Theoretical Background for the Magnetotelluric Inversion Program MT3Dinv

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Introduction

ZTEM_MTInv is a program library for carrying out forward modelling and inversion of magnetotelluric (MT), magnetivariational (MV) and joint data. Modelling and inversion of MT data closely parallels that for controlled-source data, and thus programs **ZTEM_MTInv** and **EH3DInv** share many computational routines. There are, however, some significant differences between the theoretical backgrounds of the two inversion procedures. This document describes these differences, and, as such, should be considered a companion to the document "Overview of Inversion Code EH3Dinv".

Forward Modelling

The MT forward modelling algorithm, like that for the controlled-source case, is built upon Maxwell's curl equations (and the constitutive relations), the conservation of charge, and Ohm's law:

$$\nabla \times \mathbf{E} - i\omega\mu_0\mathbf{H} = 0, \tag{1a}$$

$$\nabla \times \mathbf{H} - \mathbf{J} = 0, \tag{1b}$$

$$\nabla \cdot \mathbf{J} = 0, \tag{1c}$$

$$\mathbf{J} - \sigma\mathbf{E} = 0, \tag{1d}$$

where **E** is the total electric field, **H** is the total magnetic field intensity, **J** is the volume current density, **ω** is the angular frequency, and $\boldsymbol{\sigma} = \sigma(\mathbf{r})$ is the electrical conductivity of the Earth model. For program **ZTEM_MTInv**, the magnetic permeability is assumed to be constant and equal to its free space value, μ_0. A time-dependence of $e^{-i\omega t}$ is assumed.

There is effectively no source term in eqs. (1a–d). The source that is inducing electromagnetic fields in the MT case is considered to be outside what will be the computational domain. This is modelled by specifying the tangential components of the H-field and the normal component of the current density on the boundaries of the domain. In other words, and in contrast to the controlled-source case, the forward-modelling problem for the MT case involves homogeneous equations with inhomogeneous boundary conditions.

As for the controlled-source case, the electric field is decomposed into the sum of a vector potential and the gradient of a scalar potential:

$$\mathbf{E} = \mathbf{A} + \nabla\varphi, \tag{2}$$

with uniqueness obtained by imposition of the Coloumb gauge condition:

$$\nabla \cdot \mathbf{A} = 0. \tag{3}$$

Eliminating the **H**-field from Maxwell's two curl equations (eqs. 1a & b), and

introducing eqs. (2) & (3) gives

$$\nabla^2\mathbf{A} + i\omega\mu_0\sigma(\mathbf{A} + \nabla\varphi) = 0, \tag{4}$$

The algorithm used for the MT forward modelling is based on the separation of the total electric and magnetic fields into primary parts that exist in a background conductivity model, and secondary parts that exist because of the difference between the actual conductivity model and the background model. That is,

$$\mathbf{E} = \mathbf{E_p} + \mathbf{E_s}, \tag{5a}$$

$$\mathbf{H} = \mathbf{H_p} + \mathbf{H_s}, \tag{5b}$$

where the primary fields E_p & H_p satisfy eqs. (1a–d) for the background conductivity σ_b and the inhomogeneous boundary conditions. Equivalently, the vector and scalar potentials can be thought of as being divided into primary and secondary parts:

$$\mathbf{A} = \mathbf{A_p} + \mathbf{A_s}, \tag{6a}$$

$$\varphi = \varphi_p + \varphi_s, \tag{6b}$$

where A_p & φ_p satisfy eqs. (1c) & (4) for the background conductivity model and the inhomogeneous boundary conditions. Substituting eqs. (6a–b) into eqs. (1c) & (4) gives

$$\nabla^2\mathbf{A_s} + i\omega\mu_0\sigma\,\mathbf{A_s} + \nabla\varphi_s = -i\omega\mu_0\Delta\sigma\mathbf{E_p}, \tag{7a}$$

$$\nabla\cdot\sigma\mathbf{A_s} + \nabla\cdot\sigma\nabla\varphi_s = -\nabla\cdot\Delta\sigma\mathbf{E_p}\ , \tag{7b}$$

where $\Delta\sigma = \sigma - \sigma_b$. The preceding pair of simultaneous equations are the equations that are solved in the MT forward-modelling algorithm. The secondary potentials are assumed to vanish on the boundaries of the computational domain, that is, satisfy homogeneous boundary conditions. This pair of inhomogeneous equations, and the homogeneous boundary conditions, match the boundary value problem that is solved for the controlled-source case.

The discretization and solution of eqs. (7a–b) is done in exactly the same way as for the controlled-source case. However, one more step is required in the forward-modelling procedure for the MT case. Because, in practice, the source field for the MT case is never known, its

effects are "cancelled" by considering ratios of the E- & H-fields. Specifically, observations in the MT case, and hence the data to be calculated by the forward-modelling procedure, are the impedances $\mathbf{Z_{xx}}$, $\mathbf{Z_{xy}}$, $\mathbf{Z_{yx}}$ & $\mathbf{Z_{yy}}$ (or functions of these impedances), where the impedances are obtained by the solution of:

$$\begin{pmatrix} E_x^{(1)} & E_x^{(2)} \\ E_y^{(1)} & E_y^{(1)} \end{pmatrix} = \begin{pmatrix} Z_{xx} & Z_{xy} \\ Z_{yx} & Z_{yy} \end{pmatrix} \begin{pmatrix} H_x^{(1)} & H_x^{(2)} \\ H_y^{(1)} & H_y^{(1)} \end{pmatrix} \tag{8}$$

The superscripts in the above equation indicate the E & H fields computed in the same conductivity model for two different polarizations of the source field, and the subscripts denote the components of the fields. Two invocations of the forward modelling algorithm are therefore required, once using a primary field calculated for boundary conditions corresponding to an inducing H-field polarized in the x-direction, and again using a primary field calculated with boundary conditions for an inducing H-field polarized in the y-direction. The MT case therefore requires the solution of two systems of equations:

$$A(m)u_s^{(1)} = \hat{q}^{(1)}(m), \tag{9a}$$
$$A(m)u_s^{(2)} = \hat{q}^{(2)}(m), \tag{9b}$$

here the vector $u_s^{(1)}$ contains the values of the components of the secondary vector potential and the values of the secondary scalar potential on the mesh for the first polarization, $\hat{\mathbf{q}}^{(1)}$ represents the discretization of the right-hand side of eqs. (7a–b) for the first polarization, and A represents the discretization of the left-hand side of eqs (7a–b). Equation (9b) is the equivalent equation for the second polarization. Each of these equations is analogous to the matrix equation that is solved for the controlled-source case.

The two kinds of data-types originally accepted by the program **MT3DInv** were the real & imaginary parts of the elements of the impedance tensor (as functions of position and frequency), or the apparent resistivities and phases associated with the elements of the impedance tensor:

$$\rho_{ij} = \frac{1}{\omega\mu_0}\left|Z_{ij}\right|^2 \quad \textbf{and} \tag{10a}$$

$$\phi_{ij} = \tan^{-1}\left(\frac{\Im Z_{ij}}{\Re Z_{ij}}\right) \tag{10b}$$

The main modification to the old version of the package (**MT3DInv**) implemented in the code **ZTEM_MTInv** is the added capability to accept measured components of 3D transfer functions (Tippers), which are related to the electrical properties of the Earth and are defined only through the magnetic field components (measured both on the ground and in the air). In classical theory, the vertical component of the magnetic field, raised in the Earth by natural sources is linearly dependent on the horizontal components of this field (Wiese-Parkinson relation) as following:

$$\mathbf{H_z = [T]H_\tau} \tag{11}$$

Where **[T]=[T_{zx} T_{zy}]**; **H_z** is the vertical component of the raised magnetic field and

$$H_\tau = \begin{bmatrix} H_x \\ H_y \end{bmatrix} \tag{12}$$

The updated import into **ZTEM_MTInv** is designed in a manner to accept any combination of Real (In-Phase) and Imaginary (Quadrature) components of Tipper functions and or any combination of MT impedance data.

Inversion

Exactly as for the controlled-source case, the MT inverse problem is solved by finding the conductivity model that minimizes the sum of a data misfit term and a measure of the amount of structure in the model, where this model is determined using an iterative, Gauss-Newton procedure. The only difference between the MT and controlled-source cases is the explicit composition of the Jacobian matrix of sensitivities. As mentioned above, the data in the MT inverse problem are impedances, or functions of the impedances, and can be represented by:

$$d_i = \mathrm{F}_i\left[Q\left(u_p^{(1)} + u_s^{(1)}\right), Q\left(u_p^{(2)} + u_s^{(2)}\right)\right] \qquad \textbf{(13)}$$

where d_i is the **i**–th datum, Q is the matrix that produces the components of the E & H-fields at the observation locations given the values of the vector and scalar potentials on the mesh, and the function F_i represents the operation of calculating the **i**–th datum, whether it is an impedance or an apparent resistivity or phase, from the E- & H-fields at its observation location. The sensitivity of the **i**–th datum with respect to the **j**–th model parameter is therefore

j

$$J_{ij} \equiv \frac{\partial d_i}{\partial m_j} = \frac{\partial F_i}{\partial F_k^{(1)}} \frac{\partial F_k^{(1)}}{\partial m_j} + \frac{\partial F_i}{\partial F_k^{(2)}} \frac{\partial F_k^{(2)}}{\partial m_j} = S_{ij}^{(1)} \frac{\partial F_k^{(1)}}{\partial m_j} + S_{ij}^{(2)} \frac{\partial F_k^{(2)}}{\partial m_j} \qquad \textbf{(14)}$$

where $F_k^{(1)}$ represents an E or H-field component (for the first polarization) at the observation location and

$$\frac{\partial F_k^{(1)}}{\partial m_j} = \frac{\partial}{\partial m_j}\left[Q_k\left(u_p^{(1)} + u_s^{(1)}\right)\right] = Q_k \frac{\partial u_s^{(1)}}{\partial m_j} \qquad \textbf{(15)}$$

since the primary fields are not dependent on the model parameters in the inversion.

The expressions for the derivatives of the secondary vector and scalar potentials for both polarizations with respect to the **j**–th model parameter are obtained by differentiation both sides of eqs. (9a–b):

$$A(m)\frac{\partial u_s^{(1)}}{\partial m_j}+\frac{\partial}{\partial m_j}\left(A(m)u_s^{(1)}\right)=\frac{\partial \hat{q}^{(1)}}{\partial m_j},\Rightarrow \frac{\partial u_s^{(1)}}{\partial m_j}=A^{-1}(m)\left\{\frac{\partial \hat{q}^{(1)}}{\partial m_j}-\frac{\partial}{\partial m_j}\left(A(m)u_s^{(1)}\right)\right\}. \quad \textbf{(16)}$$

The structure of the right-hand sides of eqs. (9a–b) (see eqs. 7a–b) is very similar to the model-dependent parts of the left-hand sides of these equations. Hence,

$$\frac{\partial \hat{q}^{(1)}}{\partial m_j}=\frac{\partial}{\partial m_j}\left(A(m)u_p^{(1)}\right) \quad \textbf{(17)}$$

and similarly for the second polarization. Introducing the same notation as for the controlled-source case, the derivative of the discretization of the vector and scalar potentials can be expressed as

$$\frac{\partial u_s^{(1)}}{\partial m_j}=A^{-1}(m)\left\{G\left(m,u_p^{(1)}\right)-G\left(m,u_s^{(1)}\right)\right\}, \quad \textbf{(18)}$$

and the product of Jacobian matrix of sensitivities with a vector, as

$$Jv=\left(J^{(1)}+J^{(2)}\right)v=S^{(1)}QA^{-1}\left\{\left(G_p^{(1)}-G_s^{(1)}\right)+S^{(2)}QA^{-1}\left(G_p^{(2)}-G_s^{(2)}\right)\right\}v \quad \textbf{(19)}$$

where the superscripts and subscripts indicate to which polarization each term refers, and whether it involves the primary or secondary potentials.

Equation (19) also indicates the sequence of operations that are required to compute the product of the Jacobian matrix with a vector, which is one of the two computationally-intensive operations required by the iterative solution to the Gauss-Newton normal system of equations. It can be seen that for the MT case, the solution of two prototypical forward-modelling problems, $A\,x = b$, are required for one product of the Jacobian matrix with a vector. Likewise, the solution of two prototypical transpose systems, $A^T v = w$, are required to compute the product of the transpose of the Jacobian matrix with a vector, which is the other computationally-intensive operation that is required.

The size of matrix A is (*na+np*)**nf,* where na is the total number of cell faces in the discretization mesh, *np* is the number of cells and nf is the number of frequencies.

The modifications implemented in ZTEM_MT3DInv_64 include parallelization of the calculation for different frequencies and source polarizations, making the code suitable to be used with MPI (Message Pass Interface) and OpenMP. Hence, the new code is solving one frequency at a time, instead of solving all at once, which requires arrays of length (*na+np*). The frequency calculations are parallelized with MPI, while the 2 polarizations are parallelized using open MP. In a 2 frequency example (eqs. **20-23**)

Old code:

$$Jv = \begin{pmatrix} Q_1 & \\ & Q_2 \end{pmatrix} \begin{pmatrix} A_1^{-1} & \\ & A_2^{-1} \end{pmatrix} \begin{pmatrix} G_1^{(1)} \\ G_2^{(1)} \end{pmatrix} v + \begin{pmatrix} Q_1 & \\ & Q_2 \end{pmatrix} \begin{pmatrix} A_1^{-1} & \\ & A_2^{-1} \end{pmatrix} \begin{pmatrix} G_1^{(2)} \\ G_2^{(2)} \end{pmatrix} v \qquad \textbf{(20)}$$

Here $G_1^{(1)}$ corresponds to $\left(G_p^{(1)} - G_s^{(1)}\right)$ from eqt. **(19)** and index 1 in the subscript corresponds to the frequency

In new code:

$$Jv = \begin{pmatrix} J_1 v \\ J_2 v \end{pmatrix} = \begin{matrix} Q_1 A_1^{-1} G_1^{(1)} v + Q_1 A_1^{-1} G_1^{(2)} v \\ Q_2 A_1^{-1} G_2^{(1)} v + Q_2 A_1^{-1} G_2^{(2)} v \end{matrix} \qquad \textbf{(21)}$$

For the transposed matrixes:

Old code:

$$J^T v = \left(G_1^{T(1)} G_2^{T(1)}\right)\begin{pmatrix} A_1^{-T} & \\ & A_2^{-T} \end{pmatrix}\begin{pmatrix} Q_1^T & \\ & Q_2^T \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} + \left(G_1^{T(2)} G_2^{(2)}\right)\begin{pmatrix} A_1^{-T} & \\ & A_2^{-T} \end{pmatrix}\begin{pmatrix} Q_1^T & \\ & Q_2^T \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \quad \textbf{(22)}$$

Where $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$.

In the new code:

$$J^T v = \left(G_1^{T(1)} A_1^{-T} Q_1^T v_1 + G_1^{T(2)} A_1^{-T} Q_1^T v_1\right) + \left(G_2^{T(1)} A_2^{-T} Q_2^T v_2 + G_2^{T(2)} A_2^{-T} Q_2^T v_2\right) \quad \textbf{(23)}$$