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A RIGOROUS THREE-DIMENSIONAL MAGNETOTELLURIC INVERSION

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Abstract—The limited-memory quasi-Newton optimization method with simple bounds has been applied to develop a novel fully three-dimensional (3-D) magnetotelluric (MT) inversion technique. This nonlinear inversion is based on iterative minimization of a classical Tikhonov-type regularized penalty functional. But instead of the usual model space of log resistivities, the approach iterates in a model space with simple bounds imposed on the conductivities of the 3-D target. The method requires storage that is proportional to $n_{cp} \times N$, where the N is the number of conductivities to be recovered and n_{cp} is the number of the correction pairs (practically, only a few). This is much less than requirements imposed by other Newton type methods (that usually require storage proportional to $N \times M$, or $N \times N$, where M is the number of data to be inverted). Using an adjoint method to calculate the gradients of the misfit drastically accelerates the inversion. The inversion also involves all four entries of the MT impedance matrix. The integral equation forward modelling code *x3d* by Avdeev et al. [1, 2] is employed as an engine for this inversion. Convergence, performance and accuracy of the inversion are demonstrated on a 3D MT synthetic, but realistic, example.

1. INTRODUCTION

Limited memory quasi-Newton (QN) methods are becoming a popular tool for the numerical solution of three-dimensional (3-D) electromagnetic (EM) large-scale inverse problems [11, 7]. The reason is that the methods require calculation of gradients of the misfit only,

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while at the same time avoiding calculations of second-derivative terms. They also require storing merely several pairs of so-called correction vectors that dramatically diminish the storage requirements. A more complete review on this subject may be found in [4].

In this paper we apply a limited memory QN optimization method with simple bounds (hereinafter, referred to as LMQNB) to solve the 3–D magnetotelluric (MT) inverse problem. In Section 2 we briefly describe the setting of the inverse problem, as well as some key features of our implementation, referring the reader to the paper [3] for details.

In Section 3, we develop the theory and basic equations for the calculation of gradients of the misfit. We demonstrate that the calculation of gradients at a given period is equivalent to only two forward modellings and does not depend on the number of conductivities to be recovered. The mathematical details of the approach are not presented here except the key formula (3), which is central to the method.

In Section 4 we demonstrate how our inversion practically works on a synthetic, but realistic numerical example. This example includes a tilted conductive dyke in a uniform half-space (see [17]). The results presented are encouraging and suggest that the inversion may be successfully applied to solving realistic 3-D inverse problems with real MT data.

2. 3-D MT INVERSION

Let us first consider a 3-D earth conductivity model discretized by N cells, such that $\sigma(\mathbf{r}) = \sum_{k=1}^{N} \sigma_k \chi_k(\mathbf{r})$, where $\chi_k(\mathbf{r}) = \begin{cases} 1, \mathbf{r} \in V_k \\ 0, \mathbf{r} \notin V_k \end{cases}$, V_k is the volume occupied by k-th cell and $\mathbf{r} = (x, y, z)$. In the frame of MT inversion conductivities σ_k $(k = 1, \dots, N)$ of the cells are sought. This is a typical optimization problem, such that $\varphi(\sigma, \lambda) \underset{\sigma,\lambda}{\rightarrow} \min$, with a penalty function φ given as

$$\varphi(\sigma, \lambda) = \varphi_d(\sigma) + \lambda \varphi_s(\sigma), \tag{1}$$

where $\varphi_d = \frac{1}{2} \sum_{j=1}^{N_S} \sum_{i=1}^{N_T} \alpha_{ji} tr[\overline{\mathbf{A}}_{ji}^T \mathbf{A}_{ji}]$ is the data misfit. Here $\sigma = (\sigma_1, \dots, \sigma_N)^T$ is the vector consisting of the electrical conductivities of the cells; hereinafter superscript T means transpose and the upper bar stands for the complex conjugate; N is the number of the cells; N_S is the number of MT sites, $\mathbf{r}_j = (x_j, y_j, z = 0)$, where $j = 1, \dots, N_S$; N_T is the number of the frequencies ω_i, where $i = 1, \dots, N_T$; the $2{\times}2$ matrices $\mathbf{A}_{ji}$ are defined as $\mathbf{A}_{ji} = \mathbf{Z}_{ji} - \mathbf{D}_{ji}$, where $\mathbf{Z}_{ji} =$

$\begin{pmatrix} Z_{xx} & Z_{xy} \\ Z_{yx} & Z_{yy} \end{pmatrix}_{ji}$ and $\mathbf{D}_{ji} = \begin{pmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{pmatrix}_{ji}$ are matrices of the complex-valued predicted $\mathbf{Z}(\mathbf{r}_j, \omega_i)$ and observed $\mathbf{D}(\mathbf{r}_j, \omega_i)$ impedances, respectively; $\alpha_{ji} = \frac{2}{N_S N_T} \epsilon_{ji}^{-2} \left(tr[\overline{\mathbf{D}}_{ji}^T \mathbf{D}_{ji}] \right)^{-1}$ are the positive weights, where ϵ_{ji} is the relative error of the observed impedance $\mathbf{D}_{ji}(\sigma)$; and λ is a Lagrange multiplier. The sign $tr\,[\cdot]$ introduced above means the trace of its matrix argument, which is defined as $tr\,[\mathbf{B}] = B_{xx} + B_{yy}$, for any $\mathbf{B} = \begin{pmatrix} B_{xx} & B_{xy} \\ B_{yx} & B_{yy} \end{pmatrix}$. As prescribed by the Tikhonov regularization theory [15] the penalty function φ of (1) has a regularized part (a stabilizer) $\varphi_s(\sigma)$. This stabilizer can be chosen in different ways. However, this aspect of the problem is out of the scope of this paper. It is of importance that, as the conductivities $\sigma_k\,(k = 1, \ldots, N)$ must be non-negative and realistic, the optimization problem (1) is subject to the bounds

$$\mathbf{l} \leq \sigma \leq \mathbf{u}, \tag{2}$$

where $\mathbf{l} = (l_1, \ldots, l_N)^T$ and $\mathbf{u} = (u_1, \ldots, u_N)^T$ are respectively the lower and upper bounds and $l_k \geq 0\,(k = 1, \ldots, N)$.

Optimization method. We notice that problem (1)-(2) is a typically optimization problem with simple bounds (see [12]). To solve this problem we apply the limited memory quasi-Newton method with simple bounds. Our implementation of this method is described in a companion paper [3], which demonstrated the application of the method to the 1-D problem. At each iteration step l, we find the search direction $\mathbf{p}^{(l)}$ as $\mathbf{p}^{(l)} = -\mathbf{G}^{(l)}\mathbf{g}^{(l)}$, where $\mathbf{g}^{(l)} = (\frac{\partial\varphi}{\partial\sigma_1}, \ldots, \frac{\partial\varphi}{\partial\sigma_N})^T$ is the gradient vector and $\mathbf{G}^{(l)}$ is an approximation to the inverse Hessian matrix, that is updated at every iteration using the limited memory BFGS formula (see [12], formula (9.5), p. 225). The next iterate $\sigma^{(l+1)}$ is then found as $\sigma^{(l+1)} = \sigma^{(l)} + \alpha^{(l)}\mathbf{p}^{(l)}$, where the step length $\alpha^{(l)}$ is computed by an inexact line search. What is crucial in this approach it is that it requires 1) relatively small storage proportional to $n_{cp} \times N$, where n_{cp} is the number of the correction pairs, and 2) only the calculation of gradients rather than the time-consuming sensitivities and/or the Hessian matrices.

Calculation of gradients. To derive derivatives $\frac{\partial\varphi_d}{\partial\sigma_k}$ we apply an adjoint method. This method uses the EM field reciprocity and has been applied previously to calculate the sensitivities [16, 9] and for forward modelling and inversion [6, 13, 11, 5]. Let us now describe our implementation of such a technique.

It can be proven with some effort that

$$\frac{\partial \varphi_d}{\partial \sigma_k} = Re\left\{\sum_{i=1}^{N_T} \int_{V_k} tr\left[\mathbf{u}_i^T \mathbf{E}_i\right] dV\right\}, \tag{3}$$

where $tr[\mathbf{u}_i^T\mathbf{E}_i] = u_x^{(1)}E_x^{(1)} + u_y^{(1)}E_y^{(1)} + u_z^{(1)}E_z^{(1)} + u_x^{(2)}E_x^{(2)} + u_y^{(2)}E_y^{(2)} + u_z^{(2)}E_z^{(2)}$, the sign *Re* means the real part of its argument and the superscript 1 or 2 denote polarization of the source $\mathbf{J}_i$. By definition, 3×2 matrices $\mathbf{E}_i(\mathbf{r}) = \begin{pmatrix} E_x^{(1)} & E_y^{(1)} & E_z^{(1)} \\ E_x^{(2)} & E_y^{(2)} & E_z^{(2)} \end{pmatrix}_i^T$ and $\mathbf{u}_i(\mathbf{r}) = \begin{pmatrix} u_x^{(1)} & u_y^{(1)} & u_z^{(1)} \\ u_x^{(2)} & u_y^{(2)} & u_z^{(2)} \end{pmatrix}_i^T$ satisfy the following equations

$$\nabla \times \nabla \times \mathbf{E}_i - \sqrt{-1}\omega_i\mu\sigma(\mathbf{r})\mathbf{E}_i = \sqrt{-1}\omega_i\mu\mathbf{J}_i, \tag{4}$$

$$\nabla \times \nabla \times \mathbf{u}_i - \sqrt{-1}\omega_i\mu\sigma(\mathbf{r})\mathbf{u}_i = \sqrt{-1}\omega_i\mu\left(\mathbf{j}_i^{ext} + \nabla \times \mathbf{h}_i^{ext}\right), \tag{5}$$

where $\mathbf{j}_i^{ext} = \sum_{j=1}^{N_S} \alpha_{ji}\mathbf{p}^T\overline{\mathbf{A}}_{ji}(\mathbf{H}_{ji}^{-1})^T\delta(\mathbf{r}-\mathbf{r}_j)$, $\mathbf{h}_i^{ext} = -\frac{1}{\sqrt{-1}\omega_i\mu}\sum_{j=1}^{N_S}\alpha_{ji}\mathbf{p}^T \mathbf{Z}_{ji}^T\overline{\mathbf{A}}_{ji}(\mathbf{H}_{ji}^{-1})^T\delta(\mathbf{r}-\mathbf{r}_j)$, μ is the magnetic permeability, δ is the Dirac's delta-function and $i = 1, \ldots, N_T$. Here $\mathbf{p} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ is the projection matrix, 2×2 matrices $\mathbf{A}_{ji}$, $\mathbf{Z}_{ji}$ are previously explained and 2×2 matrix $\mathbf{H}_{ji} = \begin{pmatrix} H_x^{(1)} & H_y^{(1)} \\ H_x^{(2)} & H_y^{(2)} \end{pmatrix}_{ji}$ is composed of the magnetic fields calculated at the j-th MT site and at the i-th frequency. The formula (3) practically means that computational loads for calculating gradient $(\frac{\partial\varphi}{\partial\sigma_1}, \ldots, \frac{\partial\varphi}{\partial\sigma_N})^T$ are equivalent to those for the solution of $2 \times N_T$ forward problems using Eq. (4) to find $\mathbf{E}_i$ and of $2 \times N_T$ adjoint problems using Eq. (5) to find $\mathbf{u}_i$ for all $i = 1, \ldots, N_T$. Straightforward calculation of the gradient would require solution of $2 \times N_T \times (N+1)$ forward problems.

The approach described is quite general. It is not limited to magnetotellurics only, but can be applied to a variety of EM problems.

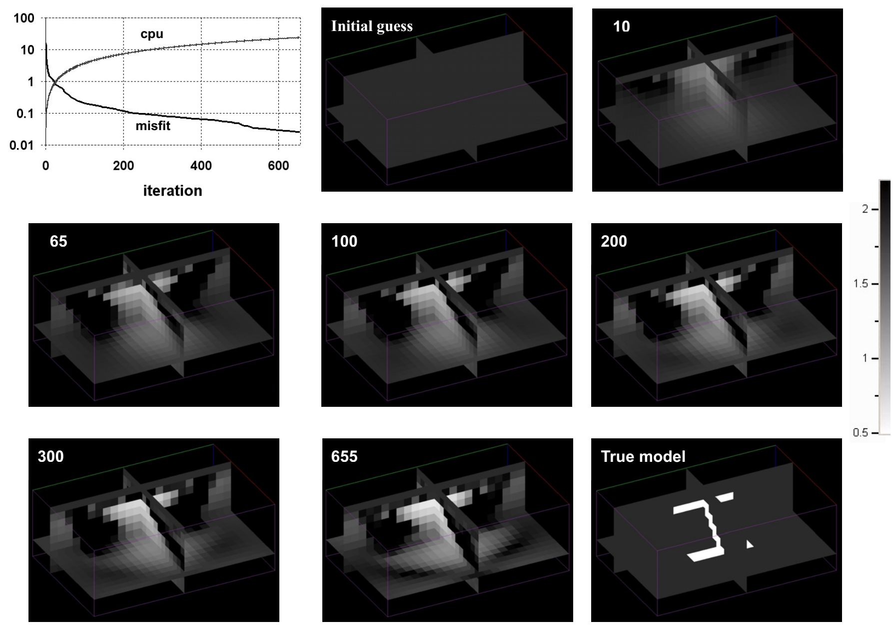

Figure 1. Convergence of the inversion for a 3-D model of a 3 ohm-m dyke in a uniform 100 ohm-m half-space. The left-upper panel presents the misfit and cpu time vs the iteration number. Other panels present images of the initial guess, the true model, as well as the models obtained at various stages of inversion. Number of iterations is given in upper-left corner of each panel.

3. MODEL EXAMPLE

Let us demonstrate on a numerical example how MT inversion allows conductivity to be recovered. In Fig. 1 we present a model including a tilted 3 ohm-m dyke embedded into a 100 ohm-m half-space. The dyke is located at depth 200 to 700 m and it consists of 5 shifted adjacent blocks of $200\times800\times100\,\text{m}^3$ size each. Our modeling domain comprises of $N_x \times N_y \times N_z$=16×24×8 rectangular prisms of $100\times100\times100\,\text{m}^3$ size that cover the dyke and the some part of the surroundings. Notice that the volume lies at depths of 100–900 m.

The inversion domain coincides with the modeling domain. This means that $N = 3072$ conductivities σ_k $(k = 1, \ldots, N)$ of the prisms need to be recovered. The *x3d* forward modeling code described in [1, 2] was exploited as an engine for inversion to solve the forward and adjoint problems given in Eq. (4) and (5). It also was used to calculate

2×2 matrices $\mathbf{D}_{ji}$ of "observed" impedances at $N_T = 4$ frequencies of 1000, 100, 10 and 1 Hz. The impedances were computed at $N_S = 168$ sites r_j $(j = 1, \ldots, N_S)$ coinciding with the nodes of a homogeneous $n_x \times n_y$=12×14 grid, where 100 m is the distance between adjacent nodes.

In addition, the number of the correction pairs n_{cp} was chosen as 6, and the relative error ϵ_{ji} of the impedance was taken as 0.05. A 100 ohm-m uniform half-space was used as an initial guess. In Fig. 1 we also present the convergence of the inversion along with a set of 3-D models recovered at various iterations. It should be mentioned, however, that during inversion we did not use the stabilizer φ_s at all; the Lagrange multiplier λ was assigned a zero value. Instead, we assigned the lower conductivity limits of Eq. (2) as $l_k = 0.005$ $(k = 1, \ldots, N)$. In other words, resistivities $\rho_k = 1/\sigma_k$ of the cells were constrained from above by a value of 200 ohm-m. This turned out to play a similar role to that of regularization.

It should be noted also that without putting constraints on l_k the iteration method without a stabilizer (i.e., when $\lambda = 0$) stagnates, when the misfit φ_d drops to a value of 1.3 and it fails to produce a good conductivity image (not presented here).

4. CONCLUSION

In this paper we have developed a novel approach to 3-D MT inversion. The most essential part of our derivation is that we developed and implemented the adjoint method to derive explicit expressions for the calculation of the gradients of the misfit. Our development is quite general and is not limited to magnetotellurics alone. It can be applied to a variety of EM problems, such as marine controlled-source EM etc. With a synthetic MT example, we have obtained the first promising results of convergence of our solution. The method still needs further development to become a user-end product of universal value to the EM community.

Further work will be concentrated on adapting various types of regularization techniques, and introducing the static shift into the penalty function (1). It is also planned to apply our inversion scheme to an experimental data set. However, previous examples from other 3-D MT inversion software developers (see [8, 10, 14, 17]) indicate that successful verification of the inversion technique even on a single practical dataset is a complex task and may take some time.

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