tau_{\kappa(p)}$ satisfying the hypothesis of Theorem 2.4.

Theorem. *Let $n \in \mathbb{N}$, let T be an arbitrary set, and let $\varphi_i \colon T \to \mathbb{R}$, $i = 1,\ldots,n$. The family of functions $\varphi_1,\ldots,\varphi_n$ is linearly independent in the vector space $\mathbb{R}^T$ if and only if there are points $t_1,\ldots,t_n \in T$ satisfying the condition*

$$\begin{vmatrix} \varphi_1(t_1) & \varphi_2(t_1) & \ldots & \varphi_n(t_1) \\ \varphi_1(t_2) & \varphi_2(t_2) & \ldots & \varphi_n(t_2) \\ \ldots & \ldots & \ldots & \ldots \\ \varphi_1(t_n) & \varphi_2(t_n) & \ldots & \varphi_n(t_n) \end{vmatrix} \neq 0\,. \tag{1}$$

◁ For convenience, introduce a notation for the matrix in (1):

$$M_n(\varphi_1, \ldots, \varphi_n; t_1, \ldots, t_n) := \begin{pmatrix} \varphi_1(t_1) & \varphi_2(t_1) & \ldots & \varphi_n(t_1) \\ \varphi_1(t_2) & \varphi_2(t_2) & \ldots & \varphi_n(t_2) \\ \ldots & \ldots & \ldots & \ldots \\ \varphi_1(t_n) & \varphi_2(t_n) & \ldots & \varphi_n(t_n) \end{pmatrix}.$$

The case $n = 1$ is trivial: if $\{\varphi_1\}$ is linearly independent then $\varphi_1 \neq 0$ and, hence, for some point $t_1 \in T$ we have $\varphi_1(t_1) \neq 0$, i. e., $|M_1(\varphi_1; t_1)| \neq 0$.

Let $n \in \mathbb{N}$ and assume that for every linearly independent family $\varphi_1, \ldots, \varphi_n \colon T \to \mathbb{R}$ there exist points $t_1, \ldots, t_n \in T$ satisfying (1). Now consider a linearly independent family $\varphi_1, \ldots, \varphi_n, \varphi_{n+1} \colon T \to \mathbb{R}$. By the induction hypothesis, there are points $t_1, \ldots, t_n \in T$ such that the matrix

$$M := M_n(\varphi_1, \ldots, \varphi_n; t_1, \ldots, t_n)$$

is invertible. We are to find a point $t \in T$ which ensures invertibility of the matrix

$$\overline{M}(t) := M_{n+1}(\varphi_1, \ldots, \varphi_n, \varphi_{n+1}; t_1, \ldots, t_n, t).$$

Assume to the contrary that $|\overline{M}(t)| = 0$ for all $t \in T$. Then, for each $t \in T$, there is a tuple $0 \neq (\alpha_1(t), \ldots, \alpha_{n+1}(t)) \in \mathbb{R}^{n+1}$ satisfying the condition

$$\overline{M}(t)(\alpha_1(t), \ldots, \alpha_{n+1}(t)) = 0$$

or, which is the same,

$$\begin{cases} \varphi_1(t_1)\,\alpha_1(t) + \cdots + \varphi_n(t_1)\,\alpha_n(t) + \varphi_{n+1}(t_1)\,\alpha_{n+1}(t) = 0, \\ \varphi_1(t_2)\,\alpha_1(t) + \cdots + \varphi_n(t_2)\,\alpha_n(t) + \varphi_{n+1}(t_2)\,\alpha_{n+1}(t) = 0, \\ \ldots, \\ \varphi_1(t_n)\,\alpha_1(t) + \cdots + \varphi_n(t_n)\,\alpha_n(t) + \varphi_{n+1}(t_n)\,\alpha_{n+1}(t) = 0, \end{cases} \tag{2}$$

$$\varphi_1(t)\,\alpha_1(t) \ + \cdots + \varphi_n(t)\,\alpha_n(t) \ + \varphi_{n+1}(t)\,\alpha_{n+1}(t) \ = 0. \tag{3}$$

The subsystem (2) is equivalent to the equality

$$M(\alpha_1(t), \ldots, \alpha_n(t)) + \alpha_{n+1}(t)(\varphi_{n+1}(t_1), \ldots, \varphi_{n+1}(t_n)) = 0$$

which implies

$$(\alpha_1(t), \ldots, \alpha_n(t)) = -\alpha_{n+1}(t)\, M^{-1}\,(\varphi_{n+1}(t_1), \ldots, \varphi_{n+1}(t_n))\,. \tag{4}$$

Due to (4), in the case $\alpha_{n+1}(t) = 0$ we would have $\alpha_1(t) = \cdots = \alpha_{n+1}(t) = 0$, which contradicts the condition $(\alpha_1(t), \ldots, \alpha_{n+1}(t)) \neq 0$. Consequently, $\alpha_{n+1}(t) \neq 0$ and

$$\left(\frac{\alpha_1(t)}{\alpha_{n+1}(t)}, \ldots, \frac{\alpha_n(t)}{\alpha_{n+1}(t)} \right) = -M^{-1}\,(\varphi_{n+1}(t_1), \ldots, \varphi_{n+1}(t_n))\,. \tag{5}$$

According to (5), the numbers $\beta_1 := \frac{\alpha_1(t)}{\alpha_{n+1}(t)}, \ldots, \beta_n := \frac{\alpha_n(t)}{\alpha_{n+1}(t)}$ do not depend on t. It remains to observe that (3) implies

$$\beta_1 \varphi_1(t) + \cdots + \beta_n \varphi_n(t) + \varphi_{n+1}(t) = 0 \quad \text{for all} \quad t \in T$$

contrary to the linear independence of the family $\varphi_1, \ldots, \varphi_n, \varphi_{n+1}$. ▷

2.6. Theorems 2.4 and 2.5 directly imply the following condition for unique solvability of the "corrected inverse problem" $Q^{-1} \circ R$.

Theorem. *Let $x \in C^1(\mathbb{R})$, $h \in C^1(\mathbb{R}^2)$. If the family of functions*

$$t \mapsto x(t)^{i_k}\, h(x(t), t)^{j_k}, \quad k = 1, 2, \ldots, \kappa(p),$$

is linearly independent in the vector space $\mathbb{R}^{\mathbb{R}}$ then there exist $\tau_1, \ldots, \tau_{\kappa(p)} \in \mathbb{R}$ such that, for all $\beta_1, \ldots, \beta_{\kappa(p)} \in \mathbb{R}$, the problem $Q^{-1} \circ R$ is uniquely solvable for the data $\tau_1, \ldots, \tau_{\kappa(p)}$, $x(\tau_1), \ldots, x(\tau_{\kappa(p)})$, $\beta_1, \ldots, \beta_{\kappa(p)}$.

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БИНАРНЫЕ СООТВЕТСТВИЯ И ОБРАТНАЯ
ЗАДАЧА ХИМИЧЕСКОЙ КИНЕТИКИ

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Аннотация. Показано, как бинарные соответствия могут быть использованы для простой формализации понятия задачи, определения основных компонентов задач, их свойств и конструкций. В частности, предложена формализация следующих понятий: условие, данные, искомые и решения задачи, разрешимость и однозначная разрешимость, обратная задача, композиция и ограничение задач, изоморфизм между задачами. Рассмотрены топологические задачи и связанные с ними понятия устойчивости и корректности. Указана связь между устойчивостью и непрерывностью однозначно разрешимой топологической задачи. Дано определение параметризации множества. Введены понятия параметризованной задачи, задачи восстановления объекта по значениям параметров, а также понятия локально свободного набора параметров и устойчивости относительно набора параметров.
В качестве иллюстрации рассмотрена сингулярно возмущенная система обыкновенных дифференциальных уравнений, описывающая процесс химической кинетики и горения. Для такой системы сформулированы прямая и обратная задача. Изучаемый класс задач расширен за счет рассмотрения многочленов произвольной степени в качестве правых частей дифференциальных уравнений. Показано, как обратная задача химической кинетики может быть скорректирована и приближена к практике посредством композиции с простой вспомогательной задачей, реализующей связь между функциями и конечными наборами измеряемых числовых характеристик. Приведены формулы решения и указаны условия однозначной разрешимости скорректированной обратной задачи. В рамках исследования разрешимости получен критерий линейной независимости вещественных функций в терминах конечных наборов их значений. С помощью установленного критерия уточнена реализуемость условия однозначной разрешимости обратной задачи химической кинетики.

Ключевые слова: бинарное соответствие, обратная задача, разрешимость, композиция, устойчивость, корректность, дифференциальное уравнение, химическая кинетика, линейная независимость.
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