Appendices
Appendix A

Additional derivations

A.1 Theorems of vector calculus

Here, the basic vector calculus definitions are given which are fundamental for some of the expressions and derivations in Chapter 1.

The gradient of a scalar field $\xi$ is defined by:

$$\nabla \xi = \left( \frac{\partial \xi}{\partial x}, \frac{\partial \xi}{\partial y}, \frac{\partial \xi}{\partial z} \right), \quad (A.1)$$

where $\nabla$ is the Nabla operator. The divergence of a vector field $\mathbf{F}$ describes the flux of $\mathbf{F}$.

$$\nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}. \quad (A.2)$$

The curl of $\mathbf{F}$ describes the rotation of $\mathbf{F}$:

$$\nabla \times \mathbf{F} = \left( \frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}, \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}, \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right). \quad (A.3)$$

The three basic operations above can be intertwined to yield the vector identities below:

$$\nabla \cdot (\xi \mathbf{F}) = \xi \nabla \cdot \mathbf{F} + \mathbf{F} \cdot \nabla \xi, \quad (A.4)$$

$$\nabla \times (\nabla \times \mathbf{F}) = -\nabla^2 \mathbf{F} + \nabla (\nabla \cdot \mathbf{F}), \quad (A.5)$$

$$\nabla \times \nabla \xi \equiv 0. \quad (A.6)$$

$\nabla^2$ is also known as the Laplace operator.
A.2 Magnetic field at the surface of Earth

Without loss of generality, we look at the \( y \)-component of the magnetic field at the surface of a homogeneous half-space. \( B_y^0 \) and \( B_y^1 \) denote the primary and secondary magnetic field at the surface, respectively. The energy of secondary magnetic field in the Earth decays with depth (see Equation (1.12a)):

\[
B_y^1 = a_1 e^{-k_1 z}.
\]  
(A.7)

In air, the energy is propagating up- and downwards:

\[
B_y^0 = a_0 e^{-k_0 z} + b_0 e^{k_0 z}.
\]  
(A.8)

Since the horizontal components of the magnetic field are continuous at the surface \( z = 0 \), the following relationship holds:

\[
a_0 + b_0 = a_1.
\]  
(A.9)

The reflexion coefficient at the surface of the half-space is defined as:

\[
\frac{Z_0 - Z_1}{Z_0 + Z_1} = \frac{b_0}{a_0}.
\]  
(A.10)

\( Z_0 \) is much larger than \( Z_1 \) as the resistivity of air goes towards infinity. Therefore, \( b_0/a_0 \approx 1 \). Therefore, \( 2a_0 = a_1 \), which means that over a homogeneous half-space and layered Earth the magnetic field \( B \) measured at the surface is twice the primary magnetic field \( B_0 \) as long as the plane-wave assumption holds.

\[
B_1 = 2B_0.
\]  
(A.11)

A.3 Invariants of the phase tensor

The phase tensor \( \Phi \) is a \( 2 \times 2 \) matrix with 4 real elements:

\[
\Phi = \begin{bmatrix} \Phi_{xx} & \Phi_{xy} \\ \Phi_{yx} & \Phi_{yy} \end{bmatrix}.
\]  
(A.12)

Each \( 2 \times 2 \) matrix has 3 simple coordinate invariants, the trace:

\[
\text{tr}(\Phi) = \Phi_{xx} + \Phi_{yy},
\]  
(A.13)

the skew,

\[
\text{sk}(\Phi) = \Phi_{xy} - \Phi_{yx},
\]  
(A.14)
and the determinant,

$$\det(\Phi) = \Phi_{xx}\Phi_{yy} - \Phi_{xy}\Phi_{yx}. \quad (A.15)$$

Written as first-order invariants:

$$\Phi_1 = \frac{\text{tr}(\Phi)}{2}, \quad (A.16a)$$
$$\Phi_2 = [\det(\Phi)]^{1/2}, \quad (A.16b)$$
$$\Phi_3 = \frac{\text{sk}(\Phi)}{2}. \quad (A.16c)$$

These invariants can conveniently be rearranged to yield the maximum, the minimum and a skew angle of the phase tensor. The new coordinate invariants are useful in depicting important phase properties, e.g. information about the polarisation of the electric field if a linear polarised magnetic field is present.

The minimum phase $\Phi_{\text{min}}$ is defined by:

$$\Phi_{\text{min}} = (\Phi_1^2 + \Phi_3^2)^{1/2} - (\Phi_1^2 + \Phi_3^2 - \Phi_2^2)^{1/2}. \quad (A.17)$$

The maximum phase $\Phi_{\text{max}}$ is:

$$\Phi_{\text{max}} = (\Phi_1^2 + \Phi_3^2)^{1/2} + (\Phi_1^2 + \Phi_3^2 - \Phi_2^2)^{1/2}. \quad (A.18)$$

Finally, the last coordinate invariant is the skew angle $\beta$:

$$\beta = \frac{1}{2} \tan^{-1} \left( \frac{\Phi_3}{\Phi_1} \right). \quad (A.19)$$

The three coordinate invariants $\Phi_{\text{max}}, \Phi_{\text{min}}$ and $\beta$ clearly define the tensor ellipse itself, but have no reference to a coordinate system. The auxiliary angle $\alpha$ defines the tensor’s position in a coordinate frame.

$$\alpha = \frac{1}{2} \tan^{-1} \left( \frac{\Phi_{xy} - \Phi_{yx}}{\Phi_{xx} + \Phi_{yy}} \right). \quad (A.20)$$

Using Equation (2.14), the following statements show the invariance of the principal values and the skew angle under rotation through an arbitrary angle $\zeta$:

$$R(\zeta) \Phi R^T(\zeta) = R(\zeta) R^T(\alpha - \beta) \begin{bmatrix} \Phi_{\text{max}} & 0 \\ 0 & \Phi_{\text{min}} \end{bmatrix} R(\alpha + \beta) R^T(\zeta)$$
$$= R^T(\alpha - \zeta - \beta) \begin{bmatrix} \Phi_{\text{max}} & 0 \\ 0 & \Phi_{\text{min}} \end{bmatrix} R(\alpha - \zeta + \beta)$$
$$= R^T(\alpha' - \beta) \begin{bmatrix} \Phi_{\text{max}} & 0 \\ 0 & \Phi_{\text{min}} \end{bmatrix} R(\alpha' + \beta), \quad (A.21)$$

and $\alpha' = \alpha - \zeta$. 
Figure B.1: Pseudosections of the TE- (left) and TM-mode (right) apparent resistivities and phases of the NLCG inversion and observed data for the Fowler survey.
Figure B.2: Pseudosection of the real and imaginary part of the geomagnetic transfer functions for the Fowler Survey.
Figure B.3: Observed and modelled responses of the diagonal impedance components $Z_{xx}$ (observed – triangles, modelled – solid line) and $Z_{yy}$ (observed – squares, modelled – dashed line) for the Fowler survey data.
Figure B.4: Apparent resistivity $\rho_a$ in [Ω m] and phase $\phi$ in [°] plots of observed data of the 2-D array. Shaded triangles and squares denote $\rho_a$ and $\phi$ of the $Z_{xx}$ and $Z_{yy}$ components of the impedance tensor, respectively. The responses shown here were manually static shift corrected (see Chapter 6.4.1). Solid and dashed lines denote the $Z_{xx}$ and $Z_{yy}$ 3-D model responses, respectively.
Table B.1: Static shift factors used in the 3-D inversion from residual analysis. Impedance tensor elements were multiplied with the static shift factors displayed here to achieve the model in Figure 6.11.

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Figure B.5: Apparent resistivity $\rho_a$ in $[\Omega \text{m}]$ and phase $\phi$ in [°] plots of remaining observed data of the 2-D array. Shaded triangles and squares denote $\rho_a$ and $\phi$ of the $Z_{xx}$ and $Z_{yy}$ components of the impedance tensor, respectively. The responses shown here were manually static shift corrected (see Chapter 6.4.1). Solid and dashed lines denote the $Z_{xx}$ and $Z_{yy}$ 3-D model responses, respectively.
Figure B.6: Cross-sections for every second of the 3-D resistivity model of the Gawler Craton in the \( x-z \) plane (compare Figure 6.11). Color scale is in \( \log_{10} \Omega \text{m} \) and open triangles mark station locations. Features A to E are nominated for comparison with Figure 6.11 and B.7. Dashed lines indicate possible former fluid pathways between the deeper conductive structures and surface conductors related to mineral systems.
Figure B.7: Cross-sections for every second of the 3-D resistivity model of the Gawler Craton in the $x$-$z$ plane (compare Figure 6.11). Color scale is in $\log_{10} \, \Omega \cdot m$ and open triangles mark station locations. Features A to E are nominated for comparison with Figure 6.11 and B.6. Dashed lines indicate possible former fluid pathways between the deeper conductive structures and surface conductors related to mineral systems.
A number of codes have been developed for this thesis which primarily aim towards the analysis of the impedance tensor and the magnetic transfer functions and the handling of the 3-D inversion code of (Siripunvaraporn et al., 2005a). All codes were developed in MATLAB, except for the expansion of the original 3-D inversion (in Fortran). In all cases, the MATLAB scripts incorporate a Graphical User Interface (GUI), which avoids the necessity to go into the code and change parameters there. Any parameters that are required will be requested by the GUI using pop-up windows. Therefore, the codes are user-friendly and can easily be used by other people. A large number of GMT scripts were written to illustrate various data sets (e.g. Figure 6.1) or $x - y$ plots (e.g. Figure 5.3). In some cases, the GMT generated figures were edited with Adobe Illustrator (e.g. Figure 4.1) to illustrate additional information, such as the geology of the area. However, here I only restrict myself to a brief explanation of the MATLAB scripts:

**MTAnalysis** The code reads in *.edi-files and converts the transfer function information into phase tensor properties (Caldwell et al., 2004), invariants according to (Weaver et al., 2000, 2003) and induction arrows. A pop-up window gives the user an option of plotting various phase tensor properties and induction arrows. The plots showing phase tensor properties mimic the figures of Caldwell et al. (2004) and are designed to provide a quick overview of the dimensionality of the data set and the strike direction of each individual station. The user can choose between plotting phase tensors across the period range for all stations, the maximum $\Phi_{\text{max}}$ and minimum $\Phi_{\text{min}}$ phases, the skew angle $\beta$, the ellipticity $\epsilon$, the azimuth of the maximum phase $\alpha = \beta$ compared with the orientation of the induction arrows. Furthermore, a background bitmap image can be loaded on top of which phase tensor ellipses and induction arrows can be plotted. It is also possible to display strike angles according to Weaver et al. (2003) following the invariant approach of Weaver et al. (2000). All figures can be saved automatically as bitmap (e.g. jpegs or tiffs) or vector graphic files (eps format).
**mt2gmt** This program has the same input function as **MTAnalysis** but does not provide a GUI for displaying computed properties. Instead, a **gmtexport** subfunction is called which produces a number of files in GMT format (Wessel and Smith, 1998). Figures that were produced using **mt2gmt** and a GMT script are for example Figure 5.3, 5.5, 5.4 and 5.6.

**edi2wsinv** This code reads in edi-files and converts them into startup file in the format required by **wsinv3dmt** (Siripunvaraporn et al., 2005a). Again, following a GUI approach, the user has the choice between implementing the whole impedance tensor or only the off-diagonal elements. Furthermore, the error floor can be reset to a new level (error floors for the diagonal components can differ) and the number of periods also has to be set.

**mtinv2gmt** Plots of observed and modelled apparent resistivity and phases are created out of output files of the **wsinv3dmt** code of Siripunvaraporn et al. (2005a). A station name file is required and the GUI asks for the observation data file of impedance tensor components (e.g. blk.data), the observation error file of impedance tensor components (e.g. blk.error) and the model response file generated by **wsinv3dmt** (e.g. blkinv.02). An example in the thesis is Figure 6.3.

**inv3d2mod** This code reads in the model and response files of the **wsinv3dmt** code and provides a GUI to display the model in all three geographic orientations. Sliders control which layer is displayed and text boxes allow cropping of the layer to the size of the array (note the model size is usually much larger than the size of the array to avoid boundary artifacts). For the cross-sections a vertical exaggeration factor can be set (default is 1). The resistivity colourbar is in logarithmic scale and the boundaries can be varied arbitrarily. Other options are the display of station locations and the display of cell boundaries. Figure 6.7 and 6.11 show figures generated by **mtinv2gmt**.

**mtinv2resid** For the static shift analysis (see Figure 6.8) the code **mtinv2resid** generates residual plots of apparent resistivity and phase for all stations. Input files are the same as for **mtinv2gmt**. This program provides a visual tool to quickly determine stations suffering from static shift. Figure 6.10 displays a comparison of model responses with and without static shift correction.

**inv3dCompare** This code generates GMT-compliant files to display phase tensor ellipses maps of the 3-D inverse code **wsinv3dmt**. The program reads in observed responses and the modelled responses and converts them into phase tensor ellipses. A comparison of the figures enables an evaluation of the model fit to the data (see Figure 6.12).

**instread** This program was developed for converting new generation long-period instrument data into time series in the format of Chave and Thomson (1989).
**wsinv3d.f & iodata.f** These Fortran routines are part of the *wsinv3dmt* code developed by Siripunvaraporn et al. (2005a) and have been extended to read in a static shift correction file. The implementation is carried out by adding another line to the startup file to read in the statics file. The static shift factors are then multiplied with the impedance tensor components to achieve static shift corrected MT responses.
Appendix D

Station locations

Table D.1: Latitude, longitude and elevation of MT stations of the Great Victorian Desert survey conducted in 2006.

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<td>E58°11'07.7&quot;</td>
<td>654</td>
</tr>
<tr>
<td>OM19</td>
<td>N22°59'07.2&quot;</td>
<td>E58°05'35.4&quot;</td>
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</tr>
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<td>E58°01'47.6&quot;</td>
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<td>E57°58'32.8&quot;</td>
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<tr>
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<td>N22°48'16.3&quot;</td>
<td>E57°53'14.5&quot;</td>
<td>504</td>
</tr>
<tr>
<td>OM23</td>
<td>N22°47'05.4&quot;</td>
<td>E57°47'28.6&quot;</td>
<td>456</td>
</tr>
</tbody>
</table>
Table D.3: Latitude, longitude and elevation of MT stations of the Fowler MT survey conducted in 2006.

<table>
<thead>
<tr>
<th>Station names</th>
<th>Latitude</th>
<th>Longitude</th>
<th>Elevation (m)</th>
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<tbody>
<tr>
<td>FOW01</td>
<td>S32°17′04.4″</td>
<td>E135°01′33.4″</td>
<td>98</td>
</tr>
<tr>
<td>FOW02</td>
<td>S32°23′33.3″</td>
<td>E134°49′14.8″</td>
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<tr>
<td>FOW03</td>
<td>S32°19′01.2″</td>
<td>E134°37′01.4″</td>
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<td>FOW04</td>
<td>S32°16′21.4″</td>
<td>E134°24′43.5″</td>
<td>83</td>
</tr>
<tr>
<td>FOW05</td>
<td>S32°13′38.0″</td>
<td>E134°12′34.2″</td>
<td>59</td>
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<tr>
<td>FOW06</td>
<td>S32°08′04.5″</td>
<td>E134°00′54.4″</td>
<td>56</td>
</tr>
<tr>
<td>FOW07</td>
<td>S32°00′47.5″</td>
<td>E133°51′27.6″</td>
<td>63</td>
</tr>
<tr>
<td>FOW08</td>
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<td>E133°27′25.5″</td>
<td>99</td>
</tr>
<tr>
<td>FOW10</td>
<td>S31°54′12.0″</td>
<td>E133°16′27.5″</td>
<td>72</td>
</tr>
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<td>S31°53′52.7″</td>
<td>E133°03′44.9″</td>
<td>46</td>
</tr>
<tr>
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<td>E132°54′37.1″</td>
<td>13</td>
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<td>E132°27′23.7″</td>
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<td>E132°09′37.6″</td>
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<td>S31°37′08.3″</td>
<td>E132°03′07.4″</td>
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<td>S31°37′03.9″</td>
<td>E131°55′58.0″</td>
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<tr>
<td>FOW19</td>
<td>S31°29′13.7″</td>
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<td>119</td>
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<tr>
<td>FOW20</td>
<td>S31°25′31.7″</td>
<td>E131°38′42.9″</td>
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<td>FOW21</td>
<td>S31°22′56.3″</td>
<td>E131°29′48.7″</td>
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<td>S31°21′37.5″</td>
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<td>FOW23</td>
<td>S31°22′14.2″</td>
<td>E131°10′39.1″</td>
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</tr>
<tr>
<td>FOW24</td>
<td>S31°25′41.6″</td>
<td>E130°58′44.9″</td>
<td>54</td>
</tr>
<tr>
<td>FOW25</td>
<td>S31°25′41.6″</td>
<td>E130°58′44.9″</td>
<td>54</td>
</tr>
</tbody>
</table>
Appendix E

Review of three-dimensional magnetotelluric inversion

This Appendix is a literature review conducted in 2004 as a partial fulfilment of the coursework requirements for the degree of Doctor in Philosophy in Geophysics at Adelaide University. It is an expansion of Chapter 3 and provides more insights into modelling approaches, specifically aimed at 3-D inversion routines.

E.1 Introduction

The magnetotelluric method (Cagniard, 1953) is becoming more fashionable in order to determine geological subsurface structures. Many of these are conducted along a two-dimensional line crossing major geological features (Thiel et al., 2005). However, the experiments often assume two-dimensional structures which is crucial for the justification of a 2-D survey. In case of highly complex 3-D structures, 3-D surveys have to be taken into consideration. These also require more effort in analysing the data and creating a realistic model of the subsurface structure. Large equation systems of ill-posed problems have to be solved and require sophisticated, fast, and accurate numerical methods. Analytical solutions cannot be used, if the subsurface contains several multi-dimensional bodies. This review shows the major approaches utilised in order to obtain a resistivity model from magnetotelluric data, a process referred to as inversion. There are several ways how to address the distribution of EM fields and other parameters in the Earth (Table E.1). The differences lie in their formulation (integral or derivative form of Maxwells’ equations) and in their representation onto a discretised model volume. This leads to a number of different approaches, which are briefly introduced here.

Several studies have examined when a 2-D survey is feasible in terms of correctness if a 3-D structure is present (Ledo et al., 2002; Wannamaker et al., 1984). The earliest inversion
techniques incorporate the integral equation method (Weidelt, 1975). It yields good results if only a few bodies are present. Wannamaker (1991); Xiong (1992) have improved this technique and it is often used for verifying accuracy in other methods or are even incorporated into their derivation (Mackie and Madden, 1993a).

Smith and Booker (1991) developed an efficient and fast iterative inversion method, that has been tested only for two-dimensional data, but has the potential tp also be used with 3-D data. The so-called rapid relaxation inversion (RRI) approximates horizontal derivative terms with their values calculated from the fields of the previous iteration. This approach results in uncoupling of the equations for each horizontal position, allowing for separate inversions beneath measurement sites. The resultant models are interpolated to form a new multidimensional model. However, RRI has problems in showing structures with little TM responses accurately and widely ignores lateral effects in computation of data sensitivities, producing possible artifacts in the conductivity profile. Other techniques are required to overcome these problems.

Finite-difference (FD) methods have proven to be a strong candidate for correctly modelling the underground structure (Mackie et al., 1993; Mackie and Madden, 1993a; Smith, 1996a; Newman and Alumbaugh, 2000). Thin-sheet modelling, similar to FD, comprises a number of simplifications to the model and speeds up the computation time (Wang and Lilley, 1999). Only recently, the finite-element (FE) method has become popular in magnetotellurics and pro-

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**Table E.1: Mathematical symbols used throughout the review.**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c \in \mathbb{R}$</td>
<td>scalar constant</td>
</tr>
<tr>
<td>$\mathcal{V}$</td>
<td>arbitrary domain</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>regularisation parameter</td>
</tr>
<tr>
<td>$S$</td>
<td>sensitivity matrix $(S_{ij} = \frac{\partial d_i}{\partial m_j})$</td>
</tr>
<tr>
<td>$d$</td>
<td>observed data vector</td>
</tr>
<tr>
<td>$m$</td>
<td>model vector</td>
</tr>
<tr>
<td>$J = (J_x, J_y, J_z)$</td>
<td>current density vector</td>
</tr>
<tr>
<td>$C_d$</td>
<td>data covariance matrix</td>
</tr>
<tr>
<td>$C_m$</td>
<td>model covariance matrix</td>
</tr>
<tr>
<td>$G$</td>
<td>dyadic Green’s function</td>
</tr>
<tr>
<td>$F$</td>
<td>Fréchet derivative matrix</td>
</tr>
<tr>
<td>$E = (E_x, E_y, E_z)$</td>
<td>electric field vector</td>
</tr>
<tr>
<td>$H = (H_x, H_y, H_z)$</td>
<td>magnetic field vector</td>
</tr>
<tr>
<td>$T = (T_{zx}, T_{zy})$</td>
<td>transfer function vector</td>
</tr>
<tr>
<td>$Z = \begin{pmatrix} Z_{xx} &amp; Z_{xy} \ Z_{yx} &amp; Z_{yy} \end{pmatrix} \in \mathbb{C}$</td>
<td>impedance matrix</td>
</tr>
<tr>
<td>$R$</td>
<td>regularisation matrix</td>
</tr>
<tr>
<td>$M$</td>
<td>preconditioning matrix</td>
</tr>
<tr>
<td>$T$</td>
<td>electric vector potential</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>magnetic scalar potential</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>objective functional in the inverse problem</td>
</tr>
</tbody>
</table>
vides a time-expensive but promising formulation of Maxwell’s equations onto a finite-element mesh (Mogi, 1996; Mitsuhata and Uchida, 2004).

Zhdanov et al. (1996) and Zhdanov and Traynin (1997) introduce a completely different method called EM migration. The EM field of natural sources in the ionosphere and its excited secondary field can be measured at the Earth’s surface. Following the concept of seismic migration (Yilmaz, 2001), the receivers can be replaced by artificial current or charge sources, which produce a propagating EM field in reverse time (migrated EM field). This can be achieved using an ordinary diffusion equation and it eventually gives information about positions of resistivity interfaces at which the primary EM field has been backscattered. Another yet very young approach is the quasi-analytical approximation, which will not be further discussed here (Zhdanov and Golubev, 2003).

In this review, the FD, Thin-sheet, and FE method are introduced in more detail. Each section will describe the basic ideas about discretisation of the underground model for each method. Furthermore, the iterative process of obtaining the final model will be described including ideas about the forward solver, the inversion procedure, boundary conditions of the model and preconditioners to enhance computation speed. In Section E.3 the regularised inversion is described in more detail and is derived so that a model with both minimum misfit and maximum smoothness can be found. In particular the FD method will be discussed thoroughly, since it has been focus of quite a number of studies.

E.2 Finite-difference methods

The basic idea behind finite-difference methods is that a model space $\mathcal{V}$ is discretised in line segments for $\mathcal{V} \in \mathbb{R}^1$, in surface areas for $\mathcal{V} \in \mathbb{R}^2$ and rectangular blocks for $\Omega \in \mathbb{R}^3$. Since the review discusses magnetotellurics in three dimensions, the latter case with $\mathcal{V} \in \mathbb{R}^3$ is considered here. The authors usually approach this discretisation with a staggered grid on which the partial differential equations are based on either a Taylor series expansion around a point $m_0$ with a small error $\xi$

$$f(m_0 + \xi) = \sum_{\nu=0}^{\infty} \frac{f^{(\nu)}(m_0)}{\nu!} \xi^\nu = f(m_0) + f'(m_0)\xi + \mathcal{O}(\xi^2) \quad (E.1)$$

or integral equations (Mackie and Madden, 1993a). A starting model is updated in an iterative fashion to find a solution that minimises the observed data and model data response. In Section E.2 two different forward operators are introduced, the methods seeking a direct (matrix inversion) solution (Mackie et al., 1993; Mackie and Madden, 1993a) and iterative solutions (Mackie and Madden, 1993b; Smith, 1996a; Newman and Alumbaugh, 2000). Boundary conditions are crucial to every model and have significant influence on the final conductivity
distribution. Several preconditioners (operators that improve the condition number of a matrix) are shown to improve the computation time.

### E.2.1 Direct methods

In their ground-breaking paper, Mackie et al. (1993) approach a non-linear inversion problem with a maximum likelihood procedure (Mackie et al., 1988), which is similar to the Gauss-Newton equation. It represents a linearised inversion scheme, that minimises a weighted sum of the variance of the difference between model response $g(m)$ and observed data $d$, and the difference between the model parameters $m$ and an *a priori* model $m_0$ at the $k$-th iteration step:

$$\left(S_h^k C_d^{-1} S_k + C_m^{-1}\right)^{-1} \Delta m_k = S_h^k C_d^{-1} \left(d - g(m_k)\right) + C_m^{-1} \left(m_0 - m_k\right).$$

(E.2)

The data and model parameters are in logarithmic parametrisation for the following reasons:

1. bias removal associated with resistivity or conductivity parameters
2. guarantee of positiveness of model parameters
3. display of complex-valued data in the form $\ln Z = \ln |Z| + i\theta$
4. allowance of larger changes in the model parameters (e.g. conductivity) \(\Leftrightarrow\) reduction in number of iterations

Furthermore the data covariance matrix $C_d$ displays the uncertainties in the data and can be computed or measured directly. The use of the model covariance matrix $C_m$ is more diverse and is applied for weighting, filtering or applying constraints. The latter use includes smoothing between neighbouring points, parameter correlation and freedom of parameter change.

Non-linear inversion requires a sensitivity analysis, describing the Frechet derivatives which give the perturbations in the data (electric and magnetic field $\delta E$ and $\delta H$, respectively) due to perturbations in the model parameters (log conductivity $\delta\sigma$). Mackie et al. (1993) uses an integral expression to link the perturbations through a dyadic Green’s function $G$:

$$\begin{pmatrix} \delta E(r) \\ \delta H(r) \end{pmatrix} = \int \int \int G(r, s) \cdot E(s) \delta\sigma(s) \, d^3s.$$

(E.3)

The reciprocity relation shows that the effect due to a source in the interior is equivalent to having a source on the surface and solving for the effect in the interior (Weidelt, 1975).

$$G_j(s, r)_k = G_k(r, s)_j,$$

(E.4)
where \( r \) is the observation point vector, \( s \) is the source point vector and the subscripts \( j \) and \( k \) denote the observed field components \((j = 1, 2, \ldots, 6)\) refer to \( E_x, E_y, \ldots, H_z \) and the source components \((k = 1, 2, 3)\) correspond to current sources \( J_x, J_y, J_z \) (Lanczos, 1961).

This approach decreases the computation time significantly. Furthermore, Mackie et al. (1993) show that the actual sensitivity matrix need not to be explicitly known, but only its effect on an arbitrary vector \( x \). Moreover, the sensitivity matrix multiplied with \( x \) is just the sum over all model parameters of the sensitivity term multiplied by the vector component \( x_i \) for that model block:

\[
p = Sx \sim \sum_{\text{model parameters}} \frac{\partial(E, H)}{\partial \sigma_i} x_i.
\]  

Maxwell’s equations represent a linear transformation system \( T \), which underlies the superposition principle:

\[
T[a + b] = T[a] + T[b] \quad \text{and} \quad T[ca] = cT[a].
\]  

\( a \) and \( b \) are input parameters and \( c \) denotes a scalar constant.

Using Equations (E.4), (E.5) and (E.6), it can be shown that there is only one forward run necessary including all sources distributed at the surface simultaneously. Mackie et al. (1993) interpret this forward operator as a downward propagation of surface fields in backwards time.

The reciprocity principle \((G_{ij}(s, r)_k = G_{kj}(r, s)_j)\) involves a computation of \( S^H x = S^T x \) (the Hermitian sensitivity matrix multiplied with an arbitrary vector \( x \) is equal to the complex conjugate transpose of \( S \) multiplied with \( x \)). However, this involves a complex conjugate of the Green’s function \( -\sigma \nabla \times (\nabla \times \frac{1}{\mu \omega}) \), yielding negative frequencies and therefore backwards time.

Algorithm 1 and 2 show the entire numerical approach. The forward operator is the direct solution described in Mackie and Madden (1993a) and a modified boundary condition approach has been chosen. The model is simply repeated in the horizontal directions, hence no side boundary terms are assigned. Tests on synthetic models show the usefulness of a priori information in the inversion routine. Mackie et al. (1993) apply \( C_m \) constraints to keep the bottom layers one-dimensional. The results illustrate a removal of smearing effects of shallow conductive bodies (Mackie et al., 1993, Fig.12). Results with only one relaxation step per iteration are reasonably good compared to three and ten relaxation steps per inversion step. However, that algorithm has not been tested on real data.

Mackie and Madden (1993a) show a slightly different approach as they start from the integral forms of Maxwell’s equation rather than the differential forms. They have developed an impedance propagator algorithm using finite-differences on a staggered-grid. The main issue is that of computing averages rather than approximating derivatives of the fields or Earth properties. This also provides a simple geometrical understanding of the coupling between Faraday’s
Algorithm 1: 3-D inversion algorithm of Mackie et al. (1993) in mathematical form.

Outer loop describes the inverse operator and inner loop shows the forward operator (linear conjugated gradient relaxation solution (Hestenes and Stiefel, 1952)).

input: Observed data
output: Resistivity model

1 for $k = 1$ to $k_{\text{max}}$ of iterations do

2 \hspace{1cm} $g(m_k)$
3 \hspace{1cm} $d - g(m_k)$
4 \hspace{1cm} $m_0 - m_k$
5 \hspace{1cm} $b = S^h C_d^{-1} (d - g(m_k)) + C_m^{-1} (m_0 - m_k)$
6 \hspace{1cm} $\Delta \sigma_0 = 0$, $r_0 = b$

7 for $i = 1$ to $i_{\text{max}}$ of relaxation iterations do

8 \hspace{1.5cm} $\beta_i = \frac{r_i^T r_i - 1}{r_{i-2}^T r_{i-2}}$
9 \hspace{1.5cm} $p_i = r_{i-1} + \beta_i p_{i-1}$
10 \hspace{1.5cm} $Bp_i = (S^h C_d^{-1} S_k + C_m^{-1}) p_i$
11 \hspace{1.5cm} $\alpha_i = \frac{r_i^T r_i - 1}{p_i^T Bp_i}$
12 \hspace{1.5cm} $\Delta \sigma_i = \Delta \sigma_{i-1} + \alpha_i p_i$
13 \hspace{1.5cm} $r_i = r_{i-1} - \alpha_i Bp_i$

14 end

15 \hspace{1cm} $\sigma_{k+1} = \sigma_k + \Delta \sigma$

end

Law and Ampere’s Law (Equation E.7a and E.7b, respectively).

$$\oint H \cdot dl = \iint J \cdot dS = \iint \sigma E \cdot dS, \quad (E.7a)$$
$$\oint E \cdot dl = \iint i \mu \omega H \cdot dS. \quad (E.7b)$$

In equation (E.7) displacement currents are neglected due to low frequencies involved in magnetotelluric exploration. The Earth is divided in gridded rectangular prisms which are transformed to an equal grid (yielding a symmetric difference equations operator), where \(H\) is defined along the edges of each cell and \(J\) and \(E\) are defined along the normals to the block faces (Figure E.1). Since \(J\) is continuous across block interfaces and since \(J = \sigma E\), \(E\) is discontinuous if conductivity changes across the cell interface. Equation (E.7a) exactly describes the utilised difference equation geometry.

The boundary conditions have been modified from the periodic model in the horizontal directions (Mackie et al., 1993) to accommodate for local magnetotelluric fields being biased by regional features, such as the ocean-continent boundary (Parkinson and Jones, 1979). Side boundary values are calculated from 2-D TM mode calculations where each vertical plane of the 3-D model is treated as the inner part of a larger-scale 2-D model. Several graded air layers
Algorithm 2: 3-D inversion algorithm of Mackie et al. (1993) in descriptive form.

input: Observed data
output: Resistivity model

1 for Non-linear inversion do
2 respond of current model
3 data residuals
4 model residuals
5 one forward problem with surface sources per frequency
6 initialize conjugate gradient algorithm
7 for relaxation solution do
8 ($\beta_0 = 0$)
9 ($p_1 = r_0$) update search direction
10 two forward problems per frequency
11 step length along search direction
12 update model perturbations
13 update residuals
14 end
15 update model parameters
16 end

Figure E.1: The difference equation geometry based on the integral forms of Maxwell’s equations (E.7a).

are added on top of the Earth model to account for perturbations in the $H$ fields from lateral current gradients. The $E$ and $H$ fields are related with a 1-D impedance matrix at the bottom of the Earth model.

Mackie and Madden (1993a) use a direct solution for solving the system of equations, similar to the Riccati equation approach (Eckhardt, 1963). The Earth impedance matrix $Z_{Earth}$ is propagated from the bottom of the model to the surface. Same procedure applies for the air impedance matrix $Z_{air}$ propagated from the top down to the surface. A uniform current sheet $J_{es}$ at the Earth’s surface acts as a source field with the $H$ field boundary terms $z_e$ being zero.
Therefore any $H$ field in the air is due to conductivity structures underneath the surface. This information can be summarised as:

$$E_{\text{air}} = Z_{\text{air}} H_{\text{air}},$$  \hspace{1cm} (E.8a)

$$E_{\text{Earth}} = Z_{\text{Earth}} H_{\text{Earth}} + z_e,$$  \hspace{1cm} (E.8b)

$$H_{\text{air}} = H_{\text{Earth}} - J_{cs}.$$  \hspace{1cm} (E.8c)

Results have been compared with Wannamaker (1991) integral solutions showing only small differences over more resistive bodies and near resistivity contrasts due to differences in the $E$ field geometry between the two algorithms and to different model discretisations.

### E.2.2 Iterative methods

Mackie and Madden (1993b) extended their earlier treatment (Mackie and Madden, 1993a) by introducing a conjugate direction relaxation solution, which is an iterative technique and not a direct solution. In order to restrict the eigenvalue spread of a coefficient matrix $A$, which solves $Ax = b$, a preconditioner is applied. In the case of 3-D electromagnetic equations, coefficient matrices are highly elliptical making a preconditioner a very useful tool to improve the condition of the matrix and reduce the computation time. Equation (E.9) is the coefficient matrix $A$ for the second order system of equations in $H$ and the preconditioning matrix $M^{-1}$ containing the inverse diagonal matrices $M$ of the 2-D operators for the transverse magnetic (TM) mode in each direction:

$$M^{-1}A = \begin{pmatrix} M_{xx}^{-1} & 0 & 0 \\ 0 & M_{yy}^{-1} & 0 \\ 0 & 0 & M_{zz}^{-1} \end{pmatrix} \begin{pmatrix} M_{xx} & N_{xy} & N_{xz} \\ N_{yx} & M_{yy} & M_{yz} \\ N_{zx} & M_{zy} & M_{zz} \end{pmatrix}. \hspace{1cm} (E.9)$$

To improve the results of the relaxation algorithm a multiple scaling approach is introduced. A coarser grid is solved using direct solutions outlined in Mackie and Madden (1993a). The obtained field values are interpolated onto a finer grid, which is then solved with the iterative solution described above. These steps are repeated until the finest grid is achieved or the 3-D model is solved.

Smith (1996a) introduced an improvement to the restriction of having an equally staggered-grid in Mackie and Madden (1993a) by developing a staggered-grid, finite-difference (SFD) method on a possibly non-uniform rectangular grid. He showed that it is non-relevant which differential equations are discretised. Both the coupled first-order equations (E.10) and the single second-order equation (E.11) in either $E$ or $H$ result in consistent systems.

$$\nabla \times E = i\omega \mu_0 H,$$  \hspace{1cm} (E.10a)

$$\nabla \times H = J = \sigma E.$$  \hspace{1cm} (E.10b)
Equation (E.10) is equivalent to Equation (E.7) in integral form.

\[
\nabla \times (\nabla \times E) = i\omega \mu_0 \sigma E, \tag{E.11a}
\]

\[
\nabla \times \left( \frac{1}{\sigma} \nabla \times H \right) = i\omega \mu_0 H. \tag{E.11b}
\]

In the Equations (E.10) and (E.11) the displacement currents are regarded as negligible due to low frequencies used in MT. Furthermore, Maxwell’s equations have a time-dependant component \( e^{i\omega t} \). In case of currents being conserved, which means no sources or sinks are present, the following relationship is true:

\[
\nabla \cdot \sigma E = 0. \tag{E.12}
\]

When the conductivity to be modeled is comprised of domains of uniform conductivity with no anisotropy, Equation (E.12) simplifies to \( \nabla \cdot E = 0 \) and with \( \nabla \times (\nabla \times E) = \nabla (\nabla \cdot E) - \nabla^2 E \), Equation (E.11a) can be written as:

\[
\nabla^2 E = -i\omega \mu_0 \sigma E, \tag{E.13}
\]

which has a general solution using the separation of variables technique.

\[
E = (\alpha, \beta, \gamma) e^{-i(xk_x + yk_y + zk_z)}. \tag{E.14}
\]

\( \alpha, \beta \) and \( \gamma \) are undetermined coefficients and \( k_x, k_y \) and \( k_z \) are separation constants corresponding to horizontal and vertical wavenumbers. Equation (E.14) is a general solution to the SFD equations. Comparison with analytical solutions reveal discrepancies at the Nyquist wavenumber, where analytical solutions attenuate much quicker. Smith (1996a) shows that the wavenumber content leads to an accurate estimate for SFD solutions, which is achieved when a reasonable portion of the grid is evenly spaced.

The staggered-grid approximation results in a linear system of equations

\[
Ax = b, \tag{E.15}
\]

with \( A \) being symmetric and non-Hermitian, and \( b \) the source vector that depends on boundary condition and source field polarisation. This system can also be solved using the biconjugate-gradient method and a modified, partial Cholesky decomposition preconditioner (Smith, 1996b). This shows significant improvement in computation time except for low frequencies, where the incomplete Cholesky decomposition has to be altered to conserve currents and satisfy Equation (E.12).

Newman and Alumbaugh (2000) utilise the conjugate gradient solution to solve for Equation (E.11a) and (E.15). However, a Yee (1966) staggered grid is applied which defines the electric field \( E \) along the edges of a block and \( H \) across the block faces (Figure E.2). Dirichlet boundary
E.2. Finite-difference methods

conditions are applied to Equation (E.11a) so that tangential electric field boundary values are specified:

\[ E_\parallel(0) = E_0. \] (E.16)

Condition (E.12) is explicitly enforced, too, closely following the approach of Smith (1996b). They employ a Tikhonov regularisation for the inverse problem, which imposes a smoothing constraint on the least-squares solution (Tikhonov and Arsenin, 1977). This procedure significantly stabilises the inversion process damping the influence of small eigenvalues on the least-squares solution (K. Spitzer, pers. comm. 2002), hence reducing the ill-posed nature. The corresponding objective functional \( \varphi \) of the Tikhonov regularisation is as follows (Newman and Alumbaugh, 2000):

\[
\varphi = \sum_{n=1}^{2N} \left( \frac{Z_{n,\text{obs}} - Z_{n,\text{m}}}{\varepsilon_n} \right)^2 + \frac{\lambda m^T R^T R m}{\text{smoothness constraint}}. \] (E.17)

The magnetotelluric tensor \( Z \) is split into the real and imaginary part and the data error \( \varepsilon_n \) reduces the influence of noisier data on the objective function \( \varphi \). The regularisation matrix

Figure E.2: Yee (1966) staggered grid employed by Newman and Alumbaugh (2000). Note that the \( E \) field is defined along the block edges and \( H \) across the block faces.
Algorithm 3: NLCG algorithm of Polyak and Ribière (1969) used to invert magnetotelluric data for a 3-D resistivity model (Newman and Alumbaugh, 2000). In this algorithm the gradient of the objective function is required.

\[ i = 1; \]
\[ \text{choose initial model } m_i; \]
\[ \text{compute } r_i = -\nabla \varphi(m_i); \]
\[ \text{set } u_i = M_i^{-1}r_i; \]

while \(|r_{i+1}| > \varepsilon|\) do
\[ \text{find } \alpha_i \text{ that minimises } \varphi(m_i + \alpha_i u_i); \]
\[ \text{set } m_{i+1} = m_i + \alpha_i u_i; \]
\[ r_{i+1} = -\nabla \varphi(m_{i+1}); \]
\[ \text{set } \beta_{i+1} = \frac{r_{i+1}^T M_i^{-1} r_{i+1} - r_i^T M_i^{-1} r_i}{r_i^T M_i^{-1} r_i}; \]
\[ \text{set } u_{i+1} = M_i^{-1} r_{i+1} + \beta_{i+1} u_i; \]
\[ i = i + 1; \]

end

\( R \) contains the finite difference approximation to the Laplacian \( \nabla^2 \) operator from Equation (E.13). The regularisation parameter \( \lambda \) controls how smooth the model will be and remains fixed throughout the inversion process. High values of \( \lambda \) result in a smoother but less well data fitted model. Unfortunately, an appropriate value of the regularisation parameter \( \lambda \) can only be found through a trial-and-error process, e.g. using the L-curve between the data and model misfit.

Newman and Alumbaugh (2000) implement a non-linear conjugate gradient forward operator similar to the linear CG method of Hestenes and Stiefel (1952). The Polyak and Ribière (1969) algorithm is identical to the linear CG method if the objective functional \( \varphi \) is quadratic and exact line searches are made with the NLCG (Algorithm 3).

The Polyak and Ribière (1969) algorithm employs the computation of the gradient of the objective function \( \nabla \varphi \). The aim is to find a minimum where the condition \( \nabla \varphi = 0 \) holds. Note the difference to the approach of Mackie et al. (1993) where a solution was sought that satisfies a trade-off between model misfit and adherence to an a priori model, scaled by the covariance matrix and the sensitivity matrix (Equation (E.2)). The gradient of the objective function can be expressed as:

\[ \nabla \varphi = \nabla \varphi_d + \lambda \nabla \varphi_m, \quad (E.18) \]

where \( \varphi_d, \varphi_m \) are functionals that relate to the data misfit and the model smoothness, respectively. Evaluation of \( \nabla \varphi_m \) is straightforward:

\[ \nabla \varphi_m = 2 R^T R m. \quad (E.19) \]

\( \nabla \varphi_d \) is a summation of a weighted difference of observed and predicted impedances \( Z \), the sparse matrix \( A \) from Equation (E.15) and an interpolation vector linking \( E \)- and \( H \)-fields.
for two source polarisation and receiver sites (Newman and Alumbaugh, 2000, Equation 13). A modified static divergence correction is applied so that the following expression is always fulfilled:

$$\nabla \cdot \sigma \mathbf{E} + \nabla \cdot \mathbf{J} = 0.$$  \hspace{1cm} (E.20)

This correction is required since the conductivity of the air is approximated by a small, finite value. Six forward solution are required per iteration step. Four forward solutions determine the computation of the gradients and two additional are necessary for the line search to find $\alpha$ that will minimise $\varphi(m + \alpha u)$. The diagonal of a Hessian matrix is utilised as a preconditioner, since computation of the full Hessian matrix would prove to be too time-consuming. A quasi-Newton formula, the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update, the diagonal Hessian can be computed without even knowing its off-diagonal components:

$$M_{i+1} = M_i + \left( \frac{\nabla \varphi(m_i) \nabla \varphi(m_i)^T}{\nabla \varphi(m_i)} \right)^T u_i + \frac{y_i y_i^T}{\alpha_i y_i^T u_i},$$  \hspace{1cm} (E.21)

with $y_i = \nabla \varphi(m_{i+1}) - \nabla \varphi(m_i)$. Parameters are represented in logarithmic form. To further improve the computation time, the NLCG algorithm is parallelised.

Newman and Alumbaugh (2000) reported that they could not achieve the desired target misfit of 1 (Figure E.3). Static shift effects, slow convergence near the minimum and numerical differences between the forward operator and the inverse operator are mentioned to cause the offset.
The major difference to the linear CG scheme in Mackie et al. (1993) lies in the implementation of a non-linear CG. Therefore, the objective functional $\varphi$ in Equation (E.17) can be non-quadratic. If only fewer steps are required to produce a model update, than a linear CG scheme would be favoured. The same conclusion can be drawn if $\varphi$ is quadratic (Newman and Alumbaugh, 2000).

### E.2.3 Conclusion

The finite-difference method allows the modelling of arbitrary complex conductivity structures. A staggered grid is a widely used tool to discretise the distribution of Maxwell’s equations in the subsurface. Due to the underdetermined nature of the magnetotelluric inverse problem, smoothing constraints have to be introduced. They provide additional information necessary for a stable solution, at the cost of data misfit. However the final models ought to display a smoothed image of the actual distribution.

In order to reduce computation time, parallelisation of the iterative solution is a further option (Newman and Alumbaugh, 2000). Another way is to utilise preconditioned matrices. Newman and Alumbaugh (2000) mention, that further improvement for the preconditioner is necessary. Li and Spitzer (2002) compared a symmetric successive overrelaxation (SSOR) preconditioner with an incomplete Cholesky decomposition preconditioner, and found that the latter was superior for 3-D resistivity modelling. However, since the preconditioner is a purely mathematical operator for large sparse systems, the results can be projected on magnetotelluric problems, too. Furthermore, Spitzer and Wurmstich (1999) show that the CG method shows shortest computation times for symmetric matrices. The biconjugate gradient method (Smith, 1996b), has been reported to converge satisfactory, and has the advantage that they can be used for non-symmetric matrices as well.

### E.3 Thin-sheet modelling

Wang and Lilley (1999) considered a thin-sheet structure in order to model synthetic and observed magnetic fluctuations responses. The underlying idea is that of a comparatively 'thin' surface layer with horizontally varying electrical conductance. Underneath the thin sheet is a one-dimensional layered Earth. The problem is non-linear as can be shown with a Fréchet derivative analysis.

$$\delta d = \iiint F \delta m \, dV,$$

(E.22)

where $F = F(r, r', m)$ denotes the Fréchet derivative of $d = d(r, m)$ with respect to $m(r')$. The transfer function $T$ relates the 'anomalous' vertical magnetic field component $H_z$ to the
'normal' magnetic field components $H_x$ and $H_y$.

$$H_z = (T_{xx}, T_{xy}) \begin{pmatrix} H_x \\ H_y \end{pmatrix}. \tag{E.23}$$

Wang and Lilley (1999) used different synthetic models to show that Fréchet derivatives of the transfer functions $T$ are model-dependent, thus showing that the observed data vector is related to the model vector in a non-linear way.

### E.3.1 Regularised inversion

For this particular problem Wang and Lilley (1999) derive an objective function, whose gradient is algebraically similar to Equation (E.2). Because of its importance a short derivation will be shown here.

$$\varphi(m) = L(m) + \lambda R(m). \tag{E.24}$$

Equation (E.24) introduces a data misfit function $L$ and a regularisation term $R$. $R$ has a significant contribution to the inverse problem since observational data alone is often insufficient in order to find a unique solution. The problem is underdetermined and needs more constraint through a smoothing operator, such as the regularisation operator in this case. The Euclidean (or $\ell^2$) norm $\|\varphi(m)\|_2$ is then sought to be minimised. In order to simplify the problem stated in Equation (E.24), a Taylor-series expansion of $\varphi(m)$ is conducted around a local point $m_0$:

$$\varphi(m_0 + \delta m) = \varphi(m_0) + (\nabla \varphi(m_0))^T \delta m + \frac{1}{2} \delta m^T H \delta m. \tag{E.25}$$

The Hessian matrix $H$ is the Jacobian of the gradient of the objective function $H = J(\nabla \varphi)$. To achieve $\|\varphi(m)\|_2 \rightarrow \text{min}$, Equation (E.25) is differentiated with respect to $\delta m$. This results in the following relation:

$$(H_L + \lambda H_R) \delta m = -(\nabla \varphi_L + \nabla \varphi_R). \tag{E.26}$$

Here $\nabla \varphi_L$ and $H_L$ are the gradient and the Hessian of the data misfit function $L(m)$, respectively. The $\ell^2$-norm of $L$ is as follows:

$$L(m) = \frac{1}{2} (d_{\text{obs}} - g(m))^T C^{-1}_{d} (d_{\text{obs}} - g(m)). \tag{E.27}$$

Accordingly, the $\ell^2$-norm of the regularisation term can be defined as:

$$R(m) = \frac{1}{2} m^T \partial_x^T \partial_x m + \frac{1}{2} m^T \partial_y^T \partial_y m. \tag{E.28}$$

$\partial_x$ and $\partial_y$ are operators that take the differences between model parameters of laterally adjacent cells in the $x$ and $y$ direction, respectively. Computing the gradient and the Hessian of Equation (E.27) and Equation (E.28) and substituting into Equation (E.26) finally yields:

$$(G^T C^{-1}_{d} G + \lambda (\partial_x^T \partial_x + \partial_y^T \partial_y)) \delta m = G^T C^{-1}_{d} ((d - g(m_0)) - \lambda (\partial_x^T \partial_x + \partial_y^T \partial_y)). \tag{E.29}$$
As stated earlier, this expression is algebraically equivalent to Equation (E.2) of Mackie et al. (1993). Wang and Lilley (1999) show that an inversion of an incomplete data set with a smoothness constraint ($\lambda \neq 0$) recovers conductive and resistive structures well for noisy synthetic data (modeled for 2% and 5%). It should be mentioned that real data always contains noise. The incorporation of smoothing is however penalised by an increase in model misfit.

The thin-sheet algorithm was applied to the Australian continent using geomagnetic data from various experiments throughout the continent. A starting model with geological \textit{a priori} information was divided into $60 \times 60$ cells with each cell of a side length of 100 km. One drawback of this technique is the implementation of one period only. Furthermore, the imaginary parts of transfer function have been left out of the inverse process leaving only the real parts. The conductance of the surrounding region were kept fixed, reducing the amount of cells to be determined for conductivity from 3600 to 861. The fixation of the ocean cell is based on the idea that ocean water largely contributes to the conductance in these cells. The final model shows a good agreement between the observed and model data in the interior of the continent. Smoothing effects and neglecting the contribution of the seafloor sediments conductivity to the conductance of the ocean cells might explain the discrepancies on the continental margins. The technique shows all major conductivity anomalies in the Australian crust and corresponds well to previous studies (Constable, 1985).

### E.4 Finite-element methods

Finite-element methods have attracted more and more interest in recent years (Mogi, 1996; Zyserman and Santos, 2000; Xie et al., 2000; Mitsuhata and Uchida, 2004), since they have the advantage that arbitrary geometries such as complex topography can be modeled. Finite elements are also able to produce good results near conductivity boundaries, but FEM methods usually take up more computation time (Li and Spitzer, 2002). Mogi (1996) developed a forward operator for the magnetotelluric problem based on the secondary field electric components. The primary electric field is solved using analytically equations, whereas the secondary fields are treated with the FEM method. A further improvement is shown in a recent paper by Mitsuhata and Uchida (2004), who developed a modelling code based on the $T - \Omega$ Helmholtz decomposition of the magnetic field $H$ in Maxwell’s equations, in which $T$ is the electric vector potential and $\Omega$ is the magnetic scalar potential.

Starting from Equation (E.10), the magnetic field $H$ can be divided into an incident magnetic field $H_0$ and a resultant magnetic field $H_c$ due to induced electric currents in the Earth. Furthermore, $\nabla \cdot J = 0$ must hold since no electric current source is present in MT. Therefore, $J$ can be expressed as:

$$J = \nabla \times T.$$  \hspace{1cm} (E.30)
Another assumption is that in the air region \( J = 0 \) and with \( \nabla \times \mathbf{H}_c = \mathbf{J} \), \( \mathbf{H}_c \) can be represented as:

\[
\mathbf{H}_c = \mathbf{T} - \nabla \Omega.
\]  

(E.31)

This expression leads to the governing equations that determine the \( \mathbf{T} - \Omega \) method. Equation (E.30) and (E.31) substituted into Equation (E.10) yield for the interior of the Earth \( \mathcal{V}_c \) (Figure E.4):

\[
\nabla \times \left( \frac{1}{\sigma} \nabla \times \mathbf{T} \right) + i\omega\mu_0(\mathbf{T} - \nabla \Omega) = -i\omega\mu_0 \mathbf{H}_0 \quad \text{in} \quad \mathcal{V}_c.
\]  

(E.32)

With the conservation law for the magnetic flux density

\[
\nabla \cdot \mathbf{H}_c = 0,
\]  

(E.33)

Equation (E.31) can be transformed into:

\[
\nabla \cdot (\mathbf{T} - \nabla \Omega) = 0 \quad \text{in} \quad \mathcal{V}.
\]  

(E.34)
### E.4.1 Interface and boundary conditions

At the interface between two media with different values of conductivity the tangential component of the electric vector potential $\mathbf{T}$ is continuous:

$$\mathbf{n} \times (\mathbf{T}_1 - \mathbf{T}_2) = 0.$$  \hfill (E.35)

and

$$\Omega_1 = \Omega_2.$$  \hfill (E.36)

The unit normal vector with respect to the interface is $\mathbf{n}$. At Earth’s surface, $\mathbf{T}$ is parallel to the unit vector $\mathbf{n}$:

$$\mathbf{n} \times \mathbf{T} = 0 \quad \text{at} \quad S_c.$$ \hfill (E.37)

The mutual dependance of Equation (E.32) and (E.34) can be overcome with following expression including the Coulomb gauge $\nabla \cdot \mathbf{T} = 0$:

$$\nabla^2 \Omega(\mathbf{r}) = -\mathbf{n} \cdot \mathbf{T}(\mathbf{r}) \left| \nabla f \right| \delta(\mathbf{r} \in S_c) \quad \text{in} \quad \mathcal{V},$$ \hfill (E.38)

where $\delta$ is the Dirac delta function, $\mathbf{r}$ is a position vector, and $f$ describes the topography function $f = z - g(x,y)$.

Equation (E.32) and (E.38) are solved to determine $\mathbf{T}$ and $\Omega$. Mitsuhata and Uchida (2004) mention that solving these equations requires significantly less computer memory since in the air domain $\mathcal{V}_a$ only $\Omega$ is the only unknown variable. Using a conventional approach, solving second order differential equations for $\mathbf{E}$ or $\mathbf{H}$ (Equation (E.11)) with a staggered-grid FD method, the divergence correction (Equation (E.20)) must always be applied and leads to ill-conditioned systems of equations due to small values of conductivity in the air. With the $\mathbf{T} - \Omega$ method a correction is not necessary.

At the boundary of $\mathcal{V}$, $\Omega$ is equal to 0 (Dirichlet boundary condition). $\mathbf{T}_z$ is zero at the side boundaries of $\mathcal{V}_c$, because $\mathbf{T}$ is produced by 2-D or 3-D conductivity anomalies only. At the x-z boundaries and y-z boundaries, $\mathbf{T}_x = \mathbf{T}_0$, and $\mathbf{T}_y = 0$, respectively (given a uniform incidence field $\mathbf{H}_0$ parallel to $x$). $\mathbf{T}_0$ is a general solution for a uniform halfspace. At the bottom of $\mathcal{V}_c$, $\mathbf{T}_z = -\mathbf{H}_0$, assuming the model reaches several skin-depths and no anomalous fields are present at the bottom boundary. The model is fully defined with these boundary conditions, it should be noted again that $\mathbf{T}$ equals zero in the air $\mathcal{V}_a$ and the boundary condition for $\mathbf{T}$ at the surface is defined by Equation (E.37).

### E.4.2 Finite-element formulation

The domain $\mathcal{V}$ is divided into so-called bricks where the electric vector field $\mathbf{T}$ is defined along the edges and $\Omega$ is defined at the nodes (Figure E.5). The volume of each brick has a constant
E.4. Finite-element methods

Figure E.5: Sampling points in the brick element. The electric vector field $\mathbf{T}$ is defined along the edges and $\Omega$ is defined at the nodes. The entire volume of each brick has a constant conductivity value $\sigma$.

The conductivity value $\sigma$. $\mathbf{T}$ and $\Omega$ are represented in the $e$th element as edge and nodal elements:

$$\mathbf{T}^e = \sum_{i=0}^{11} N_i^e T_i^e, \quad (E.39a)$$
$$\Omega^e = \sum_{j=0}^{7} N_j^e \Omega_j^e. \quad (E.39b)$$

$N_i^e$ and $N_j^e$ are the vector and scalar interpolation functions, respectively. The finite-element method equations can be derived from Equation (E.32) and (E.38) using the Galerkin method. A residual vector $\mathbf{r}$ and and a scalar residual $r$ for Equation (E.32) and (E.38) is defined, respectively.

$$\mathbf{r} = \nabla \times \left( \frac{1}{\sigma} \nabla \times \mathbf{T} \right) + i\omega \mu_0 (\mathbf{T} - \nabla \Omega) + i\omega \mu_0 \mathbf{H}_0 \quad (E.40a)$$
$$r = -\nabla^2 \Omega (\mathbf{r}) - \mathbf{n} \cdot \mathbf{T}(\mathbf{r}) |\nabla f| \delta (\mathbf{r} \in S_e) \quad (E.40b)$$
The residuals are incorporated into the following Galerkin method conditions:

\[
R_{Tk} = \iiint_{\mathcal{V}_c} N_k \cdot r \, dV = \sum_{e=1}^{NE} \iiint_{\mathcal{V}_e} N^e_{r(k)} \cdot r \, dV = 0 \quad (E.41a)
\]

\[
R_{Gl} = \iiint_{\mathcal{V}} N_l r \, dV = \sum_{e=1}^{NT} \iiint_{\mathcal{V}_e} N^e_{r(l)} r \, dV = 0. \quad (E.41b)
\]

\(N_k\) is assigned over the \(k\)th edge and \(N_l\) is assigned over the \(l\)th node. \(NE\) and \(NT\) is the number of brick elements in \(\mathcal{V}_c\) and \(\mathcal{V}\), respectively.

The next step will be only described here, since the derivation is rather lengthy. The reader is referred to Mitsuhata and Uchida (2004) for more detail. Equations (E.41) are computed for every brick element leading to a matrix expression of the form \(Ax = b\), with \(A\) a asymmetrical sparse matrix, \(x\) is a vector comprising the unknowns \(\Omega^e\) and \(T^e\), and \(b\) includes source terms and Dirichlet boundary conditions.

A BI-CGSTAB (Biconjugate gradient stabilised) method is used to solve the matrix system, preconditioned with an incomplete LU preconditioner (Van der Horst, 1992; Saad, 1996). The method is applied to two COMMEMI models (Zhdanov et al., 1997) and compared to a staggered grid FD solution. A general similarity in modeled resistivity can be observed with the highest discrepancies of about 5%.

### E.5 Conclusion

The methods that have been introduced here are able to model subsurface structure that is believed to be a smooth equivalent to the true Earth resistivity distribution. Thin-sheet modelling has been applied to the Australian continent, but only one period has been inverted for conductivity structure (Wang and Lilley, 1999). The thin-sheet modelling approach also imposes an \textit{a priori} constraint to the geometry, since it is believed that the conductivity structures are only in the top layer,’the thin sheet’. However this is not always the case. FD and also FE methods are more flexible in this sense as they allow one to model more complex structures. Especially the FE method has advantages here, even though it requires more computation time. However, it has emerged only in recent years and further improvement of this method can be expected.

For both methods the discretisation of Maxwell’s equations onto a staggered grid or brick elements for FD and FE methods, respectively, leads to a sparse matrix-vector equation \(Ax = b\). There are several methods in order to solve for \(x\). The conjugate gradient solution is clearly superior to other techniques such as conjugate directions or steepest descent methods. Direct solutions are not attempted anymore as they require vast amounts of time. In case of non-symmetric matrices the bi-conjugate gradient solution is a possible alternative. However,
transformations to an equal grid or transformations of the form

\[ \mathbf{S} = \begin{pmatrix} 0 & \mathbf{A} \\ \mathbf{A}^T & 0 \end{pmatrix} \]  \hspace{1cm} (E.42)

yield a symmetric matrix.

The review clearly shows that boundary conditions are an important part of each relaxation procedure. Dirichlet boundary condition have been applied quite often. However, this type of boundary formulation required a large model where the edges are sufficiently far away form the geological structures of interest. Another possibility would be the implementation of boundaries obtained from 2-D cross sections.

Preconditioners improve the eigenvalue spread of a matrix. Since a full inverse of the system matrix \( \mathbf{A} \) would be too time-consuming, several other preconditioning procedures are suggested. Clearly one of the best candidates is the Incomplete Cholesky decomposition. The symmetric successive overrelaxation preconditioning method requires less memory, but converges slower.

The inverse operator usually consists of a data misfit function and a regularisation term, whereas the latter improves the ill-conditioning of the solution. Wang and Lilley (1999, Figure 5) have shown that without the regularisation term, which is in most cases a smoothing operator, the inversion procedure cannot recover the true model.

The FD method has been studied thoroughly and Newman and Alumbaugh (2000) have demonstrated that the finite-difference method is a powerful tool to obtain resistivity models of the subsurface. The FE method seems to be very promising, and recently Franke et al. (2007c) showed results of simulation of magnetotelluric fields at Stromboli using a 3-D FE code (Franke et al., 2007b).


References


References


Colophon

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