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Inverse Problems of Natural Science

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Abstract—A brief definition of inverse and ill-posed problems is given, the history of studying such problems is presented, and the relations of inverse problems to computer simulation is discussed.

Keywords: inverse and ill-posed problems, instability of solution, minimization of functional

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1. ON THE DEFINITION OF INVERSE PROBLEMS

The first publications on inverse and ill-posed problems appeared in the 1950s. They were related to various branches of natural sciences—physics (quantum scattering theory, electrodynamics, and acoustics), geophysics (electro-, seismo-, and geomagnetic exploration), and astronomy. With the emergence of high-performance computers, the field of application of inverse and ill-posed problems became much wider and covered almost all academic disciplines in which mathematical models are used; they include, medical and industrial tomography, nondestructive testing, ecology, economics, and even linguistics and social sciences.

Before discussing inverse problems, we should first define direct problems. In direct problems of mathematical physics, it is desired to find (explicitly or approximately) functions describing various physical phenomena (propagation of sound, heat, seismic vibrations, electromagnetic waves, a drug in an organism, news on the Internet, etc.). These functions are solutions to equations of mathematical physics. To find these solutions, the coefficients of the equations, the domain in which they are defined, and the initial and boundary conditions must be specified. However, the properties of the medium are often not known in practical problems. This implies that inverse problems must be formulated and solved. In inverse problems, given additional information about the solution to the corresponding direct problem, it is required to determine the coefficients of the equations or, e.g., boundary conditions, location and shape of inclusions, boundaries and other properties of the domain in which the process is examined. In some inverse problems, even the form of the equation describing the phenomenon is not known.

It is clear that in order to solve an inverse problem, one must have additional information, such as the values of the solution inside the domain or on its boundary, spectral or kinematic characteristics of the process, topological or group properties, etc. In the majority of cases that are of interest from the theoretical and practical points of view, inverse problems are ill-posed; i.e., at least one of the tree well-posedness properties is violated; these are the properties of existence, uniqueness, and stability of the solution with respect to small variations of the problem data. The inverse and ill-posed problems have a common important property—they are unstable under small errors in data measurements. In the majority of interesting cases, inverse problems are ill-posed, and ill-posed problems can usually be formulated as inverse problems with respect to certain direct (well-posed) problems. However, since the inverse and ill-posed problems have often been formulated and studied independently and simultaneously, both terms are currently used in the scientific literature.

Summarizing the aforesaid, we conclude that the researchers in the field of inverse and ill-posed problems study the properties and regularization methods for unstable problems and develop and study stable methods for approximating unstable mappings.

2. A BIT OF HISTORY

Many mathematical concepts and problems arose as a result of studying various physical processes or phenomena, and this is especially true for inverse and ill-posed problems. The philosophical claim of

Plato that a man in the process of cognition has access only to shadows on a cave wall and echo (the data of an inverse problem) became the precursor of the problem of reconstructing the Earth shape on the basis of its shadow on the Moon (the inverse problem of projective geometry) solved by Aristotle.

The introduction of the physical concept of instantaneous velocity led Newton to the discovery of derivative, and the instability (ill-posedness) of the problem of numerical differentiation of the function specified approximately remains important up to the present day. The studies of Lord Rayleigh in acoustics stimulated him to formulate the question of finding the density of an inhomogeneous string from its sounding (the inverse acoustics problem), which anticipated the development of prospecting seismology on one hand and the theory of inverse spectral problems on the other. The study of the motion of celestial bodies and the problem of estimating unknown quantities given measurements containing random errors led Legendre and Gauss to studying the overdetermined systems of algebraic equations and to the development of the least squares method. Cauchy proposed the steepest gradient descent method for finding the minimum of multivariate functions, and Kantorovich in 1948 generalized, elaborated, and applied these ideas to operator equations in Hilbert spaces.

Even though certain inverse and ill-posed problems have long been the subject of research of various scientists, the mathematical features of ill-posed problems were first formulated by Hadamard in the beginning of the 20th century. The example of ill-posedness of the Cauchy problem for the Laplace equation gave rise to doubts in the expedience of studying ill-posed problems. The thesis that there are no ill-posed problems but there are wrongly formulated problems dampened the enthusiasm of some researchers and on the contrary urged others to seek new techniques for their solution.

For example, in the beginning of the 20th century, Courant studied the ill-posed problem of reconstructing a function from its spherical means. The prominent Soviet mathematician Sobolev became the academic adviser of the doctoral thesis by Ivanov called *Studies on the Inverse Problem of Potential Theory,* which provided a theoretical foundation for solving the inverse (and sverely ill-posed) problem of gravity prospecting; this problem is used for the exploration of lithosphere and prospecting for mineral resources.

It is impossible to give an account of all aspects of the theory of inverse problems and its applications. Here we mention only two directions of research a significant contribution to the emergence and development of which was made by V.E. Zakharov and A.B. Shabat, who worked in Akademgorodok (Novosibirsk, Russia)—inverse scattering transform—and A.S. Alekseev and S.V. Gol'din—inverse problems of geophysics. The inverse scattering transform was used for solving nonlinear equations of mathematical physics, such as the Korteweg–de Vries, nonlinear Schrödinger, and Kadomtsev–Petviashvili equations, and it stimulated studies in various fields of mathematics and physics (spectral theory of differential operators, classical algebraic geometry, relativistic strings, etc.). The inverse scattering transform is often called the pearl of the 20th century mathematical physics. The results obtained by Alekseev and Gol'din on the application of the spectral theory of inverse problems and integral geometry provided the theoretical foundation for many geophysics methods (inverse kinematic and dynamic problems of seismicity). Note that the generally recognized successes of the current generation of Siberian geophysicists are to a large extent determined by their good mathematical background gained on the faculty of geology and geophysics of the Novosibirsk State University. The author of this paper was lucky to work in the chair of geophysics of the Novosibirsk State University in the team of researchers and professors of geophysics (Gol'din, Tabarovskii, Epov, Dashevkii, and others) and mathematics (Lavrent'ev, Alekseev, Romanov, Godunova, and others). Discussions of how and what amount of mathematics should be taught to geophysicists were regularly held in meetings of teachers, and debates were often like discussions in scientific conferences.

A tremendous contribution to the foundations of the theory of inverse and ill-posed problems was made by our compatriots Tikhonov, Ivanov, and Lavrent'ev. A basic idea was that in the investigation of ill-posed problems, the class of possible solutions must be restricted. An important role is played by the choice of the correctness set in which an approximate solution is sought. This set is most often chosen to be compact, which makes it possible to prove the convergence of regularizing algorithms, helps choose the regularization parameter, and estimate the deviation of the approximate solution form the exact solution of the ill-posed problem.

Even though the foundations of the theory of inverse and ill-posed problems were laid in the Soviet Union as early as in the middle of the 20th century, the Russian school began to lose its leading position in the field. A lot of Russian gifted researchers, especially young ones, work abroad. While more than 14 thousands of books the title of which includes the words *inverse problems* have been published in the world, such books are rarely published in Russia. Nevertheless, the theory and numerical methods for solving inverse and ill-posed problems of natural sciences remain a priority direction of research in Russia.

3. MATHEMATICAL STATEMENT

The definition of the inverse problem is well known: the equation $Lu = g,$ initial data and boundary conditions are given in a domain D with the boundary Γ. In the inverse problem, it is assumed that some coefficients of the equation and (or) its right-hand side g, the initial and boundary value data and (or) the function describing the boundary Γ are not known. All these unknown data will be denoted by q. To find q, we assume that, for the solution of the direct problem $u,$ additional information is given, more precisely, the values of u at some points of the space and (or) at some points in time, kinematic and (or) dynamic properties described by the function u, spectral properties of the operator L, scattering data, and group or topological properties of the solution. The set of all additional data will be denoted by f. Thus, the inverse problem can be written in the form of a (generally nonlinear) operator equation $A(q) = f$, in which A is the inverse problem operator. In the general case, A maps a space Q (Euclidian, Hilbert, Banach, metric, or topological) to a space F, and this mapping has no bounded inverse mapping.

The numerical methods for solving inverse problems can be divided into two large groups—direct and iterative. The direct methods include linearization, inversion of the difference scheme, Gelfand–Levitan–Krein–Marchenko methods, the methods of boundary control and singular value decomposition. The iterative methods include gradient descent, Kantorovich–Newton methods and their generalizations.

The application of the Kantorovich–Newton method

$$q_{n+1} = q_n - [A'(q_n)]^{-1}(Aq_n - f)$$

requires, due to the ill-posedness of the inverse problem, the regularization of the inversion of the (generally compact) Frechét derivative of the operator A.

The solution of the operator equation $A(q) = f$ is often reduced to finding the minimum of the functional

$$J(q) = \langle A(q) - f, A(q) - f \rangle \to \min$$

using the gradient descent method

$$q_{n+1} = q_n - a_n J'(q_n)$$

in which the gradient is found by the rule

$$J'(q) = 2[A'(q)]^*(Aq - f).$$

4. COMPUTER SIMULATION AND INVERSE PROBLEMS

Today, the field of applications of the theory of inverse problems is extremely wide—if we make a search query with the words "inverse problems" in Google, the result contains more than 200 million references!

With the emergence of computers, mathematics, as was noted by the founder of the Russian mathematical modeling and simulation Samarskii, acquired the property of experimental science. This property becomes especially important due to active intrusion of supercomputer technologies in our life. Nowadays, one can store data in the cloud and, having certain skills, process it using only a small personal computer with the Internet access. We can not only buy various goods on the Internet, but also get opinions, including medical and legal ones; large-scale computer simulation problems can also be solved.

It is extremely important to learn how to control computational errors. For this reason, works on the optimization of models, creation of special algorithms for parallel computer architectures, estimation and analysis of computational errors are carried out. For example, when a 10-petaflops supercomputer was designed in Japan, an alternate computer based on GPUs was designed for debugging and testing software and investigating features of parallel algorithms.

It is important that along with the growth of computational performance, the probability of errors also increases. Godunov noted that an "ecological catastrophe" is imminent in computer simulation. The point is that even the elementary machine instructions (multiplication or summation) give computational errors, and these errors increase with increasing number of machine instructions used in the algorithm. For example, simulation of the formation of only one protein using molecular dynamics requires about 10^{25} machine instructions!

Nowadays, scientific research is often interdisciplinary—problems should be considered comprehensively. From the side of mathematics, this involves the study of direct and inverse problems, creation of mathematical models, and the development and justification of algorithms. With the emergence of high-performance computing, the mathematical modeling and simulation becomes an experimental tool. In many cases, full-scale experiments can be replaced by computer simulation.

5. INVERSE PROBLEMS IN EDUCATION

In higher education, the theory of inverse and ill-posed problems becomes an efficient means for teaching natural sciences for a number of reasons.

Firstly, this theory to the fullest extent meets the principle of integration of science by combining all main directions of natural sciences on the basis of mathematical equations, which makes it possible to use the interdisciplinary approach in education. When taking the course of inverse and ill-posed problems, students once more examine the disciplines they learned earlier and get deeper understanding of their mathematical features and interrelations. Secondly, the studying of the theory of inverse and ill-posed problems gives deeper understanding of the role of mathematics in society and the internal unity and beauty of mathematics itself. Finally, the study of this theory helps gain deeper understanding of the role of simulation in the cognition of the world around us.

6. CONCLUSIONS

The popularity of inverse problems grows proportionally to the growth of computer performance because one of the most simple and clear for application scientists method of solving inverse problems is the fitting method. Having at his disposal a reliable numerical method for solving a direct problem (and, therefore, a good model of the phenomenon under examination), the researcher can solve the inverse problem by purposefully varying the parameters of the model. The emergence of supercomputers open new possibilities for using gradient methods, stochastic and genetic algorithms and neural networks.

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