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Review Article

General Tikhonov Regularization with Applications in Geoscience

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Abstract. The article is devoted to a review of the following new elements of the modern theory of solving inverse problems: (a) general theory of Tikhonov's regularization with practical examples is considered; (b) an overview of a-priori and a-posteriori error estimates for solutions of ill-posed problems is presented as well as a general scheme of a-posteriori error estimation; (c) a-posteriori error estimates for linear inverse problems and its finite-dimensional approximation are considered in detail together with practical a-posteriori error estimate algorithms; (d) optimality in order for the error estimator and extra-optimal regularizing algorithms are also discussed. In addition, the article contains applications of these theoretical results to solving two practical geophysical problems. First, for inverse problems of computer microtomography in microstructure analysis of shales, numerical experiments demonstrate that the use of functions with bounded VH-variation for a piecewise uniform regularization has a theoretical and practical advantage over methods using BV-variation. For these problems, a new algorithm of a-posteriori error estimation makes it possible to calculate the error of the solution in the form of a number. Second, in geophysical prospecting, Tikhonov's regularization is very effective in magnetic parameters inversion method with full tensor gradient data. In particular, the regularization algorithms allow to compare different models in this method and choose the best one, MGT-model.

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1 Introduction: Inverse problems in geoscience

Geophysics is one of the sciences in which mathematical methods have been used for more than 100 years. It was in the study of geophysical problems that many mathematical models were developed, which were successfully applied not only in Earth sciences, but also in other applications [48, 56, 79, 82, 83, 87]. The development of many geophysical research methods led to the creation of the theory of inverse problems and then to the methods and algorithms for solving these problems, which are mostly ill-posed. It is for solving inverse problems in Earth sciences that the method of regularization of A. N. Tikhonov was created in the 60s of the XX century [67, 68]. The theory of Tikhonov regularization marked the beginning of the fruitful development of stable methods for solving inverse ill-posed problems. These methods are successfully developed and adapted to the solution of inverse problems in geophysics and other branches of science to the present. In order to understand this, it is enough to indicate that about 100 monographs on this subject have already been published. Among them, for example, are the following [4, 6, 9, 13, 14, 17, 20, 22, 30, 44, 60, 62, 69–72, 79, 89] and many others.

Hundreds of new geophysical models have been established during past decades to be applied for solving inverse problems. The model-based inversion in solid geophysics and atmospheric science has been well understood, as well as the model-based inverse problems for land surface and data-based inverse problems that received much attention from scientists only in recent years (see, e.g. [38, 51, 58, 59, 85–87]). The solution of inverse ill-posed problems is impossible without taking into account a-priori information about the desired solution. For example, in solid geophysics, using gravimetric, magnetic, electromagnetic and seismic data to dig out anomalies underground is always severely ill-posed due to very limited data acquisition during scanning the deep earth [81, 87, 90]. Therefore, integrating different geophysical exploration methods is a tendency. At the same time, the appearance of hyperspectral and multiangular remote sensor enhanced the exploration means, and provided us more spectral and spatial dimension information than before [80, 81]. For this reason, the development and improvement of existing methods for solving ill-posed inverse problems is required, so as to take into account more and more detailed a-priori information about solutions. However, stable solving inverse problems is only part of the processing of geophysical information. As a rule, it is also required to estimate the error of solutions obtained. It is desirable to have this estimate as a number, rather than an asymptotic formula. This requires solving rather complicated math questions for ill-posed problems.

In this article we try to give an overview of two directions in the study of methods for solving ill-posed problems (Section 2). First, we describe modern regularization methods, and in a fairly general form, suitable for solving complex inverse problems (Section 2.1). Secondly, in consideration of error estimation for solutions (Section 2.2), we want to point out the complexity of such a task and show constructive ways to solve it (Sections 2.3, 2.4). We will also present a new error estimation algorithm that allows us to obtain practical estimates (Section 2.5). The important notion of an extra-optimal regularizing algorithm, that is a method for solving ill-posed problems having an optimal a-posteriori error estimate, is also considered (Sections 2.6). The effectiveness of the methods used for regularization and error estimation is demonstrated by examples of solving practical inverse problems of geoscience (Sections 3, 4).

2 General theory of Tikhonov's regularization

2.1 Statement of the problem

In this paper, we study ill-posed problems and their applications in general statement, i.e. as extremal (optimization) problems. The general theory for the solution of such problems in topological spaces is presented, e.g., in [60,71]. Here we restrict ourselves to a special statement of optimization problems (see [34]). Suppose that Z is Banach space and $\mathcal{D} \neq \varnothing$ is a given set in Z. Let a functional $J_0[z]$ be defined for all $z \in \mathcal{D}$ and bounded from below on $\mathcal{D}$. We formulate the following extremal problem: it is required to obtain elements $z^* \in \mathcal{D}$ for which

$$J_0[z^*] = \inf\{J_0[z] : \ z \in \mathcal{D}\} \stackrel{def}{=} J^*. \tag{2.1}$$

The set $\mathcal{D}$ can be considered as restrictions on solutions to be found. We assume that the problem (2.1) has a nonempty set of solutions, Z^*. This set can contain more than one element. In order to select admissible solutions, we introduce an auxiliary functional $\Omega[z]$, which is defined and bounded from below on the set $\mathcal{D}$. The properties of the functional $\Omega[z]$ are listed below. The selection of a solution $\bar{z} \in Z^*$ to the problem (2.1) is performed so that the equality

$$\Omega[\bar{z}] = \inf\{\Omega[z^*] : z^* \in Z^*\} = \inf\{\Omega[z^*] : J_0(z^*) = J^*\} \tag{2.2}$$

is satisfied. Such solutions are called Ω-optimal. Denote the set of Ω-optimal solutions as $\bar{Z}$. We are interested in any Ω-optimal solution as well as in the value J^*. In practice, the functional $J_0[z]$ can be specified with an error. Assume that instead of $J_0[z]$, we have at our disposal a functional $J_\eta[z]$, which is defined on $\mathcal{D}$ and meets the following approximation condition

$$|J_0[z] - J_\eta[z]| \leq \Psi(\eta, \Omega[z]), \quad \forall z \in \mathcal{D}, \tag{2.3}$$

where the vector (or the number) η indicates the proximity of $J_\eta[z]$ to $J_0[z]$ on the set $\mathcal{D}$. The given function $\Psi(\eta,\Omega)$ is called an approximation measure.

The central problem of the theory of ill-posed extremal problems is to determine from the data $(J_\eta[z], \eta, \Psi)$ a stable estimate J^*_η of the number J^*: $J^*_\eta \to J^*$ as $\eta \to 0$, as well as a stable approximation to the set $\bar{Z}$, i.e. an element $z_\eta \in \mathcal{D}$ for which the convergence $z_\eta \to \bar{Z}$ holds, that is

$$\lim_{\eta \to 0} \inf\{\|z_\eta - \bar{z}\| : \bar{z} \in \bar{Z}\} = 0. \tag{2.4}$$

Below we give typical examples that illustrate the problems (2.1), (2.2). One can find more information about them, e.g., in [9,14,69–71] and other publications.

Example 2.1. Solving linear operator equations in Hilbert spaces via variational method.

Let Z,U be Hilbert spaces, $A:Z\to U$ be linear bounded operators and $\Omega[z]=\|Lz\|_Z$. Here $L:Z\to Z$ is a linear closed operator with a domain $D(L)$, which is dense in Z. In addition, suppose that $\|Lz\|_Z\geq k\|z\|_Z$ for all $z\in D(L)$ (k=const>0). We are interesting in solving on the set $\mathcal{D}=D(L)$ the operator equation

$$Az=u \tag{2.5}$$

with a right-hand side $u\in U$. To do this, we apply the variational approach, i.e. the solution of the problem (2.1) with $J_0[z]=\|Az-u\|_U$. Assume that solutions $z^*\in\mathcal{D}$ of such extremal problem exist and form the set Z^*. Then the value $J^*=\inf\{\|Az-u\|_U: z\in\mathcal{D}\}$ is the measure of incompatibility for Eq. (2.1) on the set $\mathcal{D}$. Let us select from the set Z^* so called *L-pseudosolution*, i.e. the unique element $\bar{z}\in Z^*$ which solves the problem (2.2) with $\Omega[z]=\|Lz\|_Z$ (see [44]). When Eq. (2.5) is uniquely solvable, its solution coincides with L-pseudosolution and $J^*=0$. Suppose that the data (A,u) of the problem (2.5) are known approximately. We are given a linear bounded operator $A_h:Z\to U$ and an element u_δ instead of A and u such that $\|A_h-A\|\leq h$ and $\|u_\delta-u\|_U\leq\delta$. The numbers $\eta=(h,\delta)$ are known. Therefore, an approximate functional $J_\eta[z]=\|A_hz-u_\delta\|_U$ is defined and the condition (2.3) is fulfilled with $\Psi(\eta,\Omega[z])=\delta+H\Omega[z], H=\frac{h}{k}$. Solving the problem (2.5), we would like to obtain stable estimates for the incompatibility measure J^* and L-pseudosolution $\bar{z}$. Note that in the simplest case, we can assume that $L=I$.

Example 2.2. Solving non-linear operator equations in Banach spaces via variational method.

In this example, Z and U are Banach spaces; $F(z)$ is an operator (generally, non-linear), which is defined on a given set $\mathcal{D},\mathcal{D}\subset Z$, and continuous from $\mathcal{D}$ to U. We shall solve on the set $\mathcal{D}$ the operator equation

$$F(z)=u, \quad u\in U, \tag{2.6}$$

by minimizing on $\mathcal{D}$ the functional $J_0[z]=\|F(z)-u\|_U$. This means solving the problem (2.1). If the set of solutions Z^* to Eq. (2.6) is nonempty, we can find Ω-optimal solutions of the equation from the problem (2.2). To this end, the approximate data $\{F_h,u_\delta\}$ of the problem (2.6) are used. Here the operator $F_h:\mathcal{D}\to U$ is supposed to be continuous and $u_\delta\in U$. Moreover, the approximation conditions $\|F_h(z)-F(z)\|_U\leq\psi(h,\Omega[z]),\forall z\in\mathcal{D}$, $\|u_\delta-u\|_U\leq\delta$ are fulfilled, where the function $\psi(h,\Omega)$ and the value $\eta=(h,\delta)$ are known. So, the approximate functional for $J_0[z]$ can be defined in the form $J_\eta[z]=\|F_h(z)-u_\delta\|_U$ with the function $\Psi(\eta,\Omega[z])=\delta+\psi(h,\Omega[z])$ in approximation condition (2.3). As a result of solving our inverse problem, we want to obtain a stable evaluations for the incompatibility measure $J^*=\inf\{\|F(z)-u\|_U: z\in\mathcal{D}\}$ in (2.6) and for the set of Ω-optimal solutions $\bar{Z}$. If Eq. (2.6) has a unique solution $\bar{z}$, then $\bar{Z}=\{\bar{z}\}$ and $J^*=0$.

In the sequel, we assume the following assumptions to be satisfied (see [30,71]).

Assumptions

(A) The functionals $J_0[z]$, $J_\eta[z]$ and $\Omega[z]$ are bounded from below and lower semicontinuous on the set $\mathcal{D}$. Without loss of generality, we assume that $J_0[z]\geq 0, J_\eta[z]\geq 0$ and $\Omega[z]\geq 0$ $\forall z\in\mathcal{D}$.

(B) Any nonempty set $\Omega_C=\{z\in\mathcal{D}:\Omega[z]\leq C\}$, $C=$const, is compact in Z.

(C) The function $\Psi(\eta,t)=\Psi(\eta_1,\cdots,\eta_m,t)$ is continuous in the domain $\{\eta\in\mathbb{R}^m_+\}\times\{t\geq 0\}$, i.e. for all $\eta_1,\cdots,\eta_m,t\geq 0$. In addition, the function $\Psi(\eta,t)$ is increasing with respect to t for every fixed $\eta\in\mathbb{R}^m_+$, $\|\eta\|>0$, and $\Psi(0,t)=0,\forall t\geq 0$. Moreover, $\Psi(\eta,t)>0$ for all (η,t), if $\|\eta\|>0$ and $t>0$. One can find examples of such functions $\Psi(\eta,t)$ for non-linear inverse problems in [71].

(D) The problem (2.1) has a unique solution, that is $\bar{z}=z^*$.

The central problem can be solved by application of regularizing algorithms (RAs) [69,71]. In this case, the approximate solution is specified in the form $z_\eta=P_\eta(J_\eta,\eta,\Psi)\in\mathcal{D}$, where $\{P_\eta\}$ is a certain parametric family of operators that act on the approximate data and explicitly depend on the estimate η of the data errors. If the RA P_η ensures the validity of so-called *regularity conditions*

$$\overline{\lim_{\eta\to 0}}\Omega[z_\eta]\leq\text{const},\quad \lim_{\eta\to 0}J_\eta[z_\eta]\leq J^* \tag{2.7}$$

for the approximate solution z_η, then under Assumptions (A)–(D), together with the condition (2.3), the convergences $z_\eta\to\bar{z}$, $J_\eta[z_\eta]\to J^*$ take place as $\eta\to 0$ [71, Sec. 2.5].

The operators P_η can be introduced in different ways (see, e.g. [6,9,71,72]). Often, variational RAs are preferable. The most popular RAs for ill-posed extremal problems are described in the following examples.

Example 2.3. Tikhonov regularization with the choice of the regularization parameter according to Generalized Discrepancy Principle (GDP) in application to the convex optimization. In this example, we introduce instead of the assumption (D) an additional assumption.

(E) The functionals $J_0[z]$, $J_\eta[z]$ are convex on the convex set $\mathcal{D}$, while the functional $\Omega[z]$ is strictly convex on $\mathcal{D}$.

Below, we follow the theory worked out in [71]. Let us introduce an auxiliary convex function $f(x)\geq 0$ assuming that $f(x)\in C^l[0,\infty)$ $(l\geq 1)$, and moreover $f^{(n)}(x)\geq 0$ for $n=1,\cdots,l-1$ and $f^{(l)}(x)\geq\kappa_0=\text{const}>0$. In practice, the most useful example is $f(x)=x^l$. Furthermore, we introduce the convex functional $I_\eta[z]=f(J_\eta[z])$ and determine for any $\alpha>0$ Tikhonov's functional

$$M^\alpha[z]=\alpha\Omega[z]+I_\eta[z],\quad z\in\mathcal{D}. \tag{2.8}$$

It follows from the assumptions (A) and (E) that the constrained optimization problem

$$M^\alpha[z^\alpha_\eta]=\inf\{M^\alpha[z]:z\in\mathcal{D}\}, \tag{2.9}$$

has a unique solution $z_\eta^\alpha \in \mathcal{D}$ for any $\alpha > 0$. Hence, we can determine the auxiliary functions

$$\beta(\alpha) = J_\eta[z_\eta^\alpha], \quad \pi(\alpha) = C\Psi(\eta, \Omega[z_\eta^\alpha]) + \lambda_\eta, \quad \rho(\alpha) = \beta(\alpha) - \pi(\alpha). \tag{2.10}$$

Here $C \geq 1$ is a fixed constant and the value λ_η is a stable upper estimate for J^*, i.e. $\lambda_\eta \geq J^*, \lambda_\eta \to J^*$ as $\eta \to 0$. For instance, if the assumptions (A)–(C) are fulfilled, one can accept $\lambda_\eta = \inf\{J_\eta[z] + \Psi(\eta, \Omega[z]) : z \in D\}$. The functions (2.10) are continuous for $\alpha > 0$ and also $\beta(\alpha), \rho(\alpha)$ are non-decreasing, while $\pi(\alpha)$ is non-increasing. The *generalize discrepancy principle* consist in a choice of the regularization parameter α_η as a root of the equation $\rho(\alpha) = 0$. If $\Omega[\bar{z}] > \inf\{\Omega[z] : z \in \mathcal{D}\}$, then under conditions (A)–(C) the equation has a solution $\alpha_\eta > 0$ at least for sufficiently small η (see [71, p. 77]). In this case, the element $z_\eta = z_\eta^{\alpha_\eta}$ can be taken as an approximate solution to the problem (2.1). One can obtain from the equality $\rho(\alpha_\eta) = 0$ that

$$J_\eta[z_\eta] = \lambda_\eta + C\Psi(\eta, \Omega[z_\eta]). \tag{2.11}$$

It was shown in [71] that, if the functionals $J_0[z]$, $J_\eta[z]$, $\Omega[z]$ and the functions $f(x)$, $\Psi(\eta, t)$ fulfill the above assumptions, then the convergences $z_\eta \to \bar{z}, \Omega[z_\eta] \to \Omega[\bar{z}]$, $J_\eta[z_\eta] \to J^*$ take place as $\eta \to 0$.

The GDP algorithm can be simplified essentially for solving linear operator equations in Hilbert spaces (see Example 2.1). In this case, we can accept $\Omega[z] = ||Lz||_Z^2$ and $I_\eta[z] = ||A_h z - u_\delta||_U^2$. It is well known (see, e.g. [16, 44]), that

$$z_\eta^\alpha = (\alpha L^* L + A_h^* A_h)^{-1} A_h^* u_\delta \tag{2.12}$$

and the root $\alpha(\eta)$ of the equation $\rho(\alpha) = 0$, i.e. $\left\|A_h z_\eta^\alpha - u_\delta\right\| - C(\delta + H\left\|L z_\eta^\alpha\right\|) - \lambda_\eta = 0$, unique. Calculating it, we can find unique approximate solution $z_\eta^{\alpha(\eta)}$ to Eq. (2.5), for which the convergences $z_\eta^{\alpha(\eta)} \to \bar{z}, \Omega[z_\eta^{\alpha(\eta)}] \to \Omega[\bar{z}]$, $f\left(J_\eta[z_\eta^{\alpha(\eta)}]\right) \to f(J^*)$ are fulfilled. Note that the number λ_η can be omitted in (2.10), (2.11) when Eq. (2.5) is solvable.

Remark 2.1. The GDP algorithm can be also applied to the solution of non-linear operator equations from Example 2.2, if the problem (2.9) possesses a unique solution for every $\alpha > 0$. When the elements z_η^α are not defined uniquely, one should apply special variants of the GDP (see for instance [54, 71] and etc.).

Example 2.4. Generalized method of discrepancy (GDM) for solving ill-posed optimization problems in Banach spaces.

This approach to approximate solution of the problem (2.1) consist in obtaining elements $z_\eta = z_\eta(J_\eta, \Psi, \eta)$ for which the relation holds:

$$\Omega[z_\eta] = \inf\{\Omega[z] : \ z \in \mathcal{D}, \ J_\eta[z] \leq C\Psi(\eta, \Omega[z]) + \lambda_\eta\}. \tag{2.13}$$

It was established in [71] that under assumptions (A)–(C) the optimization problem (2.13) has solutions z_η with the convergence properties $z_\eta \to \bar{z}, \Omega[z_\eta] \to \Omega[\bar{z}]$, $J_\eta[z_\eta] \to J^*$ as $\eta \to 0$.

2.2 A-priori and a-posteriori error estimates for solutions of ill-posed problems

The theory of *a-priori error estimates* for methods of solving ill-posed problems has been developed in many works. Here we note only a part of them, namely [7–9, 14, 41, 47, 62, 64, 71, 72], with comprehensive bibliography therein.

We now describe briefly major difficulties in this area considering the simplest case of error estimating for solutions of a linear operator equation $Az=u$ with exact operator A and approximate right-hand side u_δ, $||u-u_\delta||\le\delta$ (see [37]). We want to analyse the accuracy of the approximate solution $z_\delta=P_\delta(u_\delta)$ found by a method P_δ as a function of the error level $\delta>0$ of the data u_δ. Usually the accuracy could be estimated as $||z_\delta-\bar{z}||\le K\varphi(\delta)$. Here K does not depend on $\delta>0$ and the function $\varphi(\delta)$ defines the convergence rate of the approximation z_δ to the exact solution $\bar{z}$. We distinguish *pointwise* and *uniform* estimates. In pointwise estimates $\bar{z}$ is fixed; K and $\varphi(\delta)$ are dependent on $\bar{z}$. Uniform estimates are valid for a set M of solutions $\bar{z}$ with K dependent on characteristics of the set. Pointwise estimates have no significant sense because corresponding values $\varphi(\delta)$ are connected with the unknown $\bar{z}$. The same accuracy rate does not exist for approximate solutions of the problem with different data u_δ. More precisely, this result from [74] can be formulated as follows.

Proposition 2.1. *Let the operator $A:Z\to U$ have an unbounded inverse. Suppose that $\varphi(\delta)$ is an arbitrary positive function such that $\varphi(\delta)\to 0$ as $\delta\to 0$, and P_δ is an arbitrary method of solution. Then the following equality holds for elements $\bar{z}$ except maybe for their set of Baire first category in Z:*

$$\overline{\lim}_{\delta\to 0}\left\{\frac{\Delta(P_\delta,\delta,\bar{z})}{\varphi(\delta)}\right\}=\infty.$$

Here $\Delta(P_\delta,\delta,\bar{z})=\sup\{\|P_\delta(u_\delta)-\bar{z}\|:\ \forall u_\delta\in U,\ \|A\bar{z}-u_\delta\|\le\delta\}$ is a characterization of a pointwise accuracy for the method P_δ. The value $\Delta(P_\delta,\delta,\bar{z})$ is generally accepted in the theory of error estimates (see, e.g. [6, 9, 14, 30, 44, 62, 64, 71, 72]). In uniform estimates the rate of accuracy of an approximate solution $\varphi(\delta)$ does not depend on an exact solution. That is why uniform accuracy estimates are widely spread in the theory of ill-posed problems. However, uniform accuracy estimates do not exist on any set M. This was shown in [75] and can be expressed as:

Proposition 2.2. *Let A be a linear continuous injective operator acting in Banach space Z and the inverse operator A^{-1} is unbounded on its domain. Then a uniform error estimate can only exist on a first category subset in Z.*

A compact set is a typical example of the first category set in a normed space Z. Proposition 2.2 can be supplemented as follows (see [14]).

Proposition 2.3. *Let a bounded set M be such that there exists a uniform error estimate for the solution of Eq.* (1.1) *with a compact linear operator A. Then M is a compact set in Z.*

Thus, to construct uniform accuracy estimates for approximate solutions of ill-posed problems we must consider admissible sets of solutions with special properties as defined in Propositions 2.2 and 2.3. So, a-priori error estimates can be obtained with very strict additional constraints on the desired solution. Moreover, these estimates often contain constants, the practical calculation of which is difficult. Therefore, it is impossible to obtain an a-priori error estimate in the form of a number in most cases.

The same difficulties arise in general case of ill-posed extremal problems. In this case, an appropriate scheme for a-priori error estimation is presented in [71]. We describe it shortly. Let M, $M\subset\mathcal{D}$, be a certain set of elements such that $\sup\{\Omega[z]:z\in M\}\le b=\text{const}$. Introduce a class of problems of the type (2.1). Namely, for any functional $J[z]$ with the property (A) it is necessary to obtain an element $\bar{z}\in\mathcal{D}$ for which the relation holds

$$J[\bar{z}]=\inf\{J[z]:\ z\in\mathcal{D}\}. \tag{2.14}$$

It is supposed here that the solution $\bar{z}=\bar{z}(J)$ of the problem (2.14) is unique. Denote by $\{J\}_M$ the set of all functionals J from the problems like (2.14) with the property $\bar{z}(J)\in M$. If $J\in\{J\}_M$ then the problem (2.14) is equivalent to the problem

$$J[\bar{z}]=\inf\{J[z]:\ z\in M\}.$$

Let us fix approximate data of the problem (2.1), i.e. the values $(J_\eta[z],\eta,\Psi)$, and find a stable valuation J^*_η for J^*: $J^*_\eta\to J^*$ as $\eta\to 0$, using these data. The condition (2.3) leads on the set M to the inequality

$$|J_0[z]-J_\eta[z]|\le H,\quad \forall z\in M;\quad H\overset{def}{=}\Psi(\eta,b).$$

Here we can regard the number H as an accuracy measure for the approximation of the functional $J_0[z]$ by the functional $J_\eta[z]$ on M.

Now we define the set of functionals

$$\mathcal{F}_M(J_\eta,\eta)=\Big\{J:\ J\in\{J\}_M,\ |J[\bar{z}(J)]-J^*_\eta|\le H,\ |J[z]-J_\eta[z]|\le\bar{C}H,\ \forall z\in M\Big\}$$

with a fixed constant $\bar{C}>1$. The set $\mathcal{F}_M(J_\eta,\eta)$ represents a certain class of exact problems (2.14) with functionals $J[z]$, for which the functional $J_\eta[z]$ can serve as an approximate functional in the sense of the condition of the uniform approximation:

$$|J[z]-J_\eta[z]|\le\bar{C}H,\quad \forall z\in M.$$

Obviously, $J_0[z]\in\mathcal{F}_M(J_\eta,\eta)$.

Obtaining a-priori estimates is based on the use of the following characteristic of the accuracy of the method (i.e., the regularizing algorithm) P_η:

$$\Delta(P_\eta;J_\eta,\eta;M)=\sup_J\{\|P_\eta(J_\eta,\eta,\Psi)-\bar{z}(J)\|:\ J\in\mathcal{F}_M(J_\eta,\eta)\}.$$

In general, the a-priori estimates on the set M have the form $\Delta(P_\eta;J_\eta,\eta;M)\le K_1\xi(\eta)$. Here, K_1 does not depend on η and the function $\xi(\eta)$ is determined by the chosen method of solution and the set M. Finding this function is often difficult. However, there is a way to estimate the error without the function $\xi(\eta)$.

A-priori error estimates are usually applied to prove some optimal properties of the accuracy of the considered method, or to compare different methods in terms of their order of accuracy. Correspondingly, the key points of the theory are the determination of the optimal accuracy and the optimal method of solution for the problem as well as the notion of the optimal in order method.

The quantity $\Delta(P_\eta;J_\eta,\eta;M)$ is said to be the accuracy of the method P_η on a set M, and the quantity

$$\Delta_{opt}=\Delta_{opt}(\eta,J_\eta;M)=\inf\{\Delta(P;J_\eta,\eta;M):P\in\mathcal{P}\}$$

is said to be *the optimal accuracy* on the class $\mathcal{P}$ of various methods P. The method P_η is said to be of *optimal order* on the set M if its accuracy satisfies the condition $\Delta(P_\eta;J_\eta,\eta;M)/\Delta_{opt}(\eta,J_\eta;M)\le k=\text{const}$ as $\eta\to 0$, where k does not depend on η and M.

So, if it is possible to find the constant k for the method P_η, then the a-priori error estimate $\Delta(P_\eta;J_\eta,\eta;M)\le k\Delta_{opt}(\eta,J_\eta;M)$ is valid. This estimate shows how close is the method P_η to the optimal one.

Such a-priori estimates can be obtained in the case when Z is a reflexive Banach space, and the set M has the form $M=M_r=\{z:z=Bv,v\in V,\|v\|\le r\}$. Here, V is some auxiliary reflexive Banach space, $B:V\to Z$ is the given linear continuous operator, and r is a fixed number. Thus, it is assumed a-priori that the exact solution can be represented as $\bar{z}=B\bar{v}$, where $\|\bar{v}\|\le r$. It has been shown in [30, 34, 71] that many of known regularizing algorithms for extremal problems are optimal in order on classes M_r that are defined by the operator B of the compact embedding of the space V in the space Z.

The well-known examples of optimal in order RAs are the generalized discrepancy principle (GDP) and the generalized method of discrepancy (GDM) as well as a number of other methods [71]. For these RAs, it is established that $\Delta(P_\eta;J_\eta,\eta;M_r)\le 2\Delta_{opt}(\eta,J_\eta;M_r)$ (see [71, Sec. 2.13]). Therefore, the application of these methods on its own ensures the optimal order of accuracy of the obtained approximate solutions and the a-priori error estimate

$$\|z_\eta-\bar{z}\|=\|P_\eta(J_\eta,\eta,\Psi)-\bar{z}(J_0)\|\le 2\Delta_{opt}.$$

Note once more that the order of accuracy rendered by the function $\xi(\eta)=\Delta_{opt}(\eta,J_\eta;M_r)$ can be found in an explicit form (analytically) only for a relatively narrow range of ill-posed extremal problems and the sets M_r. The most success is reached here for the solution of operator equations from Examples 2.1 and 2.2 (see [6, 9, 14, 72] and so on).

The difficulty of a-priori error estimation for the practical accuracy evaluation of calculated approximate solutions led to the development of the theory of *a-posteriori error estimates*. The theory has been based in [10] and improved in [65, 66, 88] for solving operator equations with monotone, convex and other solutions with analogous descriptive properties. Many other works about solution, convergence and error estimation for linear and nonlinear ill-posed problems are also developed, e.g., [1,2,12,42,45,49,50,78] and references therein. In [31–35], a new scheme of a-posteriori estimates has been proposed for more general sets of solutions. In this paper, we consider the scheme for the case of ill-posed extremal problems (2.1) [36]. An alternative approach is presented in [5].

2.3 The scheme of a-posteriori error estimation used in the work

Suppose that the optimization problem (2.2) is solved by a regularizing algorithm, which generates a family of approximate solutions $\{z_\eta\}\subset\mathcal{D}$ such that $z_\eta\to\bar{z}$ in Z, and $\Omega[z_\eta]\to\Omega[\bar{z}]$, $J_\eta[z_\eta]\to J^*$ as $\eta\to 0$ (see, e.g. Examples 2.3, 2.4).

After application of an RA, the quantities $J_\eta[z_\eta],\Omega[z_\eta]$ are known. We fix the estimation constant $C>1$ and calculate the values $\Delta_\eta=CJ_\eta[z_\eta]$, $R_\eta=C\Omega[z_\eta]$. After that, we introduce the set $\mathcal{Z}_\eta=\{z\in\mathcal{D}:\Omega[z]\le R_\eta,J_\eta[z]\le\Delta_\eta\}$, which includes automatically the element z_η. Then the following a-posteriori error estimate for the approximate solution $z_\eta\in\mathcal{D}$ holds true:

$$\|z_\eta-\bar{z}\|\le\sup\{\|z_\eta-z\|:z\in\mathcal{Z}_\eta\}\overset{def}{=}\varepsilon(\eta), \tag{2.15}$$

if the exact solution $\bar{z}$ meets the constrains of the extremal problem (2.15). One can find the numerical error estimate for the approximate solution by computing the function $\varepsilon(\eta)=\sup\{\|z_\eta-z\|:z\in\mathcal{D},\Omega[z]\le R_\eta,J_\eta[z]\le\Delta_\eta\}$.

Now we clarify when the inclusion $\bar{z}\in\mathcal{Z}_\eta$ is satisfied.

Lemma 2.1. *Suppose that inequalities $\Omega[\bar{z}]>0$ and $J^*+\Psi(\eta,\Omega[\bar{z}])<\Delta_\eta$ holds at least for sufficiently small η, $||\eta||>0$. Then $\bar{z}\in\mathcal{Z}_\eta$.*

Sometimes in the sequel, we will replace the words "at least for sufficiently small η" by the inequality $0<||\eta||\le\eta_0=\text{const}$.

The condition of Lemma 2.1 is fulfilled for many regularizing algorithms. Hence, as follows from Lemma 2.1, the a posteriori error estimate (2.15) holds for these RAs when $||\eta||\le\eta_0=\text{const}$. In particular, the following theorem is true.

Theorem 2.1. *The a-posteriori error estimate* (2.15) *is valid for approximate solutions obtained by the generalized discrepancy principle when $0<||\eta||\le\eta_0$.*

Now we study the estimator $\varepsilon(\eta)$ and the extremal problem (2.15).

Theorem 2.2. *Under the assumptions (A)–(D), the least upper bound*

$$\varepsilon(\eta)=\sup\{\|z_\eta-z\|:\ z\in\mathcal{D},\ \Omega[z]\le R_\eta,J_\eta[z]\le\Delta_\eta\} \tag{2.16}$$

is attained on an element $\tilde{z}_\eta\in\mathcal{D}$ for every fixed $\eta,\|\eta\|>0$. Moreover, the limit relation $\lim_{\eta\to 0}\varepsilon(\eta)=\lim_{\eta\to 0}\|\tilde{z}_\eta-z_\eta\|=0$ holds.

Theorem 2.2 demonstrates that the function $\varepsilon(\eta)$ can be calculated for every fixed $\eta=(h,\delta)$ by solving extremal problem (2.16), i.e. by finding an approximate global maximizer $\tilde{z}_\eta$ of the functional $E[z]=\|z-z_\eta\|$ on the set $\mathcal{Z}_\eta$. There is no difficulty to understand that this problem can have many local and global maximizers. Thus, a possible approach to the solution consists in finding elements, that realize all local maxima, and after that calculating the functional $E[z]$ for these maximizers with subsequent selection from thereby calculated values the maximal one.

2.4 A-posteriori error estimate for linear inverse problems and its finite-dimensional approximation

In this section, we consider Eq. (2.5) with $\mathcal{D}=Z$. Specify what was said in Section 2.3. After finding an approximate solution, z_η, we fix a constant $C>1$ and calculate the values $\Delta_\eta=C\|A_h z_\eta-u_\delta\|$, $R_\eta=C\Omega[z_\eta]$. Further, we introduce the set $\mathcal{Z}_\eta=\{z\in Z:\ \|A_h z-u_\delta\|\le C\Delta_\eta,\ \Omega[z]\le CR_\eta\}$. Suppose that $\bar{z}\in\mathcal{Z}_\eta$ (see Lemma 2.1). Then the inequality similar to (2.15) holds:

$$\|z_\eta-\bar{z}\|\le\sup\{\|z_\eta-z\|:\ z\in Z,\ \|A_h z-u_\delta\|\le C\Delta_\eta,\ \Omega[z]\le CR_\eta\}=\varepsilon(\eta). \tag{2.17}$$

Here the function $\varepsilon(\eta)$ is a so called *global a-posteriori error estimate* for the approximate solution z_η of the operator equation (2.5). A finite dimensional approximation of this estimate can be found as follows [33].

Let a sequence of finite-dimensional spaces Z_n, U_n of dimensions $N(n)$ and $M(n)$ be defined and $N(n),M(n)\to\infty$ as $n\to\infty$. Suppose that $Z_1\subset Z_2\subset\cdots\subset Z_n\subset\cdots\subset Z$, $\bigcup_{n=1}^{\infty}Z_n=Z$, $U_1\subset U_2\subset\cdots\subset U_n\subset\cdots\subset U$, $\bigcup_{n=1}^{\infty}U_n=U$. For each n, we assume that a continuous operator $A_n:Z_n\to U_n$ and element $u_n\in U_n$ are given, which approximate the fixed data (A_h,u_δ) of the problem (2.5). Let the approximation conditions be fulfilled: $\|A_n z-A_h z\|\le\psi(h_n,\|z\|)$, $\forall z\in Z$, $\|u_n-u_\delta\|\le\delta_n$. Here $\psi(h_n,t)$ and δ_n are estimates of the accuracy for such approximation and h_n, $\delta_n\to 0$ as $n\to\infty$. The function $\psi(h,t)$ has the same properties as Ψ. In addition, we assume that a sequence of functionals $\Omega_n[z]$ is given defined on Z_n and approximating the functional $\Omega[z]\ge 0$ in the following sense: $0\le\Omega_n[z]-\Omega[z]\le\kappa_n\theta(\Omega[z])$, $\forall z\in Z_n$. Here $\kappa_n\to 0$ as $n\to\infty$ and a function $\theta(t)$ is continuous for $t\ge 0$. We also assume that a family of projectors $\mathcal{P}_n:Z\to Z_n$ is defined with the property $\lim_{n\to\infty}\|\mathcal{P}_n z-z\|=0$, $\forall z\in Z$.

Let us apply some RA to solve the problem (2.5). Then the RA gives for the data (A_h,u_δ,h,δ) an approximate solution $z_\eta\in Z$, the accuracy of which we want to evaluate using the data of finite-dimensional approximation, (A_n,u_n,h_n,δ_n). Suppose that there is a finite-dimensional version of this RA and it allows us to construct for the values (A_n,u_n,h_n,δ_n) an element $z_{\eta n}\in Z_n$ such that $z_{\eta n}\to z_\eta$ in Z as $n\to\infty$. We will use the following extremal problem for a-posteriori error estimate of a finite-dimensional approximate solution $z_{\eta n}$: find an element $\tilde{z}_{\eta n}\in Z_n$ such that

$$\|\tilde{z}_{\eta n}-z_{\eta n}\|=\sup\{\|z-z_{\eta n}\|:z\in Z_n,\|A_nz-u_n\|\le C\|A_nz_{\eta n}-u_n\|,\\ \Omega_n[z]\ \le C\Omega_n[z_{\eta n}]\}\overset{def}{=}\varepsilon_n(\eta). \tag{2.18}$$

The task (2.18) is a finite-dimensional analogue of the problem (2.17). It can be verified that the problem (2.18) has a solution under the assumptions made. The connection of the a-posteriori estimator $\varepsilon(\eta)$ and its finite-dimensional analog $\varepsilon_n(\eta)$ is indicated by the following theorem [33].

Theorem 2.3. *If the set $\mathcal{Z}_\eta=\{z\in Z:\ \|A_hz-u_\delta\|\le\Delta_\eta,\ \Omega[z]\le R_\eta\}$ satisfies the condition $\operatorname{int}\mathcal{Z}_\eta\neq\varnothing$ for each $\eta, 0<\|\eta\|\le\eta_0$, then $\lim_{n\to\infty}\varepsilon_n(\eta)=\varepsilon(\eta)$.*

The error estimate of the finite-dimensional analog, $\mathcal{P}_n\bar{z}$, of the exact solution $\bar{z}$ presents in the following theorem.

Theorem 2.4. *If $\bar{z}\in\operatorname{int}\mathcal{Z}_\eta\neq\varnothing$ for each η, $0<\|\eta\|\le\eta_0$, then $\|\mathcal{P}_n\bar{z}-z_{\eta n}\|\le\varepsilon_n(\eta)$.*

Approximate finite-dimensional data of the form Z_n,A_n,u_n,Ω_n with the properties listed above often arise in applications. In the next section, we describe a special algorithm for calculating the estimator $\varepsilon_n(\eta)$. For brevity, we will use the notation $\sigma_n=(\eta_n,\kappa_n)$ for complete set of given data errors and $m_n=z_{\eta n}$ for finite-dimensional approximate solution. Also, we use everywhere finite-dimensional Euclidean norm, $\|\cdot\|=\|\cdot\|_E$, and the scalar product $(\cdot,\cdot)$ in finite dimensional spaces Z_n and U_n.

2.5 Practical a-posteriori error estimate for linear inverse problems

We will solve a variant of the problem (2.18) to get a-posteriori error estimate for the finite-dimensional approximate solutions, m_n. As above, we set the constant $C>1$ and calculate the quantities $\Delta_n=C\|A_nm_n-u_n\|$ and $R_n=C\|m_n\|$. Next, we introduce the set $\mathcal{Z}_n=\{m\in Z_n:\ \|A_nm-u_n\|\le C\Delta_n,\ \|m\|\le CR_n\}$. Suppose that $\bar{m}=\mathcal{P}_n\bar{z}\in\mathcal{Z}_n$, where $\bar{m}$ is a finite-dimensional approximation of the exact solution $\bar{z}$. Then, the following inequality holds:

$$\|m_n-\bar{m}\|\le\max\{\|m_n-m\|:\ m\in\mathcal{Z}_n\}\overset{def}{=}E(\sigma_n), \tag{2.19}$$

in which $E(\sigma_n)$ is the *global a-posteriori error estimate* of an approximate solution m_n. It can be found by approximate calculation of the maximum (2.19).

The problem (2.19) can be written in an equivalent form, if we use the equality $m=m_n+tw$. Here, $w=(m-m_n)/\|m-m_n\|$, $\|w\|=1$, and $t=\|m-m_n\|\ge0$:

$$E^2(\sigma_n)=\max_{t,w}\Big\{t^2:\ \|w\|=1,\ \|tA_nw-v_n\|^2\le C^2\|v_n\|^2,\ \|tw+m_n\|^2\le C^2\|m_n\|^2,\ t\ge0\Big\},$$

where $v_n=u_n-A_nm_n$. Inequalities in the constraints of this extremum problem can be rewritten taking into account the equality $\|w\|=1$:

$$\|A_nw\|^2t^2-2(A_nw,v_n)t-D_n^2\le0,\quad t^2+2(w,m_n)t-r_n^2\le0,\quad t\ge0, \tag{2.20}$$

where $D_n^2 = (C^2-1)\|v_n\|^2$ and $r_n^2 = (C^2-1)\|m_n\|^2$. Solving the inequalities (2.20) for every admissible w, we obtain $t \in [0, t_n(w)]$. Here, $t_n(w) = \min\{t_n^{(A)}(w), t_n^{(I)}(w)\}$ and

$$t_n^{(I)}(w) = \sqrt{(w,m_n)^2 + r_n^2} - (w,m_n) > 0,$$

$$t_n^{(A)}(w) = \left\{ \frac{\sqrt{(A_n w, v_n)^2 + D_n^2 \|A_n w\|^2} + (A_n w, v_n)}{\|A_n w\|^2}, \ \|A_n w\| \neq 0 \right\} \geq 0.$$

If $\|A_n w\| = 0$, then formally we set $t_n^{(A)}(w) = +\infty$. Thus, the following equality holds:

$$E(\sigma_n) = \max_{t,w} \{t: \ t \in [0, t_n(w)], \ \|w\| = 1\} = \max_w \{t_n(w): \ \|w\| = 1\},$$

and the a-posteriori error estimate $E(\sigma_n)$ can be calculated from the solution of the optimization problem

$$E(\sigma_n) = \max_w \{t_n(w): \ \|w\| = 1\}$$

with a target functional $t_n(w) = \min\{t_n^{(A)}(w), t_n^{(I)}(w)\}$. This approach, however, is inconvenient, since the functional $t_n(w)$ can be non-differentiable for some w. In this regard, we will apply the following method.

We introduce the function $\xi_\nu(a,b) = \frac{ab}{\sqrt[\nu]{a^\nu + b^\nu}}$, $a,b > 0$, $\nu \in \mathbb{N}$. It is easy to verify that inequality $\xi_\nu(a,b) \leq \min\{a,b\} \leq \sqrt[\nu]{2}\xi_\nu(a,b)$ holds. Therefore,

$$\xi_\nu\left(t_n^{(A)}(w), t_n^{(I)}(w)\right) \leq \min\left\{t_n^{(A)}(w), t_n^{(I)}(w)\right\} \leq \sqrt[\nu]{2}\xi_\nu\left(t_n^{(A)}(w), t_n^{(I)}(w)\right).$$

Hence, if we solve the extremum problem: find the number

$$\rho_\nu(\sigma_n) = \max\left\{\xi_\nu\left(t_n^{(A)}(w), t_n^{(I)}(w)\right): \ \|w\| = 1\right\}, \tag{2.21}$$

then, we get the inequality $\rho_\nu(\sigma_n) \leq E(\sigma_n) \leq \sqrt[\nu]{2}\rho_\nu(\sigma_n)$. Choosing a sufficiently large ν, we can take a number $\rho_\nu(\sigma_n)$ as an estimate of the value of $E(\sigma_n)$ with relative accuracy $\epsilon = \sqrt[\nu]{2} - 1$. For example, if $\nu = 30$ then the accuracy is $\epsilon \approx 0.0234$.

The functional $K(w) := \xi_\nu(t_n^{(A)}(w), t_n^{(I)}(w))$ is differentiable on the set $\{w: \ \|w\| = 1\}$, and therefore one can apply well-known optimization methods implemented in the software packages MATLAB, SciLab, Python, etc. for solving the problem (2.21). We used the method of conjugate gradients projection described in detail in [70] with the multistart (as it is done in MATLAB).

Note that the a-posteriori error estimate, based on the application of the function $\rho_\nu(\sigma_n)$, is more preferable from a computational point of view than calculating $E(\sigma_n)$. The problem (2.21) contains only one constraint, while the original problem (2.19), for calculating the function $E(\sigma_n)$, includes two constraints defining the set $\mathcal{Z}_n$. Therefore, problem (2.21) should be solved numerically faster than (2.19).

2.6 Optimality in order for the estimator $\varepsilon(\eta)$ and extra-optimal regularizing algorithms

Let us return to the statement of the problem from Section 2.1 with the assumptions (A)–(D). In particular, we emphasize that the problem (2.1) has a unique solution $\bar{z}\in\mathcal{D}$. We introduce the number $R=\Omega[\bar{z}]$ and the set $M_R=\{z\in\mathcal{D}:\Omega[z]\le R\}$. Then the set of constraints in the problem (2.16) can be presented as $\mathcal{Z}_\eta=\left\{z\in\mathcal{D}:\ z\in M_{R_\eta},\ J_\eta[z]\le\Delta_\eta\right\}$.

Theorem 2.5. *Let the inequalities*

$$R_\eta\le C_0R,\quad \Delta_\eta\le\lambda_\eta+C_0\Psi(\eta,R), \tag{2.22}$$

are valid for $0<\|\eta\|\le\eta_0$*, where* $C_0>1$ *is a fixed constant. Then, the estimator* $\varepsilon(\eta)$ *from* (2.16) *has the optimal order of accuracy on the set* M_{C_0R}*, namely,* $\varepsilon(\eta)\le2\Delta_{opt}(\eta,J_\eta;M_{C_0R})$.

It is possible to prove as in Lemma 2.1 that the first condition in (2.22) is fulfilled for any RA, if $\Omega[\bar{z}]>0$.

Remark 2.2. Theorem 2.5 holds true for error estimates in GDP and GDM algorithms (see [34]).

Definition 2.1. *The regularizing algorithm* $z_\eta=P_\eta(J_\eta,\eta,\Psi)$ *is said to be extra-optimal if its a-posteriori error estimate, the function* $\varepsilon(\eta)$ *of type* (2.16)*, is of optimal order on the set* M_{C_0R}.

We can see from Theorem 2.5 that the sufficient condition of extra-optimality for an RA is the fulfillment of the inequalities (2.22). Theorem 2.5 along with the inequality (2.15) implies that any extra-optimal RA is optimal in order on the set M_{C_0R}. Generally speaking, the reverse is not true that is, not every optimal in order RA can be extra-optimal. The relevant example is given in [31] for linear ill-posed problems of the form (2.5). It follows from Remark 2.2 that Tikhonov regularization with the parameter α selection according to the (generalized) discrepancy principle is extra-optimal method as well as the GDM.

3 Piecewise uniform regularization for the inverse problem of microtomography with a-posteriori error estimate

In geological studies, the problem of microstructure analysis of samples often arises. Traditional methods based on surface observations, such as optical and scanning electron microscopy, are common tools for providing valuable information of microstructures [19, 21]. Recently for these purposes, the methods of computed tomography (CT) are increasingly being used, especially X-ray tomography [19,43,77]. One variant of this approach seems to be more preferable, namely, computed tomography with synchrotron radiation (SR) source. Such approach was applied in [84] for the microanalysis of shale specimens. It was noted in [84] that the SR X-ray beams have many advantages for CT:

(1) monochromatized beams eliminate beam hardening which induces artifacts in CT image, (2) it is energy-tunable and has a wide frequency spectrum and (3) it has high spatial resolution.

Using SR parallel X-ray beams for tomography we can formulate the direct problem by the use of Radon transform [46] of a function $\mu(x,y)\in Z$

$$R[\mu(x,y)](\theta,r)=\int_{l(\theta,r)}\mu(x,y)ds.$$

Here Z is appropriate Banach space (space of solutions) and $l(\theta,r):\ xcos(\theta)+ysin(\theta)=r$ is a straight line in the plane $\mathbb{R}^2_{xy}$ that depends on two parameters θ and r. In fact, we apply a more convenient form of Radon transform, that is

$$R[\mu(x,y)](\theta,r)=\iint\limits_{\mathbb{R}^2_{xy}}\mu(x,y)\delta(x\cos\theta+y\sin\theta-r)dxdy, \tag{3.1}$$

where $\delta(\cdot)$ is Dirac function. Then the inverse problem can be written as the integral equation $R[\mu(x,y)](\theta,r)=u(\theta,r)$ with data $u(\theta,r)$ which are known as projections and belong to a normed space U. Briefly, this equation can be written in the operator form $\mathcal{A}\mu=u$. Here $\mathcal{A}$ is an integral operator of the form (3.1) acting from Z into U. We shall denote the exact solution of this equation as $\bar{\mu}\in Z$. The uniqueness of the solution is investigated, for example, in [46]. The choice of the space Z is determined by the available a-priori information about the desired solution.

Usually, the exact data of such a problem are unknown, and we have at our disposal their approximations, i.e. right-hand side $u_\delta(\theta,r)\in U, \|u(\theta,r)-u_\delta(\theta,r)\|\leqslant\delta$ and an approximate kernel of Eq. (3.1), $K_h(\theta,r,x,y)=\delta_h(x\cos\theta+y\sin\theta-r)$, which is determined by a family of functions $\delta_h(\cdot)$ that approximates the delta function (see, e.g. [73]). Thus, we solve in fact the integral equation

$$\iint\limits_{\mathbb{R}^2_{xy}}K_h(\theta,r,x,y)\mu(x,y)dxdy=u_\delta(\theta,r),\quad \mu\in Z. \tag{3.2}$$

In the operator form we will write it as $\mathcal{A}_h\mu=u_\delta$, where $\mathcal{A}_h:Z\to U$ is an integral operator presented in (3.2). In what follows we assume that $U=L_2(\mathcal{D})$, where $\mathcal{D}$ is a range of variables (θ,r). The operator $\mathcal{A}_h$ approximates the operator $\mathcal{A}$ on the element $\bar{\mu}\in Z$ with an error $\varepsilon_{\mathcal{A}}=\|\mathcal{A}_h\bar{\mu}-\mathcal{A}\bar{\mu}\|_U$. This error must be taken into account in the method of solving the inverse problem (3.2). In some cases, when there is additional a-priori information about the solution, one can find an upper estimate h for $\varepsilon_{\mathcal{A}}$ and then solve problem (3.2) on the class of functions μ for which the inequality $\|\mathcal{A}_h\mu-\mathcal{A}\mu\|_U\leq h$ holds (see, e.g. [71]). Therefore, the residual of Eq. (3.2) on the element $\bar{\mu}$ approximates the exact residual, $\|\mathcal{A}\bar{\mu}-u\|_U=0$, with an accuracy $h+\delta$:

$$\big|\|\mathcal{A}\bar{\mu}-u\|_U-\|\mathcal{A}_h\bar{\mu}-u_\delta\|_U\big|\leq\|\mathcal{A}_h\bar{\mu}-\mathcal{A}\bar{\mu}\|_U+\|u-u_\delta\|_U\leq h+\delta.$$

This means that when a regularization method is applied to solve the inverse problem, we must use $\eta = h + \delta$ instead of δ in a procedure of choosing the regularization parameter. The quantity h can often be neglected if condition $h \ll \delta$ is valid.

The integral equation (3.2) can be conveniently solved using the Tikhonov regularization method [70]. In doing so, we obtain a solution in the form $\mu^{\alpha(\eta)} \in Z$, where

$$\mu^{\alpha} = \operatorname{argmin}\left\{\alpha\Omega(\mu) + \|\mathcal{A}_h\mu - u_\delta\|_U^2 : \mu \in Z\right\}, \tag{3.3}$$

$\Omega(\mu)$ is a regularizing functional, and $\alpha = \alpha(\eta) > 0$ is a regularization parameter chosen in a special way, for example, according to the discrepancy principle (DP) [44]. The regularizing functional must be chosen so as to provide the required type of convergence of approximate solution to the exact one when data errors vanish, $\eta \to 0$.

Similar procedure for solving inverse problems was applied by many authors (see, for example, [9, 71], etc.) for various spaces Z, functionals $\Omega(\mu)$ and parameters $\alpha(\eta)$. In particular, for the discrete problem (3.2), the space ℓ_1 was taken as the solution space in [84]. This provides the so-called sparse regularization. Another approach is proposed in [3] where the space $\mathcal{BV}$ of functions with BV-variation (see, e.g. [18]) was applied as the space of solutions. This allows considering discontinuous or close to discontinuous solutions of inverse problems. Consideration of such functions is important, for example, when analyzing the internal structure of geological samples that have a granular or crystalline structure. The choice of a regularizing functional in the form $\Omega(\mu) = \|\mu\|_{BV}$ then ensures L_1-convergence of the approximate solutions to the exact one.

In this paper, we use the space $\mathcal{VH}$ of functions with bounded VH-variation as Z. This space was introduced in [23, 24] by generalizing the concept of a function with a bounded Hardy-Krause variation. Properties of functions from this space are described in [23–27]. In particular, such functions can be discontinuous, and this allows us to use such functions in solving inverse problems along with functions from $\mathcal{BV}$. It turns out that in the Tikhonov regularization with $Z = \mathcal{VH}$ a piecewise uniform convergence of approximate solutions to the exact solution can be obtained. This makes it possible to reconstruct the solution sufficiently well outside the vicinity of the lines of discontinuity which themselves can be well contrasted (see [26, 27]).

The second feature of this paper is the method of a-posteriori error estimation for the obtained approximate solutions. In most works (see, for example, [9] and the references therein), theoretical a-priori error estimates are carried out. They, as a rule, are obtained with very strict additional constraints on the desired solution. Moreover, these estimates often contain constants, the practical calculation of which is difficult. Therefore, it is impossible to obtain an a-priori error estimate in the form of a number in most cases. In this regard, the theory of a-posteriori error estimates has recently been developed (see [5, 33–35, 66, 88]). Using the methods of this theory, one can obtain numerical estimates of the accuracy of approximate solutions. In this paper, we apply the approach to an a-posteriori error estimate given in [33–35]. More importantly, we propose and test a new algorithm for obtaining a-posteriori error estimate in the solution space L_2 for the inverse tomography problem (3.2).

3.1 Solution of the inverse microtomography problem in the class of VH-functions

We shall assume for simplicity that $\operatorname{supp}(\bar{\mu}) \subseteq \Pi = [0,1]\times[0,1]$. Suppose that the function $\bar{\mu}(x,y)$ is continuous everywhere in Π except on a set $G, G\subset\Pi$, of unknown discontinuity points. We assume that the set G has a zero 2D-measure. Given the data of our inverse problem we wish to construct a function $\mu_\eta(x,y)$, such that $\mu_\eta(x,y)\to\bar{\mu}(x,y)$ as $\eta\to 0$ uniformly on any closed subset $D, D\subset\Pi$, containing no discontinuity points of the function $\bar{\mu}(x,y)$. The procedure of constructing such functions $\mu_\eta(x,y)$ is called piecewise uniform regularization. The piecewise uniform regularization in N-dimensional case has been studied theoretically in [23–27]. In these investigations the functions of bounded variation were widely used. Note that in the N-dimensional case the concept of the variation of a function can be represented in several ways. The properties of corresponding functions of bounded variation depend essentially on the particular construction of variation and, in general, can differ from some standard properties in the one-dimensional case. Therefore, not all constructions of N-dimensional variation are theoretically suitable for piecewise-uniform regularization. For instance, the application of the BV-variation (cf. [18]) to the Tikhonov regularization only ensures convergence in $L_p, 1\le p<\frac{N}{N-1}$, of the approximate solutions (see, e.g., [3]). Also, a counterexample is presented in [25] demonstrating that, in general, the use of BV-variation does not guarantee pointwise (and therefore, piecewise-uniform) convergence. For piecewise uniform regularization, the most suitable is the construction of the VH-variation. Readers can learn more about the theory of VH-variation in [23–26]. Here, for brevity, we give only the main facts without proofs.

First, we formulate the definition of a total VH-variation given in [23, 24].

Let K,L be arbitrary numbers in $\mathbb{N}\backslash\{1\}$. We introduce a grid S_{KL} of the size $K\times L$ in Π: $S_{KL}=\{x_{k,l}\}_{k=1,l=1}^{KL}$ with $x_{k,l}=(x_k,y_l)$, $0=x_1<x_2<\cdots<x_K=1$, $0=y_1<y_2<\cdots<y_L=1$.

Definition 3.1. *The value*

$$\begin{aligned}VH(\mu,\Pi)=\sup_{S_{KL}}\Bigg\{&\sum_{k=1}^{K-1}|\mu(x_{k+1,1})-\mu(x_{k,1})|+\sum_{l=1}^{L-1}|\mu(x_{1,l+1})-\mu(x_{1,l})|\\&+\sum_{k=1}^{K-1}\sum_{l=1}^{L-1}|\mu(x_{k+1,l+1})-\mu(x_{k+1,l})-\mu(x_{k,l+1})+\mu(x_{k,l})|:\\&\forall K,L\in\mathbb{N}\backslash\{1\},\ \forall S_{KL}=\{x_{k,l}\}_{k=1,l=1}^{KL}\Bigg\}\end{aligned}$$

is called the total VH-variation of the function $\mu(x,y)$ in the domain Π. If the value $VH(\mu,\Pi)$ is finite, then we say that the function $\mu(x,y)$ has bounded VH-variation.

The set of all functions with bounded VH-variation equipped with the norm $\|\mu\|_{VH}=|\mu(0,0)|+VH(\mu,\Pi)$ is a Banach space, which we denote by $\mathcal{VH}(\Pi)$. If $\mu\in\mathcal{VH}(\Pi)$ then $\mu(x,y)$ is bounded and continuous in Π everywhere except perhaps in points of discontinuity belonging to no more than a countable set of coordinate lines. Hence, $\mathcal{VH}(\Pi) \subset L_p(\Pi)$, $p \geq 1$.

We will further assume that $\bar{\mu} \in \mathcal{VH}(\Pi)$ and $\bar{\mu}(x,y)|_{\partial\Pi} = 0$. From the results of [23–27] (see, for example, Theorem 4 and Theorem 5 in [24]) it follows in particular that the Tikhonov regularization with $\Omega(\mu) = \|\mu\|_{VH}$ and with a choice of the regularization parameter by the discrepancy principle guarantees the piecewise uniform convergence of approximate solutions to the exact one when $\eta \to 0$. This means that the convergence $\mu^{\alpha(\eta)} \to \bar{\mu}$ will be uniform in any closed region where the function $\bar{\mu}$ is continuous.

Consider a discrete version of the inverse problem and an algorithm for solving it. Let $\mathcal{S}$ be a uniform grid in Π with $K = L = M+1$. Let's further $S_{MM} = \{x_k, y_l\}$, $k,l = 1,\cdots,M$, be a grid composed of centers (x_k, y_l) of the grid $\mathcal{S}$. We will use the set of values, $m = \{\mu(x_k, y_l)\}$, as a discretization of a function $\mu(x,y)$, which, like the function $\bar{\mu}(x,y)$, satisfies the condition $\mu(x,y)|_{\partial\Pi} = 0$. Moreover, we use the notations $d_\delta = \{u_\delta(\theta_i, r_j)\}$ for the measured projections. For these experimental data, the finite-dimensional Euclidean norm $\|\cdot\|_E$ will be used. Next, we denote by A and A_h the finite-dimensional operators obtained by the discretization of the integral operators $\mathcal{A}, \mathcal{A}_h$ in (3.1) and (3.2) on the grids S_{MM} and $\{(\theta_i, r_j)\}$. We will also assume that $\|Am - A_h m\|_E \leq h$ and the error estimate of the operator, h, is known. Then, the inverse problem (3.2) in discrete form can be formulated as a system of linear algebraic equations (SLAE) $A_h m = d_\delta$. We note that the matrix A_h is sparse, (in our computational tests the sparsity is about 0.9983 [84]).

As a regularizer, we choose the discrete version of the norm $\|\mu\|_{VH}$:

$$\Omega(m) = \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} |m(x_{k+1,l+1}) - m(x_{k+1,l}) - m(x_{k,l+1}) + m(x_{k,l})|$$

taking into account that $m|_{\partial\Pi} = 0$. The Tikhonov regularization of the form (3.3) with such a functional Ω requires the optimization of non-smooth functionals. To avoid this, the replacement of $\Omega(m)$ by a smoothed functional

$$\Omega_\varepsilon(m) = \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} f_\varepsilon(m(x_{k+1,l+1}) - m(x_{k+1,l}) - m(x_{k,l+1}) + m(x_{k,l}))$$

was proposed and justified in [24–26]. Here $f_\varepsilon(t)$ is a smoothing function, properties of which are listed, for example, in [25]. In what follows, we take $f_\varepsilon(t) = \sqrt{t^2 + (\frac{\varepsilon}{KL})^2}$. Then, $0 \leq \Omega_\varepsilon(m) - \Omega(m) \leq \varepsilon$. The quantity ε can be taken arbitrarily small. Being applied in the Tikhonov regularization (3.3), this functional ensures the piecewise-uniform regularization of the inverse problem with the help of the approximate solutions $m^{\alpha(\eta,\varepsilon)} = \operatorname{argmin}\{\alpha\Omega_\varepsilon(m) + \|A_h m - d_\delta\|_E^2\}$, as $\eta, \varepsilon \to 0$ (see [24–27] and [71] for proofs). Here the regularization parameter $\alpha(\eta,\varepsilon)$ is chosen according to the discrepancy principle [44]. To find the approximations $m^{\alpha(\eta,\varepsilon)}$, we use a variant of the well-known method of conjugate gradients projecting (see e.g., [70, p.88,92]). Previously, we applied this version of the method to solving many practical problems and therefore we do not give a detailed description of it.

3.2 A-posteriori error estimate for the solution of the microtomography inverse problem

We tested the proposed technique of solving the microtomography inverse problem (3.2) on the class $\mathcal{VH}$ with the a-posteriori error estimate (2.21) for the standard model problem with Shepp-Logan phantom [61]. In our case, the dimension of the reconstructed image was $\dim m = K\times L = 683\times 683$, and the dimension of the projections was $\dim d_\delta = \dim\{(\theta_i, r_j)\} = 180\times 683$. The matrix A_n of the problem $A_n m = d_\delta$ was previously used to solve the inverse problem of microtomography in the work [84].

The numerical matrix A_n differs from the exact matrix A, which is used in the standard module Radon.m of the MATLAB package. For the model problem solved in this section, in which the condition $|\bar{\mu}(x,y)|\le 1$ is satisfied, we can estimate the value of h. It turned out that $h\approx 4.2\cdot 10^{-6}$. Thus, we can assume that $h+\delta\approx\delta$ for the values of δ used below. In the calculations, we also assume that $\varepsilon=10^{-8}$, $C=1.1$, $n=30$.

Fig. 1(a) shows the data of the inverse problem (projections) d_δ, and the exact solution, $\bar{m}$, is given in Fig. 1(b). In Fig. 2(a), the approximate solution $m_\sigma = m^{\alpha(\eta,\varepsilon)}$ (see Section 3.1) for unperturbed data is presented. The relative residual of the approximate solution found is $\frac{\|A_h m_\sigma - d_\delta\|_E}{\|d_\delta\|_E} = 6.6\cdot 10^{-6}$. To obtain the approximation, it took 1000 iterations. The calculation time was about 593 seconds on the PC Intel (R) Core (TM) i7-2600 CPU 3.40 GHz, RAM 8Gb. The relative a-posteriori error estimate, $e(\sigma) = \frac{E(\sigma)}{\|m_\sigma\|_E}$, approximately found by solving the problem (2.21) turned out to be $e(\sigma)\approx 0.13\cdot 10^{-5}$ against the directly found relative error $\frac{\|m_\sigma - \bar{m}\|_E}{\|\bar{m}\|_E} = 0.11\cdot 10^{-5}$. It took about 292 seconds to get the error estimate.

For comparison, the results of the solution to the inverse problem for data perturbed by normally distributed errors with $\delta = \frac{\|d_\delta - d\|_E}{\|d\|_E} = 0.01$ are presented on Fig. 2(b). Here, the relative a-posteriori error estimate was about 0.0756 against the relative error 0.0487 (see Table 1).

Now we compare the accuracy of the Tikhonov regularization for solving the inverse problem on the functional class $\mathcal{VH}$ and the class $\mathcal{BV}$, i.e. with regularizers $\Omega(\mu) = \|\mu\|_{VH}$ and $\Omega(\mu) = \|\mu\|_{BV}$. In both cases, the regularization parameter was chosen by the discrepancy principle. Results of calculations for different relative levels of data disturbance, $\delta_0 = \frac{\|u_\delta - u\|_{L_2}}{\|u\|_{L_2}}$, are presented in Table 1.

Table 1: Global errors $\Delta_C = \|\bar{m} - m_\sigma\|_{C(\Pi)}/\|\bar{m}\|_{C(\Pi)}$ in Π and errors $\Delta_C = \|\bar{m} - m_\sigma\|_{C(R)}/\|\bar{m}\|_{C(\Pi)}$ in continuity regions $R = R_{1-4}$.

	global, Π		region 1, R_1		region 2, R_2		region 3, R_3		region 4, R_4	
δ_0	Δ_C^{VH}	Δ_C^{BV}	Δ_C^{VH}	Δ_C^{BV}	Δ_C^{VH}	Δ_C^{BV}	Δ_C^{VH}	Δ_C^{BV}	Δ_C^{VH}	Δ_C^{BV}
0.01	0.0431	0.0335	1.79e-4	2.52e-4	2.06e-4	2.88e-4	1.71e-4	2.99e-4	1.52e-4	3.45e-4
0.001	0.0059	0.0036	1.72e-5	2.58e-5	2.03e-5	2.94e-5	1.63e-5	3.03e-5	1.53e-5	3.48e-5

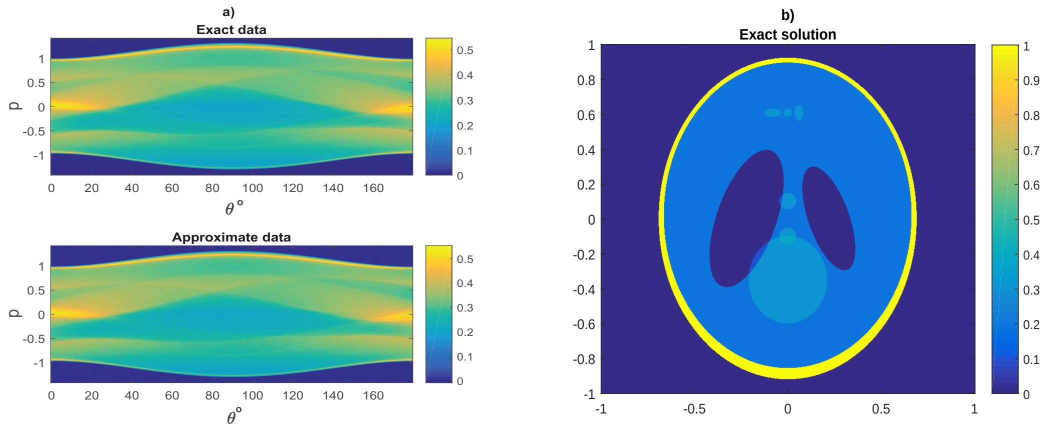

Figure 1: (a) Exact and approximate data. (b) Exact image.

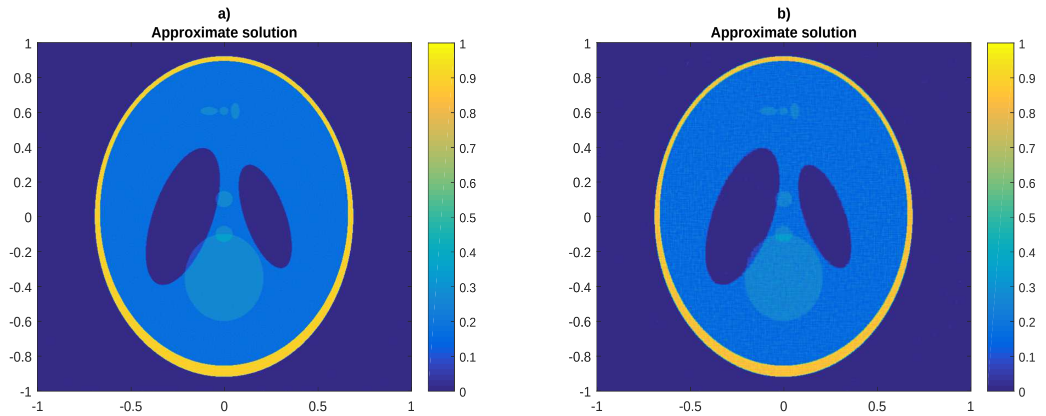

Figure 2: (a) Approximate solution for unperturbed data. (b) Approximate solution for perturbed data with $\delta = 0.01$.

Columns 2-3 show global relative uniform errors, $\Delta_C = \|\bar{m} - m_\sigma\|_{C(\Pi)} / \|\bar{m}\|_{C(\Pi)}$, of both methods. It can be seen that the BV-method gives a better global accuracy than the VH-method. However, it is known [23–26] that the VH-method has a theoretical advantage. It guarantees the piecewise uniform convergence of approximate solutions when $\delta_0 \to 0$, while the BV-method ensures only convergence in some spaces L_p [3]. Columns 4-11 of Table 1 allow to compare relative uniform errors $\Delta_C = \|\bar{m} - m_\sigma\|_{C(R)} / \|\bar{m}\|_{C(\Pi)}$ of the methods in certain areas of continuity, $R = R_{1-4}$. These areas are shown in Fig. 3 in orange color. For all domains, the errors of the VH-method turn out to be substantially less than the errors of the BV- method, and this ratio is preserved when decreasing the data error level δ_0.

Thus, as noted earlier in [23–26], the VH-method is more preferable in solving inverse problems with exact solutions that have discontinuity lines separating regions of

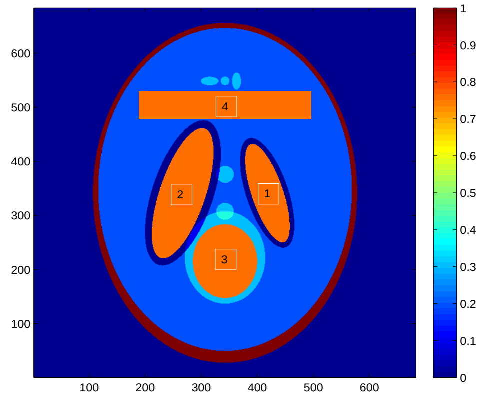

Figure 3: Selected regions of continuity R_{1-4} for error estimates.

continuity. A typical example of such solutions for tomography problems is the Shepp-Logan phantom. Solutions of this type appear in the study of shales structures by the microtomography methods [84], as well as in image processing problems [26].

Finally, we consider numerical results concerning a-posteriori error estimates of the approximate solutions m_σ, computed from the VH-method. In doing so, we note that estimates of the form (2.19) can be obtained for a part of the solution defined in a region $R\subset\Pi$: $\|m_n-\bar{m}\|_{E(R)}\le\max\left\{\|m_n-m\|_{E(R)}:\ m\in\mathcal{Z}_n\right\}\overset{def}{=}E_R(\sigma_n)$. Here, $\|\cdot\|_{E(R)}$ is the Euclidean norm calculated for the grid functions $m_n,\bar{m}$ and m restricted to the domain R. Arguing as above, we can prove that

$$E_R(\sigma_n)=\max_w\Big\{t_n(w)||w||_{E(R)}:\ \|w\|=1\Big\}.$$

Next, we can find the number $\rho_\nu^{(R)}(\sigma_n)=\max\left\{\xi_\nu\left(t_n^{(A)}(w),t_n^{(I)}(w)\right)||w||_{E(R)}:\ \|w\|=1\right\}$ and obtain the inequality $\rho_\nu^{(R)}(\sigma_n)\le E_R(\sigma_n)\le\sqrt[\nu]{2}\rho_\nu^{(R)}(\sigma_n)$ that is used to estimate the value $E_R(\sigma_n)$.

So, we use the method from Section 2.5 to estimate the quantity $\Delta_E=\|\bar{m}-m_\sigma\|_E/\|\bar{m}\|_E$ for $R=\Pi$ and $R=R_{1-4}$. Table 2 shows the true values of these errors and their relative a-posteriori estimates, $e(\sigma)=\frac{E(\sigma)}{\|m_\sigma\|_E}$ and $e_R(\sigma)=\frac{E_R(\sigma)}{\|m_\sigma\|_E}$.

Table 2: Errors Δ_E and relative a-posteriori error estimates $e(\sigma)$ in $R=\Pi$ and in continuity regions $R=R_{1-4}$.

	global, Π		region 1, R_1		region 2, R_2		region 3, R_3		region 4, R_4	
δ	Δ_E	$e(\sigma)$	Δ_E	$e_R(\sigma)$	Δ_E	$e_R(\sigma)$	Δ_E	$e_R(\sigma)$	Δ_E	$e_R(\sigma)$
0.01	0.0487	0.0756	0.0016	0.0066	0.0020	0.0092	0.0103	0.0134	0.0125	0.0152
0.001	0.0041	0.0066	0.0002	0.0008	0.0003	0.0012	0.0009	0.0009	0.0011	0.0012

These results show that the value of $e(\sigma)$ fairly well estimates the true relative errors of solutions both globally and in the areas of continuity.

4 Magnetic parameters inversion method with full tensor gradient data

In geophysical prospecting, data measured at, above, or below the ground are obtained during field survey (a forward problem), and extraction of the physical properties of the Earth from the data is a mathematical problem (an inverse problem) which is essential for processing and interpretation. Meanwhile, the use of magnetics for geophysical exploration is widely studied.

Traditional magnetic data are total magnetic intensity (TMI). With the development of a high temperature superconducting quantum interference devices (SQUIDs) operating in liquid nitrogen, a novel rotating magnetic gradiometer system has been designed. This system allows to measure components of the gradient tensor. Gradient measurements also provide valuable additional information, compared to conventional total-field measurements, when the field is undersampled. Many discussions are given on the advantages of magnetic gradient tensor surveys as compared to the conventional total magnetic intensity (TMI) surveys [11, 15, 57–59, 85, 86].

Inversion of physical parameters, such as the magnetic susceptibility and the magnetization, are main scientific problems using magnetic field data [52, 53]. Here, a lot of research works have been done so far. Wang and Hansen [76] reformulated the gravimetric-magnetic model in wavenumber domain into coordinates invariance form, and extended the original magnetic inversion method CompuDept into three-dimensional case, which allowed a large amount of airborne magnetic data being involved in inversion; Li and Oldenburg [38] recovered 3D susceptibility models by incorporating a priori information into the model objective function using one or more appropriate weighting functions; Pignatelli et al. [51] considered using dipole source to approximate the discrete gridded model of the anomaly, encompassed the depth weighting function into the discrete potential field function and employed the L–M method to solve the corresponding linear equation to get the solution with depth resolution.

According to the potential theory, the measurement points of the magnetic fields can be described by the integral equations of the first kind. This means that the observed data is far less than the desired susceptibility, as a result, magnetic inverse problems are always ill-posed [89]. The main problems are the nonuniqueness and instability of the solution. Sometimes, missing geological information in the survey area may also lead to difficulty in explanation of the inversion results. Therefore it is crucial to choose proper norm to restrict the solution space of the model. This is meaningful in reducing ill-posedness and enhancing numerical stability. The norm should be chosen according to the *a-priori* information of the model. Due to the fact that the magnetic data lack the resolution in depth, pure norm constraint on the model is not sufficient to reflect the medium layers. To overcome this problem, there are two ways. One is based on the Tarantolas statistical theory [63], assuming that the data and the model are both uncertain and obey the Gaussian distribution, and constructing the fitting function using the maximum *a-posteriori* likelihood function; another is based on Tikhonov regularization theory [70]. It can be proved these two forms are equivalent under proper conditions. Retrieval of magnetization parameters using magnetic tensor gradient measurements receives attention in recent years. The direct determination of subsurface properties (e.g., position, orientation, magnetic susceptibility) from the observed potential field measurements is referred to as inversion.

4.1 Mathematical modeling

The equation describing magnetic field $\boldsymbol{B}_{field\,dipole}$ of dipole sources $\boldsymbol{m}$ is defined as [85,86]

$$\boldsymbol{B}_{field\,dipole}=\frac{\mu_0}{4\pi}\left(\frac{3(\boldsymbol{m}\cdot\boldsymbol{r})\boldsymbol{r}}{r^5}-\frac{\boldsymbol{m}}{r^3}\right),$$

where

$$\boldsymbol{m}=m_x\boldsymbol{i}+m_y\boldsymbol{j}+m_z\boldsymbol{k},\quad \boldsymbol{r}=(x-x_s)\boldsymbol{i}+(y-y_s)\boldsymbol{j}+(z-z_s)\boldsymbol{k},$$

$r=\sqrt{(x-x_s)^2+(y-y_s)^2+(z-z_s)^2}$ is a distance between point (x_s,y_s,z_s), which corresponds to allocation of the triaxial sensor that measures magnetic field $\boldsymbol{B}_{field\,dipole}$, and point (x,y,z) of dipole source $\boldsymbol{m}$, μ_0 is a permeability in vacuum.

Transforming $\boldsymbol{B}_{field\,dipole}$ into following form

$$\begin{aligned}\boldsymbol{B}_{field\,dipole}&=B_{x\,dipole}\boldsymbol{i}+B_{y\,dipole}\boldsymbol{j}+B_{z\,dipole}\boldsymbol{k}\\&=\frac{\mu_0}{4\pi}\left(\left(\frac{3(\boldsymbol{m}\cdot\boldsymbol{r})(x-x_s)}{r^5}-\frac{m_x}{r^3}\right)\boldsymbol{i}+\left(\frac{3(\boldsymbol{m}\cdot\boldsymbol{r})(y-y_s)}{r^5}-\frac{m_y}{r^3}\right)\boldsymbol{j}\right.\\&\qquad\left.+\left(\frac{3(\boldsymbol{m}\cdot\boldsymbol{r})(z-z_s)}{r^5}-\frac{m_z}{r^3}\right)\boldsymbol{k}\right)\end{aligned}$$

and redefining the variables as $i=x,y,z$ and $p=(p_x,p_y,p_z)\equiv(x_s,y_s,z_s)$, we have following representation for components of vector $\boldsymbol{B}_{field\,dipole}$:

$$B_{i\,dipole}=\frac{\mu_0}{4\pi}\left(\frac{3(\boldsymbol{m}\cdot\boldsymbol{r})(i-p_i)}{r^5}-\frac{m_i}{r^3}\right).$$

Taking derivative of $B_{i\,dipole}$ with respect to spatial variable $i=x,y,z$ and $j=x,y,z\neq i$, we have the diagonal elements and non-diagonal elements of tensor matrix $\mathbf{B}_{tensor}$:

$$\begin{aligned}B_{ii}&=\frac{\mu_0}{4\pi}\left(\frac{6m_i(i-p_i)}{r^5}+\frac{3(\boldsymbol{m}\cdot\boldsymbol{r})}{r^5}-\frac{15(\boldsymbol{m}\cdot\boldsymbol{r})(i-p_i)(i-p_i)}{r^7}\right),\\B_{ij}&=\frac{\mu_0}{4\pi}\left(\frac{3m_i(j-p_j)}{r^5}+\frac{3m_j(i-p_i)}{r^5}-\frac{15(\boldsymbol{m}\cdot\boldsymbol{r})(i-p_i)(j-p_j)}{r^7}\right).\end{aligned}$$

Note, that we define full tensor magnetic gradient $\mathbf{B}_{tensor}$, which unlike to magnetic induction $\boldsymbol{B}_{field\,dipole}$ (that has only 3 components) has 9 components and can be written in the following matrix form:

$$\mathbf{B}_{tensor} \equiv [B_{ij}] \equiv \begin{bmatrix} \frac{\partial B_x}{\partial x} & \frac{\partial B_x}{\partial y} & \frac{\partial B_x}{\partial z} \\ \frac{\partial B_y}{\partial x} & \frac{\partial B_y}{\partial y} & \frac{\partial B_y}{\partial z} \\ \frac{\partial B_z}{\partial x} & \frac{\partial B_z}{\partial y} & \frac{\partial B_z}{\partial z} \end{bmatrix} \equiv \begin{bmatrix} B_{xx} & B_{xy} & B_{xz} \\ B_{yx} & B_{yy} & B_{yz} \\ B_{zx} & B_{zy} & B_{zz} \end{bmatrix},$$

where

$$\frac{\partial B_x}{\partial y} = \frac{\partial B_y}{\partial x}, \quad \frac{\partial B_x}{\partial z} = \frac{\partial B_z}{\partial x}, \quad \frac{\partial B_y}{\partial z} = \frac{\partial B_z}{\partial y}, \quad \frac{\partial B_x}{\partial x} + \frac{\partial B_y}{\partial y} + \frac{\partial B_z}{\partial z} = 0.$$

So, actually, we have only 5 different components of the tensor matrix.

Thus, for the whole object, for volume V of which we want to restore the magnetic moment density $\boldsymbol{M}$ ($\boldsymbol{M} = M_x\boldsymbol{i} + M_y\boldsymbol{j} + M_z\boldsymbol{k}$), we have the following 3D Fredholm integral equations of the 1^{st} kind:

$$\begin{aligned}
\boldsymbol{B}_{field\,dipole} &= \frac{\mu_0}{4\pi} \iiint\limits_V \left(\frac{3(\boldsymbol{M}\cdot\boldsymbol{r})\boldsymbol{r}}{r^5} - \frac{\boldsymbol{M}}{r^3} \right) dv, \\
B_{ii} &= \frac{\mu_0}{4\pi} \iiint\limits_V \left(\frac{6m_i(i-p_i)}{r^5} + \frac{3(\boldsymbol{M}\cdot\boldsymbol{r})}{r^5} - \frac{15(\boldsymbol{M}\cdot\boldsymbol{r})(i-p_i)(i-p_i)}{r^7} \right) dv, \\
B_{ij} &= \frac{\mu_0}{4\pi} \iiint\limits_V \left(\frac{3m_i(j-p_j)}{r^5} + \frac{3m_j(i-p_i)}{r^5} - \frac{15(\boldsymbol{M}\cdot\boldsymbol{r})(i-p_i)(j-p_j)}{r^7} \right) dv,
\end{aligned}$$

which can be rewritten as the following system of two 3D Fredholm integral equations of the 1^{st} kind:

$$\begin{cases} \boldsymbol{B}_{field\,dipole}(x_s,y_s,z_s) = \dfrac{\mu_0}{4\pi} \displaystyle\iiint\limits_V \mathbf{K}_{TMI}(x-x_s,y-y_s,z-z_s)\boldsymbol{M}(x,y,z)dv, \\ \boldsymbol{B}_{tensor\,dipole}(x_s,y_s,z_s) = \dfrac{\mu_0}{4\pi} \displaystyle\iiint\limits_V \mathbf{K}_{MGT}(x-x_s,y-y_s,z-z_s)\boldsymbol{M}(x,y,z)dv, \end{cases} \tag{4.1}$$

where $\boldsymbol{B}_{field\,dipole} = [B_x\, B_y\, B_z]^T$ and $\boldsymbol{B}_{tensor\,dipole} = [B_{xx}\, B_{xy}\, B_{xz}\, B_{yz}\, B_{zz}]^T$. Kernels $\mathbf{K}_{TMI}$ and $\mathbf{K}_{MGT}$ of these integral equations can be written as

$$\begin{aligned}
&\mathbf{K}_{TMI}(x-x_s,y-y_s,z-z_s) \\
=&\frac{1}{r^5} \begin{bmatrix} 3(x-x_s)^2-r^2 & 3(x-x_s)(y-y_s) & 3(x-x_s)(z-z_s) \\ 3(y-y_s)(x-x_s) & 3(y-y_s)^2-r^2 & 3(y-y_s)(z-z_s) \\ 3(z-z_s)(x-x_s) & 3(z-z_s)(y-y_s) & 3(z-z_s)^2-r^2 \end{bmatrix}
\end{aligned}$$

and

$$\mathbf{K}_{MGT}(x-x_s,y-y_s,z-z_s)$$
$$=\frac{3}{r^7}\begin{bmatrix} (x-x_s)[3r^2-5(x-x_s)^2] & (y-y_s)[r^2-5(x-x_s)^2] & (z-z_s)[r^2-5(x-x_s)^2] \\ (y-y_s)[r^2-5(x-x_s)^2] & (x-x_s)[r^2-5(y-y_s)^2] & -5(x-x_s)(y-y_s)(z-z_s) \\ (z-z_s)[r^2-5(x-x_s)^2] & -5(x-x_s)(y-y_s)(z-z_s) & (x-x_s)[r^2-5(z-z_s)^2] \\ -5(x-x_s)(y-y_s)(z-z_s) & (z-z_s)[r^2-5(y-y_s)^2] & (y-y_s)[r^2-5(z-z_s)^2] \\ (x-x_s)[r^2-5(z-z_s)^2] & (y-y_s)[r^2-5(z-z_s)^2] & (z-z_s)[3r^2-5(z-z_s)^2] \end{bmatrix}.$$

If we take into account that $V\subset P=\{(x,y,z): L_x\le x\le R_x, L_y\le y\le R_y, L_z\le z\le R_z\}$ and the system of sensor planes is restricted by rectangular parallelepiped $Q=\{(x_s,y_s,z_s)\equiv(s,t,r): L_s\le s\le R_s, L_t\le t\le R_t, L_r\le r\le R_r\}$, we can rewrite the system (4.1) in the following operator form

$$\mathbf{A}\boldsymbol{M}=\frac{\mu_0}{4\pi}\int_{L_x}^{R_x}\int_{L_y}^{R_y}\int_{L_z}^{R_z}\mathbf{K}(s,t,r,x,y,z)\boldsymbol{M}(x,y,z)dxdydz=\boldsymbol{B}(s,t,r), \tag{4.2}$$

where $\boldsymbol{B}(s,t,r)$ and $\boldsymbol{M}(x,y,z)$ are vector–functions: $\boldsymbol{B}=[B_x\, B_y\, B_z\, B_{xx}\, B_{xy}\, B_{xz}\, B_{yz}\, B_{zz}]^T$ and $\boldsymbol{M}=[M_x\, M_y\, M_z]^T$, kernel $\mathbf{K}(s,t,r,x,y,z)$ is a matrix-function: $\mathbf{K}=[\mathbf{K}_{TMI}\,\mathbf{K}_{MGT}]^T$ ($\mathbf{K}=\mathbf{K}_{TMI}$ in the case of total magnetic intensity model without using full tensor magnetic gradient data and $\mathbf{K}=\mathbf{K}_{MGT}$ in the opposed case).

4.2 Tikhonov regularization

We assume that $\boldsymbol{M}\in W_2^2(P)$, $\boldsymbol{B}\in L_2(Q)$, and integral operator $\mathbf{A}$ with the kernel $\mathbf{K}$ is continuous and injective. Norms of the right-hand side of Eq. (4.2) and the solution are introduces as follows:

$$\|\boldsymbol{B}\|_{L_2}=\sqrt{\|B_x\|^2_{L_2}+\|B_y\|^2_{L_2}+\|B_z\|^2_{L_2}+\|B_{xx}\|^2_{L_2}+\|B_{xy}\|^2_{L_2}+\|B_{xz}\|^2_{L_2}+\|B_{yz}\|^2_{L_2}+\|B_{zz}\|^2_{L_2}},$$
$$\|\boldsymbol{M}\|_{W_2^2}=\sqrt{\|M_x\|^2_{W_2^2}+\|M_y\|^2_{W_2^2}+\|M_z\|^2_{W_2^2}}.$$

Suppose that instead of exact data, $\bar{\boldsymbol{B}}$ and $\mathbf{A}$, their approximations $\boldsymbol{B}_\delta$ and $\mathbf{A}_h$ are known, such that $\|\boldsymbol{B}_\delta-\bar{\boldsymbol{B}}\|_{L_2}\le\delta$, $\|\mathbf{A}-\mathbf{A}_h\|_{W_2^2\to L_2}\le h$. In what follows, we denote the error levels of the data as $\eta=\{\delta,h\}$. As the inverse problem (4.2) is ill-posed it is necessary to apply a regularizing algorithm for its solving. We use the algorithm based on minimization of the Tikhonov functional [70,89] of the form

$$F^\alpha[\boldsymbol{M}]=\|\mathbf{A}_h\boldsymbol{M}-\boldsymbol{B}_\delta\|^2_{L_2}+\alpha\|\boldsymbol{M}\|^2_{W_2^2}. \tag{4.3}$$

For any $\alpha>0$, an unique element $\boldsymbol{M}^\alpha_\eta$ exists, which implements the minimum of $F^\alpha[\boldsymbol{M}]$ in $W_2^2(P)$. One can find such elements using well-known optimization methods, for example, the conjugate gradient method. When selecting the regularization parameter $\alpha=\alpha(\eta)$, we use the generalized discrepancy principle [16] that is, solve the equation

$$\rho(\alpha)=\|\mathbf{A}_h\boldsymbol{M}_\eta^\alpha-\boldsymbol{B}_\delta\|_{L_2}^2-\left(\delta+h\|\boldsymbol{M}_\eta^\alpha\|_{W_2^2}\right)^2=0 \Rightarrow \alpha=\alpha(\eta) \tag{4.4}$$

by the methods presented in [70], [71, Sect. 2.14] and based on multiple minimization of the functional (4.3) for different α. Then, using the parameter found, an approximate solution $\boldsymbol{M}_\eta^{\alpha(\eta)}$ is calculated. It is proved in [70,71] that $\boldsymbol{M}_\eta^{\alpha(\eta)}$ tends to the exact solution as $\eta\to 0$ in W_2^2.

4.3 Numerical aspects of the algorithm

The details of the algorithm for minimizing the functional in (4.3) are described in [39,40], including some recommendations of its effective parallelization.

After discretization, the necessary and sufficient condition for the minimum of the functional (4.3) can be written as

$$(A_h^TA_h+\alpha R^TR)M=A_h^TB_\delta. \tag{4.5}$$

Here R and A_h are finite-dimensional approximations, matrices, of operators $\mathbf{R}$: $\|\boldsymbol{M}\|_{W_2^2}=\|\mathbf{R}\boldsymbol{M}\|_{L_2}$ and $\mathbf{A_h}$, respectively, and M is a finite dimensional solution. The dimensions of these quantities are as follows: $\dim R=(N_R\times N)$, $\dim A=(N_A\times N)$, $\dim M=(N\times 1)$.

For numerical solving of system (4.5) we use the conjugate gradient method (CGM) in the following form. Let $M^{(s)}$ be an iterative sequence of the CGM with an initial guess $M^{(1)}$, $p^{(s)}$, $q^{(s)}$ be auxiliary vectors, and suppose that $p^{(0)}=0$. Then formulas of the CGM for searching of solution $M^{(\nu)}$ of system (4.5) can be presented as follow:

$$\begin{aligned}
&r^{(s)}=\begin{cases} A_h^T\big(A_hM^{(s)}-B_\delta\big)+\alpha R^T\big(RM^{(s)}\big), & \text{if}\quad s=1,\\ r^{(s-1)}-q^{(s-1)}/\big(p^{(s-1)},q^{(s-1)}\big), & \text{if}\quad s\geq 2,\end{cases}\\
&p^{(s)}=p^{(s-1)}+\frac{r^{(s)}}{\big(r^{(s)},r^{(s)}\big)},\\
&q^{(s)}=A_h^T\big(A_hp^{(s)}\big)+\alpha R^T\big(Rp^{(s)}\big),\\
&M^{(s+1)}=M^{(s)}-\frac{p^{(s)}}{\big(p^{(s)},q^{(s)}\big)}.
\end{aligned}$$

In numerical experiments, we assumed that $M^{(1)}=0$ and used the following rule for stopping iterations: $\nu=\min\{s\colon s\in N,\ \|A_hM^{(s+1)}-B_\delta\|\leq\delta+h\|RM^{(s)}\|\}$ to get the approximate solution $M^{(\nu)}$.

4.4 Numerical results

At first, we wanted to compare different models, namely TMI, TMI+ MGT and MGT models. To do this, we performed the simulation of the experimental data with Gaussian nose of the level $\delta \sim 4\%$, both for TMI and MGT, which are close enough to the practical field experiments. For testing calculation, we used the solution domain,

$$P=\{(x,y,z):\ -5000\leq x\leq 5000,\ -5000\leq y\leq 5000,\ -105\leq z\leq 95\},$$

with the uniform grid of the size $(Nx,Ny,Nz)=(80,80,1)$, and the observation domain,

$$Q=\{(x_s,y_s,z_s)\equiv(s,t,r):\ -400\leq s\leq 4000,\ -4000\leq t\leq 4000,\ r=2000\},$$

with the simulated field data at the points of the grid having the size $(Ns,Nt,Nr)=(350,20,1)$. The normalized magnitude of the model magnetic moment density, $\boldsymbol{M}$, is represented on Fig. 4(a). The results of calculations with TMI, TMI+MGT and MGT models are represented of Fig. 4(b,c,d). The RMS error of the components of the reconstructed vector $\boldsymbol{M}$ is 0.12263 for TMI-model, 0.12262 for TMI+MGT-model and 0.12527 for MGT-model. This means that all listed models give "equal" results, but Fig. 4(c) shows that MGT-model produce more detailed solution.

The main conclusion from testing calculations is that 1) MGT-model is able to produce the better reconstruction for the magnitude of the small details of the solution, 2) the MGT-model should be used alone without combining TMI- and MGT-data.

For calculations, we used 128 processors of the shared research facilities of HPC computing resources "Lomonosov–1" at Lomonosov Moscow State University [55]. Time of calculations is about 5 minutes.

5 Conclusions

The following theoretical points are central to our article:

(a) General theory of Tikhonov's regularization with practical examples is considered.

(b) An overview of a-priori and a-posteriori error estimates for solutions of ill-posed problems is presented as well as a general scheme of a-posteriori error estimation.

(c) A posteriori error estimates for linear inverse problems and its finite-dimensional approximation are considered in detail together with practical a-posteriori error estimate algorithms.

(d) Optimality in order for the error estimator and extra-optimal regularizing algorithms are also discussed.

We suppose that the following applications of this theory are important for practical inverse problems:

(A) The use of functions with bounded VH-variation for a piecewise uniform regularization of the inverse problem of computer tomography has a theoretical and practical

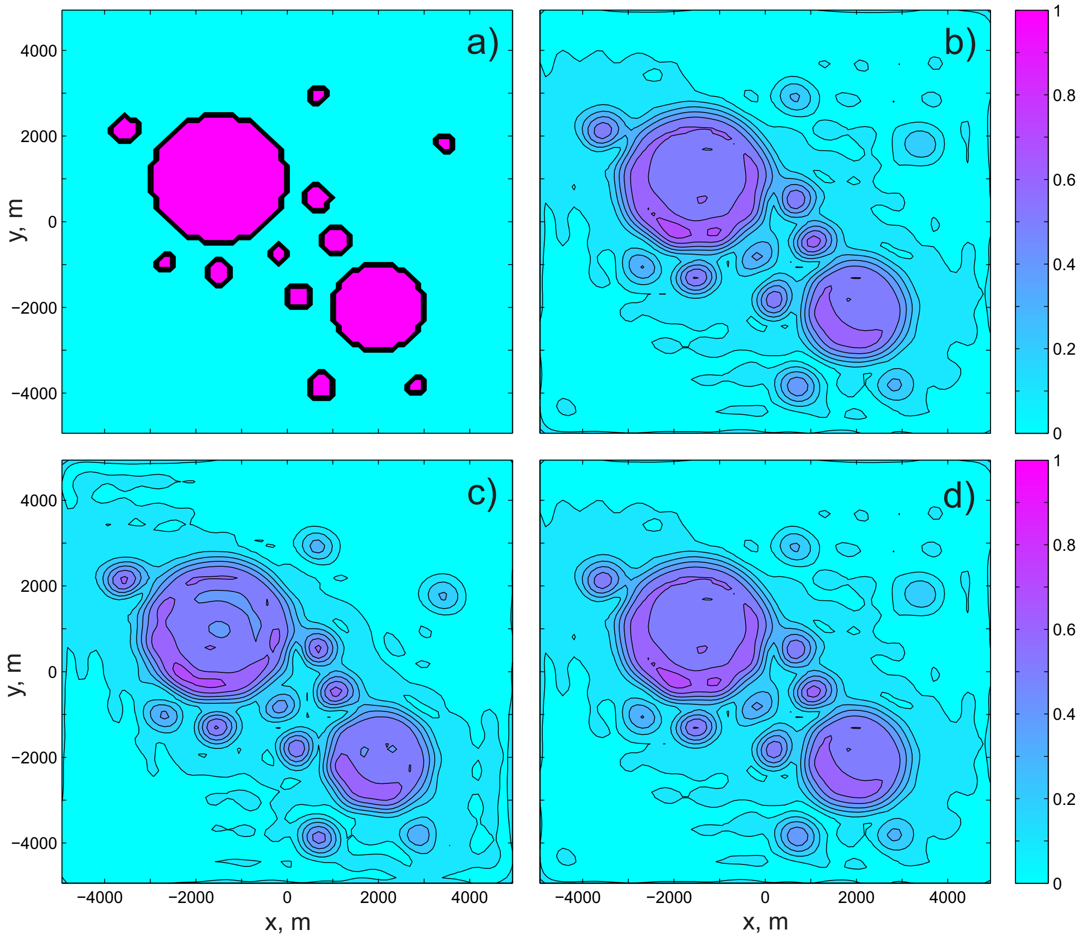

Figure 4: Results of testing calculations: a) model solution (the normalized value of the magnitude of the magnetic moment density **M**), b) retrieved solution for the TMI-model, c) retrieved solution for the MGT-model, d) retrieved solution for the TMI+MGT-model. The MGT-model produces the better reconstruction for the magnitude of the small details of the model solution. The use of the combined TMI+MGT-data does not give any advantages in reconstruction quality comparing with the using of TMI-data only.

advantage. It ensures piecewise-uniform convergence of approximate solutions. This advantage was confirmed by numerical experiments. A piecewise-uniform regularization of this problem was not considered at all before.

(B) A new algorithm for a-posteriori error estimation (see the problem (6)) makes it possible to estimate the error of the solution in the form of a number. It turns out that the a-posteriori error estimate, based on the application of the function $\rho_\nu(\sigma)$, is more preferable from a computational point of view than the algorithm proposed in [33, 34]. The problem (6) contains only one constraint, while the original problem (4) for direct calculation of the function $E(\sigma)$ includes two constraints defining the set $\mathcal{Z}_\sigma$.

(C) Tikhonov's regularization is very effective in magnetic parameters inversion method with full tensor gradient data. The regularization algorithms allow to compare different models in this method and choose the best one, MGT-model.

(D) Application of Tikhonov's regularization to magnetic inverse problem is straightforward since it belongs to volume detection. It is obvious other inverse problems in geophysical exploration can be immediate applied, such as gravimetric inversion, electromagnetic inversion, and seismic inversion.

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