Interpretation of Global EM Induction Data from Ground, Sea and Space
New Response Functions, Inversion Schemes and Conductivity Models

Author(s):
Püthe, Christoph

Publication Date:
2015

Permanent Link:
https://doi.org/10.3929/ethz-a-010531597

Rights / License:
In Copyright - Non-Commercial Use Permitted
Interpretation of global EM induction data from ground, sea and space: New response functions, inversion schemes and conductivity models

A dissertation submitted to attain the degree of

DOCTOR OF SCIENCES of ETH ZURICH
(Dr. sc. ETH Zurich)

presented by

CHRISTOPH PÜTHE

Master of Science ETH in Erdwissenschaften
born on September 18, 1986
citizen of Germany

accepted on the recommendation of

PD Dr. Alexey Kuvshinov
Prof. Dr. Andrew Jackson
Dr. Jakub Velímský
Prof. Dr. Nils Olsen

2015
Abstract

Resolving the three-dimensional (3-D) structure of Earth’s deep interior is one of the challenging tasks in modern geophysics. To date, most knowledge about heterogeneities in the mantle is gained from seismic tomography, which is used to map mechanical properties. An alternative technique to image Earth’s interior is electromagnetic (EM) induction. This technique is based on electric currents flowing in the conductive Earth, which are induced by a time-varying, external magnetic field. EM induction is used to map electrical conductivity, which is sensitive to the presence of partial melt and volatiles. Seismic tomography and EM induction can hence provide complementary information about the composition and structure of Earth’s mantle.

While in the last decades global seismic tomography has reached a certain level of maturity, the application of EM induction to global problems is far less developed. On one hand this is due to the sparsity of observations, but it is also due to a lack of methods to analyse and invert the available data. The present study aims at advancing global EM induction research. Special attention is given to handling a spatially complex source, including as many types of data as possible in the analysis, and developing algorithms that invert these data for global conductivity structure.

EM induction research makes extensive use of transfer functions. These are frequency-domain quantities that describe the response of the conductive Earth to the excitation by given sources. A particularly popular transfer function in global applications is the so-called C-response. It is commonly estimated by relating horizontal and vertical components of the magnetic field at a given site. This technique is subject to the common assumption that the inducing source at periods longer than one day consists of a large-scale, symmetric ring current in the magnetosphere.

We challenge this assumption in a model study. By numerically simulating induction due to a more complex source, which was derived from observatory magnetic data, we investigate the reliability of the estimated C-responses. The results indicate that the asymmetric part of the source has an important effect on the estimates, which might be misinterpreted for conductivity anomalies. This stimulates us to devise new transfer functions for data from ground, sea and space that can handle a more complex source structure. To estimate these transfer functions from EM data, we develop a multivariate data analysis tool.

A large part of this work is dedicated to the inversion of global EM data. We first investigate the dependence of electrical conductivity on depth. In contrast to most previous studies that tackled this 1-D problem, we take into account 3-D effects due to induction in the conductive oceans. Ten years of data from satellites and geomagnetic observatories are analysed and inverted. Deterministic and probabilistic inversion approaches yield very similar conductivity profiles. These feature a highly resistive upper mantle, an increase in conductivity in and beneath the transition zone, a marked kink...
at a depth of 900 km, and a conductive lower mantle. Information on model resolution is obtained from an analysis of the Hessian of the objective function and from an independent Monte Carlo study.

We subsequently consider the 3-D problem. We develop a modular inversion algorithm that can handle various kinds of EM data. The deterministic algorithm is based on the minimization of an objective function. To calculate its gradient, we make use of the adjoint approach, which greatly accelerates the computations. Various methods to parametrize conductivity structure and to minimize the objective function are implemented. For the forward computations (which rely on an integral equation solver), the code is parallelised over frequencies and elementary sources.

For the actual 3-D inversion of satellite and observatory data, we employ the \( Q \)-matrix. This array of transfer functions relates the external and internal coefficients of the spherical harmonic expansion of the magnetic field. In test studies, conductivity anomalies of continental size are successfully recovered. This validates the functionality of the algorithm. An application to real data fails, however, due to the difficulty to separate contributions to the magnetic field of different origin.
Zusammenfassung


Während die globale seismische Tomographie sich in den vergangenen Jahrzehnten stark entwickelt hat, fristet die erdmagnetische Tiefensondierung auf globalem Massstab ein Nischendasein. Dies liegt zum einen an der geringen Datendichte, zum anderen aber auch an fehlenden Methoden, um die vorhandenen Daten zu analysieren und invertieren. Die vorliegende Doktorarbeit setzt sich das Ziel, die Forschung in der erdmagnetischen Tiefensondierung auf globaler Ebene voranzutreiben. Besonderes Augenmerk wird dabei darauf gelegt, ein räumlich komplexes Quellsystem zu erfassen, so viele Datentypen wie möglich in die Analyse mit einzubeziehen und Algorithmen zu entwickeln, um aus den Daten die globale Verteilung der elektrischen Leitfähigkeit zu berechnen.


## Contents

Abstract 3

Zusammenfassung 5

1 Introduction 10
1.1 Motivation 10
1.2 Global EM sounding – a brief history 12
1.3 Outline of the thesis 15

2 Electromagnetic Transfer Functions 17
2.1 A basic set of equations 17
2.2 Expanding EM fields 19
2.3 The concept of transfer functions 21
2.4 Old and new transfer functions 23
2.4.1 The $C$-response 23
2.4.2 New transfer functions for global induction studies 25
2.5 Multivariate analysis 27
2.5.1 Conventional approach 28
2.5.2 Multi-frequency approach 31
2.5.3 Comparison of two approaches 32
2.5.4 A multivariate processing code 33

3 Indications for a Complex Source 34
3.1 Variability of $C$-Responses 34
3.1.1 Observed variability 35
3.1.2 Numerical modelling 35
3.2 Alternative responses for observatory data 42
3.2.1 Transfer functions for the Hermanus observatory 43
3.2.2 Analysis of coherencies 46
3.2.3 Discussion 47
3.3 Alternative responses for cable data 48

4 The Swarm Satellite Mission 51
4.1 Outline and objectives of the mission 51
4.2 The Swarm SCARF test data set 52

5 1-D Inversion for Mantle Conductivity Structure 55
5.1 Introduction 55
Contents

B.5 Recovery of the source current ........................................... 130
B.6 Analysis of day-to-day variability ...................................... 131

C Reproducing Electric Field Observations during Magnetic Storms 134
  C.1 Background .............................................................. 134
  C.2 Methods ................................................................. 135
    C.2.1 Data ................................................................. 136
    C.2.2 Calculation of the electric field .............................. 137
    C.2.3 Estimation of distortion matrices ............................ 138
  C.3 Results and discussion ................................................ 139
    C.3.1 Ocean bottom observatories .................................. 139
    C.3.2 Onshore observatories .......................................... 140
    C.3.3 Galvanic and inductive effects ............................... 143
    C.3.4 Towards real-time prediction .................................. 145
  C.4 Conclusions ............................................................. 147

List of Figures ............................................................... 149
List of Tables ............................................................... 154
Bibliography ................................................................. 156
Acknowledgements .......................................................... 167
Curriculum Vitae ............................................................ 168
Chapter 1

Introduction

1.1 Motivation

Humankind has conquered the Earth. Over the last centuries, new continents have been discovered, new territories have been settled, and each discovery has been recorded in books, maps or pictures. There was no place too far away from civilization and too inhospitable for a human being to reach and explore it. Today, satellites provide accurate photos of the most remote places on this planet. But in spite of all these achievements, the majority of the Earth is still hidden from our eyes. Even the deepest boreholes hardly reach more than 10 km – tiny scratches on the surface of a body with a mean radius of 6371 km. Any investigation of deeper parts of the Earth must rely on indirect methods. This is the field of geophysics.

Earth’s mantle extends from few tens of kilometres to the core-mantle boundary at a depth of 2890 km. This knowledge was gained from seismic studies, just as most other information we have about its structure. Similar to X-ray tomography used in medical imaging, seismic tomography (e.g. Woodhouse & Dziewonski, 1984; Becker & Boschi, 2002; Nolet, 2008) images the interior of a body by analysing waves passing through it. Based on mechanical waves, seismic tomography is sensitive to mechanical parameters such as bulk modulus, shear modulus and – to a limited degree – density. Moreover, seismic methods have proven very useful at detecting discontinuities in media. All of this information is crucial for an understanding of mantle dynamics, as it helps at illuminating structures such as cratonic roots or subducting slabs. However, the interpretation of seismic data has some inherent shortcomings, since mechanical parameters alone can hardly constrain the thermal and compositional structure of the mantle unambiguously (e.g. Khan et al., 2009). This calls for alternative methods, which can provide complementary information.

Electromagnetic (EM) induction studies aim at elucidating the distribution of electrical conductivity in the subsurface. In contrast to seismic wave speed, which typically varies by a few percent, electrical conductivity can vary by several orders of magnitude
Motivation

Figure 1.1: Concept of EM induction (courtesy of Jin Sun). According to Maxwell’s equations, a primary time-varying current generates a primary (external) time-varying magnetic field. The latter induces an electric field in the conducting Earth, which in turn drives a secondary current, generating a secondary (internal) magnetic field. Measurements taken on or above Earth’s surface contain contributions of both primary and secondary fields.

in different media. It is very sensitive to the connectivity of fluids and partial melt, but also to temperature and mineralogy. While seismology is a wave propagation method, EM induction is a diffusion method and therefore more suitable for imaging broad structures than for detecting discontinuities. To obtain reliable temperature profiles or to illuminate the role of water in the mantle, a combined interpretation of seismic and EM data will likely be beneficial.

The concept of EM induction is illustrated in Figure 1.1. Today, EM induction methods are most commonly applied in a local or regional context. The magnetotelluric (MT) method (e.g. Simpson & Bahr, 2005; Berdichevsky & Dmitriev, 2008; Chave & Jones, 2012) is used to measure and analyse EM fields that result from natural sources in order to image conductivity structure in the shallow subsurface. Global deep EM sounding – the imaging of conductivity at depths >100 km – also relies on natural sources, i.e. currents originating in the ionosphere (about 100 km above Earth’s surface) or the magnetosphere (3–8 Earth radii above the surface). It is thus similar in concept to MT, but to date much less developed. For this reason, global EM induction is still far from being an adequate complement to global seismic tomography.

This PhD project was initiated to advance the application of EM induction on a global scale. Special attention was given to handle a spatially complex source, to include as many types of data as possible in the analysis, and to develop algorithms that invert these data for the global conductivity structure. Before outlining the details of this project, however, I will summarize the history of deep EM sounding from its very beginnings to the current state of research.
1.2 Global EM sounding – a brief history

Earth’s magnetic field varies slowly in time due to changes in the fluid flow in the outer, liquid core. On top of the slow secular variation, the magnetic field is subject to fluctuations of small amplitude and short duration, which can be observed over the course of a day and which are commonly known as geomagnetic variations.

Geomagnetic variations were first reported by Graham (1724). The author made very detailed observations of the regular daily fluctuations of a compass needle, but could not explain the observed behaviour. It was not until 1882 that Stewart suggested currents in the upper atmosphere to be the cause of the oscillations already observed by Graham. In contrast to the old observer one and a half centuries before, Stewart (1882) could already rely on the principles of electromagnetism. The electromagnetic theory had been established in the first half of the 19th century based on the experimental work of Ørsted, Ampère, and Faraday. Later, it was summarized in a today well-known set of equations by Maxwell (1865).

Induction effects due to natural sources were first observed in telegraph cables during violent magnetic storms, such as the 1859 event (e.g. Clement, 1860). Early EM induction studies, however, focussed on the regular daily variations of the quiet-time magnetic field, which were the most obvious feature of the observed oscillations. Stewart’s assumption was confirmed by Schuster (1889), who analysed the daily magnetic variations measured at four magnetic observatories. He used the method of Gauss (1839) to expand the data onto Earth’s surface by a spherical harmonic analysis and separate the field into contributions from internal and external sources. Few years earlier, Lamb (1883) had developed the theory of EM induction in a uniform sphere. Schuster made use of this theory and demonstrated that the internal parts of the observed magnetic variations could be explained by EM induction in the conducting Earth. From an analysis of his results, he concluded that the Earth was not of uniform conductivity, but that “the upper layers must conduct less than the inner layers”.

This first evidence of heterogeneity gave rise to more and more complex conductivity models of the Earth as derived from EM measurements. Chapman (1919) was the first to publish a quantitative model of Earth’s conductivity structure, consisting of an insulating outer shell and a conducting core. The model was designed to reproduce the diurnal quiet-time magnetic variations. In later works (Chapman & Whitehead, 1922; Chapman & Price, 1930), the author admitted limitations of this model, as it did not consider induction in the highly conducting oceans and was incompatible with storm-time data. Lahiri & Price (1939) extended the uniform sphere-model and presented models with radially variable conductivity that were consistent with both quiet-time and storm-time data. It was already clear at that time that conductivity also varies laterally, at least in
Figure 1.2: Map of geomagnetic observatories delivering magnetic data as this thesis is written. Colours indicate topography/bathymetry.

the uppermost 10 km, where conductive oceans are located next to resistive continents. For practical reasons, this complication of the problem had to be ignored.

Modern deep EM sounding goes back to the work of Banks (1969), Berdichevsky et al. (1969), and Schmucker (1970). These studies advocated methods to derive subsurface conductivity structure locally or regionally from magnetic measurements. This facilitated the detection of lateral heterogeneities that were smoothed out in the global studies cited above. Banks (1969) moved the focus from reproducing diurnal variations to reproducing the spectral continuum of storm-induced magnetic fields at periods from two days to several months, since “it is clearly desirable that the response should be determined over as wide a range of frequency as possible if better estimates of the conductivity distribution are to be made”.

Banks demonstrated that the largest part of the measured variations in mid-latitudes and at periods >1 day could be explained by intensifications of the magnetospheric ring current. The assumption of a large-scale ring current as inducing source got known as $P_1^0$-assumption, since the magnetic field due to such a current system can be parametrized by a single zonal harmonic of degree 1. The $P_1^0$-assumption was the basis of many later studies that aimed at deriving regional 1-D conductivity profiles, such as those of Schultz & Larsen (1987) and Khan et al. (2011). The horizontal gradient method of Schmucker (1970, 1979) does not require strict assumptions about the inducing source, but its application is restricted to areas with dense coverage of observations. It was applied by Olsen (1998) to estimate the deep conductivity structure beneath Europe.

All studies mentioned above are based on data from the global network of magnetic observatories. This seems fair for local or regional studies, but can hardly yield reliable and unbiased results in global investigations. As shown in Figure 1.2, the distribution of magnetic observatories is far from uniform, with great deficiencies in oceanic regions and the entire southern hemisphere. An inversion of ground-based data for global conductivity structure will thus inevitably be biased towards continental regions.
In contrast, low-Earth-orbit platforms provide high-quality magnetic data with almost uniform spatial coverage. Past and recent satellite missions dedicated to measure the magnetic field are listed in Table 1.1. The analysis of satellite data is, however, challenging due to the difficulty in distinguishing between temporal and spatial variations in the records. Moreover, satellites pass over both continental and oceanic regions, which is why the measurements are affected by induction in the oceans in a complicated way (Tarits & Grammatica, 2000; Everett et al., 2003; Kuvshinov & Olsen, 2005). In spite of these difficulties, satellite data have been used to derive global 1-D conductivity models of Earth’s mantle within the last three decades, e.g. by Didwall (1984), Olsen (1999), Velímský et al. (2006) and Kuvshinov & Olsen (2006). The latter study takes into account the effect of a laterally heterogeneous surface layer.

For completeness, it shall be mentioned that magnetic observatories and satellites are not the only sources of long-period EM data. Currents induced by geomagnetic variations in abandoned submarine telecommunication cables reflect the conductivity structure underneath. In combination with observatory data, voltage data from such cables were used by e.g. Utada et al. (2003) and Shimizu et al. (2010a) to derive the conductivity distribution in the North Pacific.

Almost 100 years after Chapman (1919), the variation of electrical conductivity with depth is still topical in the EM community. In particular, model uncertainties are largely unknown, such that it is not clear how reliable the results of different studies are. On top of that, a consistent treatment of shallow lateral heterogeneities must be part of the analysis. Addressing these issues and deriving new models by using the maximum amount of available data was one of the goals of this project.

But is Earth’s conductivity structure underneath the surface shell really 1-D? Recent improvements in global 3-D EM forward modelling and the growth of computational resources have also made rigorous 3-D inversions on a global scale tractable. Spherical 3-D inversion schemes were presented by Koyama (2001), Kelbert et al. (2008), Tarits & Mandea (2010) and Kuvshinov & Semenov (2012). The first large-scale regional (e.g. Koyama et al., 2006; Shimizu et al., 2010b; Koch & Kuvshinov, 2015) and global (e.g.

<table>
<thead>
<tr>
<th>Name</th>
<th>Lifetime</th>
<th>Altitude</th>
<th>Type of data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magsat</td>
<td>1979-1980</td>
<td>350-580 km</td>
<td>vector/scalar</td>
</tr>
<tr>
<td>Ørsted</td>
<td>1999-2012</td>
<td>630-860 km</td>
<td>vector(until 2005)/scalar</td>
</tr>
<tr>
<td>CHAMP</td>
<td>2000-2010</td>
<td>350-450 km</td>
<td>vector/scalar</td>
</tr>
<tr>
<td>SAC-C</td>
<td>2000-2004</td>
<td>700 km</td>
<td>scalar</td>
</tr>
<tr>
<td>Swarm (3 satellites)</td>
<td>2013-2018*</td>
<td>450-550 km</td>
<td>vector/scalar</td>
</tr>
</tbody>
</table>

Table 1.1: Past and recent missions of satellites measuring the magnetic field. *Expected lifetime.
Kelbert et al., 2009; Semenov & Kuvshinov, 2012) studies revealed heterogeneous structure of mid-mantle conductivity. All of these studies were based on observatory data and, except for Koch & Kuvshinov (2015), on the $P_0$-assumption. However, bearing in mind the sparse and irregular distribution of geomagnetic observatories, reliable global images of 3-D variations of mantle conductivity can hardly be obtained at present or in the foreseeable future with the use of ground-based data alone.

The Swarm multi-satellite geomagnetic mission (Friis-Christensen et al., 2006) has prompted the initiation of efforts to develop methodologies for recovering 3-D electrical conductivity variations from space. Elaborating a consistent global 3-D inversion scheme, based on new transfer functions that can handle complex source systems and data of different origin, was thus another major goal of this project.

1.3 Outline of the thesis

The following Chapter 2 starts with Maxwell’s equations, which constitute the basis for all EM research. After some remarks on common representations of EM fields, I will introduce the important concept of transfer functions and its application to EM induction. Conventional and new transfer functions for global induction will be presented. The chapter closes with the detailed description of a multivariate time series algorithm, which was developed to estimate transfer functions from EM data.

In Chapter 3, I investigate the global variability of $C$-responses, which are transfer functions estimated locally from data of geomagnetic observatories. I conclude that part of the variability must be due to a more complex current source in the magnetosphere than commonly assumed. This asks for different transfer functions, which are tested against the conventional $C$-responses for a number of observatory sites. The text in the chapter is based on one of the papers published during my PhD (Püthe et al., 2015a).

Part of the research presented in this thesis was motivated by the Swarm multi-satellite geomagnetic mission. The mission’s objectives and the test data set used in the development phase are presented in Chapter 4.

The test data set was employed to validate the functionality of algorithms that recover the 1-D and 3-D distribution of electrical conductivity in Earth’s mantle. The 1-D algorithm, which is described in detail in Chapter 5, was subsequently applied to more than 10 years of real data. Different approaches to inversion, results including estimates of model uncertainties, and a geological interpretation are presented. The text in the chapter is based on two further papers (Püthe & Kuvshinov, 2013a; Püthe et al., 2015b).

The 3-D inverse problem is discussed in Chapter 6. In that chapter, I will first outline the mathematical foundations of a 3-D inversion algorithm and its application to different types of EM data. Thereafter, I will describe the numerical implementation in a modular code, which was developed as part of my PhD. The 3-D inversion algorithm is thoroughly
Introduction

tested and then applied to the same data as the 1-D algorithm. Parts of the chapter are based on two of my papers (Püthe & Kuvshinov, 2013b, 2014).

The work presented in this thesis is summarized in Chapter 7. I discuss implications of my results and provide an outlook for future research in the area of global EM induction.

Appendix A contains some mathematical derivations that relate to the main body of the thesis. The further appendices summarize independent side-projects of my PhD. Appendix B describes the analysis of $S_q$ variations and the quest for a more suitable parametrization of the global geomagnetic field in magnetic quiet times. That work was done during my research stay at DTU Space in Denmark. Appendix C contains a study focussing on the hazard due to geomagnetic storms in mid-latitude regions. That is a continuation of my Bachelor project; a corresponding paper was published as Püthe et al. (2014).
Chapter 2

Electromagnetic Transfer Functions

2.1 A basic set of equations

Maxwell’s equations describe the spatio-temporal behaviour of electric and magnetic fields and hence form the basis of electrodynamics. In the time-domain, they are commonly formulated as

\[ \nabla \times \mathbf{H} = \mathbf{j}, \]  
(2.1)

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \]  
(2.2)

\[ \nabla \cdot \mathbf{B} = 0, \]  
(2.3)

\[ \nabla \cdot \mathbf{D} = q. \]  
(2.4)

Maxwell’s equations (2.1)–(2.4) are completed with the constitutive relations

\[ \mathbf{B} = \mu \mathbf{H}, \]  
(2.5)

\[ \mathbf{D} = \varepsilon \mathbf{E}. \]  
(2.6)

The quantities in eqs (2.1)–(2.6) are deciphered as follows:

- \( \mathbf{H} \): magnetic field intensity, \([\mathbf{H}] = 1 \text{ A/m}\)
- \( \mathbf{E} \): electric field intensity, \([\mathbf{E}] = 1 \text{ V/m}\)
- \( \mathbf{B} \): magnetic flux density, \([\mathbf{B}] = 1 \text{ T} = 1 \text{ Vs/m}^2\)
- \( \mathbf{D} \): electric flux density, \([\mathbf{D}] = 1 \text{ As/m}^2\)
- \( \mathbf{j} \): electric current density, \([\mathbf{j}] = 1 \text{ A/m}^2\)
- \( q \): electric charge density, \([q] = 1 \text{ As/m}^3\)
- \( \mu \): magnetic permeability, \([\mu] = 1 \text{ Vs/Am}\)
• $\epsilon$: electric permittivity, $[\epsilon] = 1 \text{ As/Vm}$

All quantities introduced above generally vary in space and are thus functions of the position vector $\mathbf{r}$. In case of global studies, $\mathbf{r} = (r, \vartheta, \varphi)$ conveniently describes a spherical coordinate system, with $r$, $\vartheta$ and $\varphi$ being distance from Earth’s centre, colatitude and longitude, respectively.

Eq. (2.1), Ampère’s law, reflects the generation of magnetic fields by electric currents. Eq. (2.2), Faraday’s law, describes the induction process, in which electric fields are generated by a time-varying magnetic flux. Eq. (2.3), Gauss’ law for magnetism, states that the magnetic field is solenoidal, i.e. there are neither sources nor sinks for $\mathbf{B}$ and no magnetic monopoles. Field lines of $\mathbf{B}$ are therefore always closed. In contrast, field lines of $\mathbf{D}$ start or end at charges, as stated by eq. (2.4), Gauss’ law for electric fields. EM induction studies usually work with the assumption $\mu = \mu_0 = 4\pi \cdot 10^{-7} \text{ Vs/Am}$, i.e. magnetic permeability is assumed to be constant and equal to its value in free space.

The electric current density $\mathbf{j}$ can be further split into three constituents,

$$\mathbf{j} = \sigma \mathbf{E} + \frac{\partial \mathbf{D}}{\partial t} + \mathbf{j}^{\text{ext}}. \quad (2.7)$$

The first term on the right hand side (RHS) of eq. (2.7) is essentially Ohm’s law in matter, $\mathbf{j}_c = \sigma \mathbf{E}$, where $\sigma$ is electrical conductivity, $[\sigma] = 1 \text{ S/m}$, and $\mathbf{j}_c$ is known as conduction current. The second term on the RHS of eq. (2.7) reflects that magnetic fields can also be generated by fluctuating electric fields; $\mathbf{j}_d = \partial \mathbf{D}/\partial t$ is termed displacement current. The last term on the RHS of eq. (2.7) is known as extraneous current (or primary/impressed current). In this work, it is assumed that $\sigma$ is a scalar (no anisotropy) and is independent of frequency (no polarization effect).

For a number of reasons that will become clear later, it is advantageous to work in the frequency-domain, i.e. not to use the time series of electric and magnetic fields, but their time spectra. I adopt the Fourier transform convention

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(\omega)e^{-i\omega t}d\omega, \quad (2.8)$$

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} f(t)e^{i\omega t}dt, \quad (2.9)$$

where $f(t)$ is any function of time, $\tilde{f}(\omega)$ is its frequency-domain equivalent, and $\omega = 2\pi/T$ is the angular frequency (with $T$ being the period of variations). I will use the same nomenclature for the (complex-valued) time spectra as for the time series, namely denote them as $\mathbf{B}$, $\mathbf{E}$ etc. Using the constitutive relations (2.5)–(2.6), the above assumption on $\mu$ and the Fourier convention (2.9), Maxwell’s equations (2.1)–(2.2) can be rewritten in
the frequency-domain,

\[
\frac{1}{\mu_0} \nabla \times \mathbf{B} = (\sigma - i\omega \epsilon) \mathbf{E} + j^{\text{ext}}, \tag{2.10}
\]
\[
\nabla \times \mathbf{E} = i\omega \mathbf{B}. \tag{2.11}
\]

One last modification concerns the relative amplitudes of the terms on the RHS of Ampère’s law (2.10). Deep EM studies consider induction due to natural current systems, which vary on time scales between $10^{-3}$ s and a few months. In spite of large variations of electrical conductivity in nature, it is thus safe to assume that $\sigma \gg \omega \epsilon$, such that displacement currents can be neglected. This common simplification is known as \textit{quasi-static approximation}. The final representation of Maxwell’s equations, which form the basis of all forthcoming analyses, reads

\[
\frac{1}{\mu_0} \nabla \times \mathbf{B}(\mathbf{r}, \omega) = \sigma(\mathbf{r}) \mathbf{E}(\mathbf{r}, \omega) + j^{\text{ext}}(\mathbf{r}, \omega), \tag{2.12}
\]
\[
\nabla \times \mathbf{E}(\mathbf{r}, \omega) = i\omega \mathbf{B}(\mathbf{r}, \omega). \tag{2.13}
\]

\section{2.2 Expanding EM fields}

Eqs (2.12)–(2.13) reflect that electric and magnetic fields are linear with respect to the source $j^{\text{ext}}$. Thanks to this linearity, it is always possible to represent $\mathbf{B}$ as

\[
\mathbf{B}(\mathbf{r}, \omega) = \sum_j \alpha_j(\omega) \mathbf{B}_j(\mathbf{r}, \omega), \tag{2.14}
\]
where $\mathbf{B}_j$ are responses of the Earth to excitation by a source with a given geometry and unit amplitude, and $\alpha_j$ is an appropriate complex-valued factor.

Global EM induction studies commonly consider source currents originating in the ionosphere or magnetosphere. For an observer on Earth’s surface, such current systems are equivalent to \textit{sheet currents} flowing in an infinitely thin spherical shell at a given altitude (e.g. Olsen, 2006). Being confined to a spherical surface, the sheet current can be represented by a spherical harmonic expansion (SHE) as

\[
\mathbf{j}^{\text{ext}}(\mathbf{r}, \omega) = \sum_{n,m} \varepsilon_n^m(\omega) j_n^m(\mathbf{r}, \omega), \tag{2.15}
\]

where $j_n^m$ are spherical harmonic sheet currents of unit amplitude, $\varepsilon_n^m$ are the corresponding SHE coefficients, and the double sum is a short-hand notation,

\[
\sum_{n,m} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n}. \tag{2.16}
\]
In analogy to eq. (2.14), the magnetic field underneath the source region is given by

$$\mathbf{B}(\mathbf{r}, \omega) = \sum_{n,m} \varepsilon_n^m(\omega) \mathbf{B}_n^m(\mathbf{r}, \omega).$$  \hspace{1cm} (2.17)$$

An equivalent relation holds for the electric field,

$$\mathbf{E}(\mathbf{r}, \omega) = \sum_{n,m} \varepsilon_n^m(\omega) \mathbf{E}_n^m(\mathbf{r}, \omega).$$  \hspace{1cm} (2.18)$$

Just above Earth’s surface and in the electrically insulating atmosphere, eq. (2.12) reduces to $\nabla \times \mathbf{B} = 0$ due to vanishing conductivity and the absence of source currents. $\mathbf{B}$ is thus a potential field, i.e. we can define a scalar magnetic potential $V$ such that $\mathbf{B} = -\nabla V$. Since $\mathbf{B}$ is solenoidal, $V$ satisfies Laplace’s equation, $\nabla^2 V = 0$. The solution can be represented as sum of external and internal parts (e.g. Backus et al., 1996), $V = V^{\text{ext}} + V^{\text{int}}$, with

$$V^{\text{ext}}(\mathbf{r}, \omega) = a \sum_{n,m} \varepsilon_n^m(\omega) \left( \frac{r}{a} \right)^n Y_n^m(\theta, \phi),$$  \hspace{1cm} (2.19)$$

$$V^{\text{int}}(\mathbf{r}, \omega) = a \sum_{k,l} \iota_k^l(\omega) \left( \frac{a}{r} \right)^{(k+1)} Y_k^l(\theta, \phi).$$  \hspace{1cm} (2.20)$$

Here, $a$ is Earth’s mean radius, and $\varepsilon_n^m(\omega)$ and $\iota_k^l(\omega)$ are the SHE coefficients of the external (inducing) and internal (induced) parts of the potential, respectively. For reasons that will become clear later, I use different indices for the SHEs of external and internal parts. Note that the $\varepsilon_n^m$ in eq. (2.19), which describe the magnetic potential due to external sources, are equivalent to those in eqs (2.17)–(2.18). $Y_n^m$ is the spherical harmonic of degree $n$ and order $m$,

$$Y_n^m(\theta, \phi) = P_n^{|m|}(\cos \theta)e^{im\phi},$$  \hspace{1cm} (2.21)$$

where $P_n^{|m|}(\cos \theta)$ is an associated Legendre function. The magnetic field is derived by taking the negative gradient of $V$,

$$B_r(\mathbf{r}, \omega) = -\sum_{n,m} n \varepsilon_n^m(\omega) \left( \frac{r}{a} \right)^{n-1} Y_n^m \left[ \sum_{k,l} (k+1) \iota_k^l(\omega) \left( \frac{a}{r} \right)^{(k+2)} Y_k^l \right],$$  \hspace{1cm} (2.22)$$

$$B_\theta(\mathbf{r}, \omega) = -\sum_{n,m} \varepsilon_n^m(\omega) \left( \frac{r}{a} \right)^{n-1} \frac{\partial Y_n^m}{\partial \theta} + \sum_{k,l} \iota_k^l(\omega) \left( \frac{a}{r} \right)^{(k+2)} \frac{\partial Y_k^l}{\partial \theta},$$  \hspace{1cm} (2.23)$$

$$B_\phi(\mathbf{r}, \omega) = -\frac{1}{\sin \theta} \sum_{n,m} \varepsilon_n^m(\omega) \left( \frac{r}{a} \right)^{n-1} \frac{\partial Y_n^m}{\partial \phi} + \sum_{k,l} \iota_k^l(\omega) \left( \frac{a}{r} \right)^{(k+2)} \frac{\partial Y_k^l}{\partial \phi}. $$  \hspace{1cm} (2.24)$$
The concept of transfer functions

Note again that the representation of $\mathbf{B}$ given by eqs (2.22)–(2.24) is only valid in the source-free region above Earth’s surface, while the representation given by eq. (2.17) is also valid inside the conductor, e.g. at the sea bottom. The electric field is not a potential field; therefore, a representation analogous to eqs (2.22)–(2.24) is not possible for $\mathbf{E}$.

For completeness, a common special case of eqs (2.22)–(2.24) is introduced. If using the same indices for external and internal parts, the components of the magnetic field at Earth’s surface ($\mathbf{r} = \mathbf{r}_a$) are given by

\begin{align*}
B_r(\mathbf{r}_a, \omega) &= -\sum_{n,m} z^n_m(\omega) Y^n_m(\vartheta, \varphi), \\
B_\vartheta(\mathbf{r}_a, \omega) &= -\sum_{n,m} v^n_m(\omega) \frac{\partial Y^n_m(\vartheta, \varphi)}{\partial \vartheta}, \\
B_\varphi(\mathbf{r}_a, \omega) &= -\sum_{n,m} v^n_m(\omega) \frac{1}{\sin \vartheta} \frac{\partial Y^n_m(\vartheta, \varphi)}{\partial \varphi},
\end{align*}

with $z^n_m = n \varepsilon^n_m - (n + 1) v^n_m$, and $v^n_m = \varepsilon^n_m + i^n_m$.

\section*{2.3 The concept of transfer functions}

Transfer functions are mathematical representations of the relations between input and output signals of a system in the frequency-domain (Girod et al., 2001). By means of these functions, it is possible to determine the response of a system to a specified source. The concept is illustrated in Figure 2.1. Transfer functions are independent of the amplitude of the source, which makes their use advantageous in many applications. The term is often exclusively assigned to linear systems, for which the determination of transfer functions is simplified.

Due to the linearity of Maxwell’s equations with respect to the source, the conducting Earth itself can be seen as a linear system. Accordingly, there must also be a linear relation between the internal part of the potential $V^{\text{int}}$ (i.e., the “output” of the conducting Earth) and the external part $V^{\text{ext}}$ (i.e., its “input”; for a proof, see Egbert, 1987).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.1.png}
\caption{A system transforms an input signal into an output signal. Without knowledge of the physics, the only visible part of the system is its transfer function. By adding an appropriate physical model, it is possible to gain insight into the system’s properties from its transfer functions.}
\end{figure}
Following the notation of Egbert & Booker (1989), we can thus write

\[ V_{\text{int}}(r, \omega) = \mathcal{L}_\omega \left[ V_{\text{ext}}(r, \omega) \right]. \]  \hspace{1cm} (2.28)

The linear operator \( \mathcal{L}_\omega \) depends on frequency and on the conductivity structure. Let us illustrate the concept with a simple example. Assume that the geometry of the inducing source can be described by the single spherical harmonic \( Y^0_1 \). Also assume that conductivity in the Earth is only a function of depth. In this case, there is no transfer of energy to other spherical harmonics (Parkinson, 1983), and the double sums in eqs (2.19)–(2.20) collapse. This yields at Earth’s surface

\[ V_{\text{ext}}(r_\alpha, \omega) = a \varepsilon_0^1(\omega) Y^0_1(\vartheta, \varphi), \]  \hspace{1cm} (2.29)

\[ V_{\text{int}}(r_\alpha, \omega) = a \iota_0^1(\omega) Y^0_1(\vartheta, \varphi). \]  \hspace{1cm} (2.30)

Cancelling terms reveals that \( \mathcal{L}_\omega \) is in this case nothing but the scalar \( Q \)-response of degree 1,

\[ \iota_0^1(\omega) = Q_1(\omega) \varepsilon_0^1(\omega). \]  \hspace{1cm} (2.31)

The scalar \( Q \)-response is one of the most common transfer functions in global EM induction research and was already used by Chapman & Price (1930) and Lahiri & Price (1939), although its name was only established later.

In general, \( \mathcal{L}_\omega \) contains all information about electrical conductivity in the Earth that can be obtained from measurements on its surface (Egbert & Booker, 1989). Hence, the ultimate goal of EM studies must be to obtain as much information as possible about this operator. However, apart from very simple examples as the one above, a unique and complete determination of \( \mathcal{L}_\omega \) is not possible. This is mostly due to limited spatial and spectral data coverage. Moreover, a separation of input signals (EM fields due to primary, extraneous currents) and output signals (EM fields due to secondary, induced currents) is usually difficult, as measured EM fields contain contributions of both.

For a more practical treatment of the problem, Egbert & Booker (1989) introduced the response space. This concept is based on the assumption that the source geometry can be described by \( p \) independent spatial modes, or, in other words, that the space of source potentials has \( p \) degrees of freedom. This implies that the sum on the RHS of eq. (2.14) is finite and contains \( p \) non-zero coefficients \( \alpha_j, j = 1 \ldots p \). Suppose now that there is a complex-valued data vector \( \mathbf{f} \) that contains \( M \) time spectra of measured EM fields for a given frequency \( \omega \), with \( M > p \). The measurements can include both magnetic and electric fields at different sites and may be in an arbitrary order. In analogy to eq. (2.14), we can write

\[ \mathbf{f} = \sum_{j=1}^{p} \alpha_j \mathbf{u}_j, \]  \hspace{1cm} (2.32)
where the $u_j$ contain EM responses of the Earth. The vectors $u_j$ span the response space introduced by Egbert & Booker (1989). In matrix notation, eq. (2.32) reads

$$f = U\alpha,$$  \hspace{1cm} (2.33)

where $U$ is an $(M \times p)$-matrix consisting of the column vectors $u_j$, and $\alpha$ is a vector of length $p$ containing the $\alpha_j$. Let us now divide $f$ and $U$ into two parts,

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} \alpha,$$  \hspace{1cm} (2.34)

such that $f_1$ is of length $p$, $f_2$ is of length $(M - p)$, $U_1$ is of dimension $p \times p$, and $U_2$ is of dimension $(M - p) \times p$. Then

$$f_2 = U_2\alpha = U_2U_1^{-1}U_1\alpha = U_2U_1^{-1}f_1 = Tf_1.$$  \hspace{1cm} (2.35)

This derivation, which was presented in more detail in Egbert & Booker (1989), shows that all observables can be linearly mapped to the first $p$ observables. The linear mappings are assembled in a matrix $T$ and constitute the *inter-component* and *inter-station* transfer functions that are commonly applied in practice in EM induction research. For example, in MT the source is usually represented by $p = 2$ plane waves of different polarizations. A set of widely used transfer functions are the two elements of the so-called tipper, which relate the vertical component of the magnetic field to its two horizontal components.

### 2.4 Old and new transfer functions

#### 2.4.1 The $C$-response

At long periods (days to months) usually considered in global EM induction research, many studies rely on the $P_0^1$-assumption, i.e., they assume that the external magnetic potential can be described by the zonal harmonic $Y_0^1 = P_0^1 = \cos \vartheta$ in a coordinate system aligned with the geomagnetic axis. Hence, $p = 1$, implying the existence of transfer functions connecting any two field components. The long periods impede the use of electric data: As apparent from eq. (2.13), the electric field vanishes as frequency decreases. Moreover, $Y = B_\varphi = 0$ in a 1-D Earth excited by a $P_0^1$-source (cf. eq. 2.27), such that it is of little use for induction studies (although a transfer function involving $Y$ was proposed by Fujii & Schultz (2002) to detect lateral conductivity heterogeneities).

It is thus natural to devise a transfer function connecting $Z = -B_r$ and $X = -B_\vartheta$. This was first done by Banks (1969) and later on referred to as $Z/H$ method (as the horizontal magnetic variation $H$ equals $X$ under the given assumptions). By means of a
simple scaling, this transfer function becomes equivalent to the $C$-response (Schmucker, 1970; Weidelt, 1972), which is then given by

$$C(r_a, \omega) = -\frac{a \tan \vartheta}{2} \frac{B(r_a, \omega)}{B_\vartheta(r_a, \omega)} = -\frac{a \tan \vartheta}{2} \frac{Z(r_a, \omega)}{X(r_a, \omega)}.$$  \hfill (2.36)

The $C$-response is widely applicable and intuitively understood, as its real part corresponds to the centre depth of the induced currents and thereby is indicative of the depth to which EM fields (of a given period) can penetrate (Weidelt, 1972).

In contrast to the $Q$-response (eq. 2.31), which reflects the globally laterally averaged conductivity, the $C$-response can be used to sense the 1-D conductivity profile at a specific location. It is easily shown that $C$-responses are the same everywhere on the surface of a 1-D Earth. In other words, spatial variations of $C$-responses estimated with the $Z/H$ method reflect either conductivity heterogeneities or a violation of the $P_0^1$-assumption (or even both).

While the $Z/H$ method remains popular in global and large-scale regional EM induction studies, there has long been evidence for a more complex structure and asymmetry of the magnetospheric ring current (e.g. Daglis & Kozyra, 2002; Balasis et al., 2004; Olsen & Kuvshinov, 2004; Balasis & Egbert, 2006). The recovered conductivity structures, both in 1-D and 3-D studies, might thus be contaminated by errors originating from an inaccurate description of the source. I will demonstrate the vulnerability of $C$-responses in an environment with a complex source structure in Section 3.1.

The finding that the magnetospheric source might be more complex than commonly assumed stimulates the invention of new, alternative transfer functions that can handle such a source. But before proposing such alternatives, let me formulate general criteria for EM transfer functions. First of all, an EM transfer function must be highly sensitive to induction processes. It should show strong correlations between its input and output channels to ensure that all sources have been taken into account. For generality, it should be applicable in 3-D environments, and 3-D structures should be apparent in the estimated transfer function.

Which of these criteria does the $C$-response fulfil? Since its estimation with the $Z/H$-method involves the $Z$-component of magnetic variations, the $C$-response is highly sensitive to induction processes. $C$-responses may be applicable in 3-D environments, but whether the subsurface is 1-D, 2-D, or 3-D is usually not readily apparent in $C$-responses, just like in other scalar transfer functions. Finally, the $Z/H$-method is based on the assumption that $p = 1$. This can make a reliable interpretation of the estimated transfer function in terms of conductivity very difficult.
2.4.2 New transfer functions for global induction studies

In MT, the impedance tensor (e.g. Simpson & Bahr, 2005) has many of the desired properties stated above. It thus seems natural to also devise arrays of transfer functions for global induction studies. A consistent treatment can be envisioned by a 3-D modification of eq. (2.31), which reads

\[ \iota_{k}^{l}(\omega) = \sum_{n,m} Q_{kn}^{lm}(\omega) \varepsilon_{n}^{m}(\omega). \]  

(2.37)

\( Q_{kn}^{lm} \) is a two-dimensional array of transfer functions that was discussed before by Olsen (1999). In the following, I will refer to it as “matrix \( Q \)-response” or “\( Q \)-matrix”. The diagonal elements of this matrix mostly describe the bulk conductivity and the stratification of the subsurface – in case of a layered (1-D) Earth, they are equivalent to the scalar \( Q \)-responses. The off-diagonal elements describe a transfer of energy to coefficients of different degree and order, which only occurs if the subsurface has 3-D structure.

In practice, an estimation of the \( Q \)-matrix hinges on the precise determination of induced fields in a spherical harmonic representation. This requires a very good global data coverage, which can to date only be provided by satellite missions. I will discuss the estimation and inversion of the \( Q \)-matrix in Section 6.5.

Ground-based measurements taken at irregularly distributed geomagnetic observatories require a different approach. To this purpose, let us re-examine eq. (2.17). The \( B_{n}^{m} \) on the RHS of the equation are responses of the Earth to excitation by unit scale spherical harmonic sources; their components hence represent EM transfer functions. For the vertical component, we can write

\[ Z(r, \omega) = \sum_{n,m} \varepsilon_{n}^{m}(\omega) T_{n}^{m}(r, \omega). \]  

(2.38)

\( T_{n}^{m}(r, \omega) \) is a transfer function relating the \( Z \)-component of the magnetic variation at the measuring site to the source coefficient \( \varepsilon_{n}^{m}(\omega) \). The \( T_{n}^{m} \) form a one-dimensional, potentially infinite array. In practice, its size is limited by the number of external SHE coefficients that can be determined.

For ground-based magnetic observatories \( (r = a) \), the \( T_{n}^{m} \) are readily related to the \( Q \)-matrix as

\[ T_{n}^{m}(r_{a}, \omega) = nY_{n}^{m}(\theta, \varphi) - \sum_{k,l} (k + 1) Q_{kn}^{lm}(\omega) Y_{k}^{l}(\theta, \varphi), \]  

(2.39)

which is easily verified from eqs (2.22), (2.37) and (2.38). In contrast to the \( Q \)-matrix, the \( T_{n}^{m} \) make use of local information on conductivity structure and are thus suitable transfer functions in case of sparse and irregularly distributed observations.
The above equations are in particular also valid if the $P_1^0$-assumption holds and conductivity only depends on depth. $T_1^0$ is in this case related to the $C$- and $Q$-responses,

$$T_1^0(\vartheta, \omega) = \frac{3C(\omega)}{a + C(\omega)} \cos \vartheta = (1 - 2Q_1(\omega)) \cos \vartheta. \quad (2.40)$$

In the zero-order-approximation $|C| \ll a$ in the considered period range; therefore, $T_1^0$ is roughly proportional to $C$. We can expect a similarity in shape even if $\varepsilon_1^0$ is not the only, but the dominating source coefficient. In contrast to $C$, all $T_m^n$ vary with geographical location by definition. Note also that while estimating $C$ is a univariate problem, estimating the $T_m^n$ is generally a multivariate problem (see next section).

For the horizontal components of the magnetic variation, $X = -B_\vartheta$ and $Y = B_\varphi$, we can analogously define

$$X(r, \omega) = \sum_{n,m} \varepsilon_n^m(\omega) U_n^m(r, \omega) \quad (2.41)$$

and

$$Y(r, \omega) = \sum_{n,m} \varepsilon_n^m(\omega) V_n^m(r, \omega). \quad (2.42)$$

In case of ground-based magnetic observations, $U_n^m$ and $V_n^m$ relate to the $Q$-matrix as

$$U_n^m(r_a, \omega) = \frac{\partial Y_n^m(\vartheta, \varphi)}{\partial \vartheta} + \sum_{k,l} Q_{kn}^m(\omega) \frac{\partial Y_k^l(\vartheta, \varphi)}{\partial \vartheta} \quad (2.43)$$

and

$$V_n^m(r_a, \omega) = -\frac{i}{\sin \vartheta} \left[ mY_n^m(\vartheta, \varphi) + \sum_{k,l} lQ_{kn}^m(\omega) Y_k^l(\vartheta, \varphi) \right]. \quad (2.44)$$

This is easily verified from eqs (2.23)–(2.24), (2.37) and (2.41)–(2.42). Note that $U_n^m$ and $V_n^m$ were mainly introduced for completeness. In practice, these transfer functions do not prove very beneficial for a recovery of conductivity structure. Since they only involve the horizontal components of the magnetic variation, $U_n^m$ and $V_n^m$ are not very sensitive to induction processes. The proposed new ground-based transfer functions $T_n^m$, $U_n^m$ and $V_n^m$ are analysed in Section 3.2.

Another source of EM data are abandoned submarine telecommunication cables. The voltage induced in these cables is indicative of the distribution of electrical conductivity underneath. In previous studies (e.g. Koyama et al., 2006; Shimizu et al., 2010a), cable voltage data were combined with magnetic data from nearby observatories to estimate long-period impedances. The estimation of impedances, however, relies on the plane-wave assumption, i.e. $p = 2$. A more consistent treatment can be envisioned in analogy to the proposed ground-based transfer functions. If $U$ is the voltage induced in a cable
we can define transfer functions \( K_n^m \) as
\[
U(c, \omega) = \sum_{n,m} K_n^m(c, \omega) \varepsilon_n^m(\omega).
\] (2.46)

Transfer functions \( K_n^m \) will be analysed in Section 3.3.

The transfer functions introduced above are not only applicable to geomagnetic variations at periods >1 day, as investigated in this study, but also to the \( Sq \) variations at periods <1 day. The \( Sq \) source system is spatially complex, requiring a large number of spherical harmonics for an adequate description (cf. Appendix B). The transfer functions \( T_n^m \) were used for an analysis of the \( Sq \) variations by Guzavina et al. (2015).

2.5 Multivariate analysis

In the context of EM sounding research, usually not more than two transfer functions are estimated for a single field component. In MT, for instance, the horizontal components of magnetic and electric fields are related to each other by a \( 2 \times 2 \)-matrix \( Z \), which is known as impedance tensor:
\[
\begin{bmatrix}
E_x \\
E_y
\end{bmatrix} =
\begin{bmatrix}
Z_{xx} & Z_{xy} \\
Z_{yx} & Z_{yy}
\end{bmatrix}
\begin{bmatrix}
B_x \\
B_y
\end{bmatrix}.
\] (2.47)

This accordingly involves the determination of two transfer functions per (output) field component (e.g. \( Z_{xx} \) and \( Z_{xy} \) for \( E_x \)). The same is the case for the tippers (induction arrows) mentioned above.

One of the exceptions is the methodology of Schmucker (2003b), which combines gradient sounding and geomagnetic depth sounding, and which involves the determination of five transfer functions for one (vertical) magnetic field component. In the general case of a source with \( p \) degrees of freedom, \( p \) transfer functions need to be determined for each output channel. The output channel may be an internal coefficient \( \iota^I_k \) as in eq. (2.37), a component of the magnetic field as in eq. (2.39), or a voltage as in eq. (2.46).

In order to simultaneously estimate \( p \) transfer functions from EM data, I developed a multivariate data analysis tool based on the section-averaging approach (e.g. Olsen, 1998) and iteratively re-weighted least squares (e.g. Aster et al., 2005). In the following, two methods are presented and compared – the conventional (single-frequency) approach and the multi-frequency approach.
2.5.1 Conventional approach

Let us denote the \( p \)-dimensional vector of input signals as \( x(t) \) and the output signal as \( y(t) \). In general there might be more than one output signal, but transfer functions are estimated independently for each of them. In the conventional (single-frequency) approach, an array of transfer functions \( T(\omega) \) is estimated individually for each frequency of interest \( \omega \) with the section-averaging approach (Olsen, 1998):

1. Cut the full time series (of input channels \( x(t) \) and output channel \( y(t) \)) into \( N \) segments of length \( s = \gamma T \), where \( T = 2\pi/\omega \) is the period of interest, and \( \gamma \) is an integer >1:

\[
x(t), y(t) \rightarrow x_i(\tau), y_i(\tau), \quad i = 1 \ldots N.
\] (2.48)

Small \( \gamma \) increase \( N \), which reduces the uncertainty of the estimate, but also increase the spectral leakage (see next step). Tests revealed that a choice of \( 3 \leq \gamma \leq 10 \) usually constitutes a good compromise. The segments may partially overlap.

2. Multiply the time series of each segment with a window function to decrease the spectral leakage (e.g. Harris, 1978):

\[
x_i^\eta(\tau) = x_i(\tau) \eta(\tau), \quad y_i^\eta(\tau) = y_i(\tau) \eta(\tau).
\] (2.49)

This step is known as tapering.

3. Perform a Fourier transform on each segment:

\[
\begin{align*}
x_i(\omega) &= \int_{-\infty}^{\infty} x_i^\eta(\tau) e^{i\omega \tau} d\tau, \\
y_i(\omega) &= \int_{-\infty}^{\infty} y_i^\eta(\tau) e^{i\omega \tau} d\tau.
\end{align*}
\] (2.50)

Note that \( x_i(\omega) \) and \( y_i(\omega) \) are complex-valued quantities.

4. Assuming a linear relationship between \( x_i(\omega) \) and \( y_i(\omega) \), assemble a linear system of equations:

\[
\begin{bmatrix}
Y_1(\omega) \\
Y_2(\omega) \\
\vdots \\
Y_N(\omega)
\end{bmatrix} =
\begin{bmatrix}
X_1^{(1)}(\omega) & \cdots & X_1^{(p)}(\omega) \\
X_2^{(1)}(\omega) & \cdots & X_2^{(p)}(\omega) \\
\vdots & \ddots & \vdots \\
X_N^{(1)}(\omega) & \cdots & X_N^{(p)}(\omega)
\end{bmatrix}
\begin{bmatrix}
T^{(1)}(\omega) \\
\vdots \\
T^{(p)}(\omega)
\end{bmatrix} +
\begin{bmatrix}
\delta Y_1(\omega) \\
\vdots \\
\delta Y_N(\omega)
\end{bmatrix}
\] (2.51)

\( T(\omega) = [T^{(1)}(\omega) \ldots T^{(p)}(\omega)]^\top \) is the \( p \)-dimensional complex-valued vector of transfer functions relating input and output quantities, and \( \delta Y(\omega) = [\delta Y_1(\omega) \ldots \delta Y_N(\omega)]^\top \) is the vector of residuals. In matrix notation, eq. (2.51) can be written as

\[
Y = XT + \delta Y.
\] (2.52)
Note that the dependency on $\omega$ was omitted for the simplicity of presentation.

5. Solve the linear system of equations (2.52). If using regular least-squares, the solution is given by

$$\hat{T}_{\text{lsq}} = \left[ X^\dagger X \right]^{-1} X^\dagger Y$$

(2.53)

where $\hat{T}_{\text{lsq}}$ is a least-squares estimate of $T$, and superscript $\dagger$ denotes the complex conjugate (hermitian) transpose. The least-squares solution, however, is known to be strongly affected by outliers in the data. A robust least-squares algorithm (e.g. Aster et al., 2005) can minimize the effect of such outliers on the solution. This algorithm consists of the repeated solution of a modified system of equations, in which a weighting matrix $W$ is introduced. $W$ is a diagonal matrix, containing weights based on the residuals obtained in the previous iteration. The solution of a such weighted system (in iteration $j$) is

$$\hat{T}_{\text{rob}}^{(j)} = \left[ X^\dagger W^{(j)} X \right]^{-1} X^\dagger W^{(j)} Y.$$  

(2.54)

Eq. (2.54) is solved repeatedly with updated weighting matrix $W$ until convergence is reached.

The section-averaging approach does not only yield an estimate of the transfer functions, but also provides the framework for an analysis of uncertainties. An estimation of uncertainties is crucial to investigate the reliability of the estimated transfer functions. This is particularly important if the latter are supposed to be used in the context of a subsequent inversion for electrical conductivity.

Schmucker (2003a) pointed out that in the case of multivariate analyses with more than 3 unknowns, only jackknife estimates can handle bias errors due to noise in the input variables. I apply the jackknife method as outlined by Chave & Thomson (1989). By omitting in the (potentially robust) least-squares analysis one event after the other, $N$ estimates of $\hat{T}$ are obtained from $N - 1$ events each. Let us define $\hat{T}^{(i)}$ as the leave-one-out estimate obtained by omitting the $i$-th event. The arithmetic average of the leave-one-out estimates is calculated as

$$\bar{T} = \frac{1}{N} \sum_{i=1}^{N} \hat{T}^{(i)},$$

(2.55)

and the jackknife mean is given by

$$\hat{T}_{\text{jk}} = N \bar{T} - (N - 1) \hat{T}.$$  

(2.56)
The jackknife covariance matrix is calculated as
\[ \hat{C}_{jk} = \frac{N - p}{N} \sum_{i=1}^{N} (\hat{T}^{(i)} - \bar{T})(\hat{T}^{(i)} - \bar{T})^\dagger. \] (2.57)

Confidence limits for the estimated transfer functions can be obtained from the diagonal elements of the covariance matrix \( \hat{C} \) using \( t \)-statistics (Aster et al., 2005). In contrast to the elements of \( \hat{T} \), the confidence limits are real-valued. Note that the standard estimate \( \hat{T} \) and the jackknife estimate \( \hat{T}_{jk} \) are usually very similar; the jackknife approach is thus in first place suitable for an estimation of covariances.

An important quantity in regression analysis is the coefficient of determination \( R^2 \). It measures the proportion of the output quantity that can be explained by the considered input quantities. Let us first define \( \bar{Y}_i = X_i^\top \hat{T} \) as the predicted output for input \( X_i \), based on the estimated transfer functions \( \hat{T} \). Furthermore,
\[ \bar{Y} = \frac{1}{N} \sum_{i=1}^{N} Y_i, \] (2.58)
is the sample mean of the output quantity \( Y \). The total variation in \( Y \) is measured by the total sum of squares,
\[ SS_Y = \sum_{i=1}^{N} |Y_i - \bar{Y}|^2, \] (2.59)
which is, apart from a factor, nothing but the sample variance. Part of this variation may be explained by a variation of the input quantities, with which \( Y \) correlates, the remaining part is explained by random fluctuations (uncorrelated noise) or dependency on other sources not taken into account (correlated noise). The variation due to noise is measured by the residual sum of squares,
\[ SS_R = \sum_{i=1}^{N} |Y_i - \bar{Y}_i|^2. \] (2.60)
Eqs (2.59)–(2.60) have here been written for the case of regular (non-weighted) least-squares. If a robust least-squares method is employed, the summands in both equations are weighted by the corresponding value in the weighting matrix \( W \). In any case, however, the coefficient of determination is defined as
\[ R^2 = 1 - \frac{SS_R}{SS_Y} \] (2.61)
and by this definition varies between 0 (no correlation) and 1 (perfect correlation). In linear regression problems as considered here, \( R^2 \) is equivalent to the correlation coefficient. Another common quantity in signal processing is the squared coherency (Bendat
& Piersol, 2010). In the case considered here, the \textit{multiple} squared coherency $\text{coh}^2_{\text{mult}}$ is also equivalent to $R^2$, while the \textit{ordinary} squared coherency $\text{coh}^2$ is defined analogously for only one specific input signal.

2.5.2 Multi-frequency approach

EM transfer functions are usually estimated for a number of logarithmically spaced frequencies $N_\omega$, which are believed to be representative for the full set of frequencies contained in the data. While the single-frequency approach yields independent estimates for each of these frequencies, the newly developed multi-frequency approach solves the linear system of equations (2.52) simultaneously for all $N_\omega$ frequencies. This in particular implies a large, sparse system matrix, which in diagonal blocks contains the $X(\omega)$ for all considered frequencies $\omega$. Solving this large system is mathematically equivalent to solving $N_\omega$ small systems (2.52), but computationally more expensive. The advantage of this method is the possibility to impose additional constraints on the solution.

Bailey (1969) stated that the inverse Fourier transform of the scalar $Q$-response (eq. 2.31) must be a causal response function, since there cannot be an internal signal $\eta^m_n$ prior to excitation by $e^m_n$. An analogous reasoning holds for the array transfer functions introduced in Section 2.4. Causal response functions are analytic and bounded function of $\omega$ everywhere in the upper half of the complex $\omega$-plane (and in particular on the positive part of the real axis; e.g. Landau & Lifshitz, 1958). This theoretical finding coincides with the observation that EM transfer functions vary smoothly with respect to frequency (or its logarithm) for any realistic conductivity distribution.

The multi-frequency approach makes use of this additional information and requires the estimated transfer functions to vary smoothly with frequency by minimizing their second derivative with respect to $\log_{10}(\omega)$. Let $\mathbf{Y}$ be a vector containing the output signal $Y(\omega)$ for all $\omega$ (in increasing order), and let $\mathbf{X}$ be the system matrix containing the input signals $X(\omega)$ for all $\omega$ in diagonal blocks. The vector of transfer functions is denoted by $\mathbf{T}$. The system of equations (2.52) then reads

$$\mathbf{Y} = \mathbf{X} \mathbf{T} + \delta \mathbf{Y},$$

and its least-squares solution is analogous to eq. (2.53). Let us now define a regularization matrix $\mathbf{L}$ that connects the $T(\omega)$ of different frequencies $\omega$ and minimizes their second derivatives with respect to $\log_{10}(\omega)$. With a regularization parameter $\lambda > 0$, the solution of the regularized least squares problem (e.g. Aster et al., 2005) reads

$$\hat{\mathbf{T}}_{\text{lsq}} = \left[ \mathbf{X}^\dagger \mathbf{X} + \lambda \mathbf{L}^\dagger \mathbf{L} \right]^{-1} \mathbf{X}^\dagger \mathbf{Y}.$$  \hspace{1cm} (2.63)
Combining the regularization with the above-mentioned robust least squares algorithm finally yields the estimate

$$\hat{T}^{(j)}_{rob} = \left[ X^\dagger W^{(j)} X + \lambda L^\top L \right]^{-1} X^\dagger W^{(j)} Y, \quad (2.64)$$

where $W$ is again a diagonal weighting matrix. The optimum amount of smoothing (determined by the value of $\lambda$) can be found by using an L-curve approach (Hansen, 1992). This approach relates a norm of the data misfit,

$$\psi_d = (Y - X\hat{T})^\dagger (Y - X\hat{T}), \quad (2.65)$$

to a norm of the smoothness of the responses,

$$\psi_m = (L\hat{T})^\dagger (L\hat{T}). \quad (2.66)$$

The optimum solution minimizes both norms.

Uncertainties of the transfer functions are estimated with the jackknife method outlined above, cf. Section 2.5.1. The results, however, have to be analysed with care. The enforced smoothness of the solution decreases the spread of the leave-one-out estimates. This leads to an overall decrease of the estimated uncertainties. In turn, covariances between estimates at neighbouring frequencies are generated.

### 2.5.3 Comparison of two approaches

The two approaches presented above can be applied to any kind of EM data. For a preliminary comparison, I estimated $C$-responses with the $Z/H$-method according to eq. (2.36) from 16 years (1997–2012) of magnetic measurements taken at the observatory Irkutsk (IRT). A robust least-squares algorithm was employed, and uncertainties were estimated with the jackknife approach. Figure 2.2 shows the results. As expected,
the $C$-responses obtained with the multi-frequency approach vary more smoothly with frequency, which is due to the applied regularization. More features of the $C$-responses will disappear if the amount of regularization is increased. In line with the expectations, uncertainties are generally smaller.

The results obtained with the multi-frequency approach look ‘nicer’, but at least for the considered example, the effect does not seem to be significant. The differences are mostly within uncertainties obtained in the conventional approach. Considering that usually, a large variety of conductivity distributions can explain the estimated transfer functions within uncertainties, it is unlikely that the differences will have any relevant effect in an inversion. Since the conventional approach is computationally cheaper and error estimates are more reliable, I will use it for further investigations. I will, however, get back to the multi-frequency approach when estimating matrix $Q$-responses in Section 6.5.

### 2.5.4 A multivariate processing code

To estimate transfer functions from different types of EM data, I developed a multivariate data processing software in MATLAB. It is based on a conventional univariate processing code by Olsen (1998), which was originally designed to estimate $C$-responses. The new code can estimate both scalar and array transfer functions from any kind of EM data. Parameters such as period range, period spacing or the value of $\gamma$ can be defined in a separate parameter file. The code can handle gaps in the input/output time series. Different methods for estimating uncertainties are implemented, in particular also the jackknife approach outlined above. Transfer functions can be estimated with regular least-squares and different robust methods, but also with total least squares (e.g. Golub & van Loan, 1980) and repeated medians (Smirnov, 2003). A separate version of the code employs the multi-frequency approach outlined above. Another separate version features the use of a remote reference station for processing of field data. The code is documented in a user manual.
Chapter 3

Indications for a Complex Source

3.1 Variability of $C$-Responses

As mentioned in Section 1.2, many classical and modern global EM induction studies are based on the $P_1^0$-assumption. The authors of these studies hence assumed that the inducing source at periods $>1$ day is well-approximated by a symmetric ring current around the geomagnetic equator ($p = 1$). This permits the use of the $Z/H$-method for estimating $C$-responses, first proposed by Banks (1969). In this chapter, the validity of the $P_1^0$-assumption is investigated by an analysis of observatory magnetic data. Large parts of the chapter closely follow the paper by Püthe et al. (2015a).

![Figure 3.1: Variability of observed $C$-responses, estimated at 77 mid-latitude observatories with the $Z/H$-method from 16 years of observatory data (1997–2012). The solid lines indicate the theoretical prediction, corresponding to the 1-D conductivity profile derived from satellite data by Kuvshinov & Olsen (2006). The top panel shows squared coherencies.](image-url)
3.1.1 Observed variability

C-responses were estimated from 16 years of observatory data (1997–2012) with the \( Z/H \)-method. The results for 77 observatories, located at geomagnetic latitudes between \( \pm 10^\circ \) and \( \pm 55^\circ \), are shown in Figure 3.1. If the source was perfectly described by the first zonal harmonic and if conductivity depended only on depth, the derived \( C \)-responses at a given frequency should be the same everywhere at Earth’s surface (indicated by the solid black lines). However, Figure 3.1 reveals a huge variability both in the real and the imaginary part of \( C \) at all periods.

The top panel of Figure 3.1 shows squared coherencies between \( Z \) and \( X \) for all observatories. Average coherencies (of all observatories) increase from <0.5 at short periods to a maximum of 0.7 at a period of 32 days. Coherencies drop slightly at longer periods. This observation reveals that a significant proportion of the variations in \( Z \) cannot be explained by variations in \( X \). This challenges the assumption of \( p = 1 \).

As a measure of the uncertainties, which vary strongly between different observatories, the 90\% confidence interval is used – for clarity of presentation we, however, do not show it in Figure 3.1. The mean of the confidence interval (at all observatories) increases from about 100 km at a period of 2 days to about 180 km at a period of 32 days. It is thus in this period range considerably smaller than the overall variability of both the real and the imaginary part of \( C \) (cf. Figure 3.1). For longer periods, the mean of the confidence interval clearly exceeds 200 km and becomes comparable to the overall variability. Hence, a part of the observed variability might be explained by measurement uncertainties. However, particularly for periods <32 days, the variability is too large to be explained solely by (uncorrelated) noise in the data.

3.1.2 Numerical modelling

In order to analyse the origin of the observed variability, we tried to reproduce the pattern shown in Figure 3.1 numerically. To this purpose, we computed \( C \)-responses with the \( Z/H \)-method from synthetic magnetic data. The data were generated by simulating induction due to a complex magnetospheric source (including higher-degree terms \( \varepsilon_{mn}^m \) in addition to \( \varepsilon_1^1 \)) in a 3-D conductivity model.

The chosen conductivity model consists of a thin spherical shell of laterally variable conductance at Earth’s surface (with a resolution of \( 1^\circ \times 1^\circ \)), and a radially symmetric (1-D) conductivity structure underneath. The shell conductance is obtained by considering contributions both from seawater and sediments. The conductance of seawater was taken from Manoj et al. (2006) and accounts for ocean bathymetry, ocean salinity, temperature and pressure. The conductance of the sediments (in continental as well as oceanic regions) is based on the global map of sediment thickness of Laske & Masters (1997) and is calculated by a heuristic procedure similar to that described in Everett et al. (2003). The
The inducing source is described by coefficients $\varepsilon_n^m$ of the SHE of the magnetic field due to signals of magnetospheric origin. These coefficients were recovered from observatory magnetic data with the following algorithm:

- Numerical simulation of EM induction in a given conductivity model (Figure 3.2) due to unit amplitude spherical harmonic sources in frequency domain at a set of logarithmically spaced frequencies $\omega_j$. To this purpose, we use the x3dg code (Kuvshinov, 2008), which is based on a contracting integral equation approach (Pankratov et al., 1995). The calculations yield model responses to unit scale spherical harmonic sources at Earth’s surface, termed $B_n^m(r_a, \omega_j)$.

- Calculation of scalar $Q$-responses $Q_n(\omega_j)$ from the $B_n^m(r_a, \omega_j)$. This calculation involves eq. (6.44), which will be introduced in Section 6.2.3.

- Collection of magnetic data from all available observatories at mid-latitudes and removal of core and crustal field by fitting the data with a low-degree polynomial.

- The horizontal components of the measured magnetic variations can be represented by eqs (2.26)–(2.27). In vector notation, the time domain equivalents of these equations can be combined to

\[
B_r(r_a, t) = - \sum_{n,m} v_n^m(t) \nabla_{\perp} Y_n^m(\vartheta, \varphi), \tag{3.1}
\]
Variability of C-Responses

Figure 3.3: Time series of the external coefficients $q^m_n$, $s^m_n$ (in nT) that describe the source in our model study. Ticks indicate January 1 of the respective years. Note that the real coefficients $q^m_n(t)$, $s^m_n(t)$ shown in this figure are related to the complex coefficients $\varepsilon^m_n(t)$ in the following way: $\varepsilon^m_n = (q^m_n - is^m_n)/2$ if $m > 0$, $\varepsilon^m_n = (q^m_n + is^m_n)/2$ if $m < 0$, and $\varepsilon^0_n = q^0_n$. Also note the different scales of the individual plots.

where subscript $\tau$ denotes the horizontal part of $B$ and $\nabla_\perp$ is the angular part of the gradient operator. The linear system of equations (3.1) is solved for the unseparated coefficients $v^m_n$ for each instant $t$.

- Fourier transformation of the unseparated coefficients, yielding $v^m_n(\omega)$.
- Spectral interpolation of $Q_n$ to the full set of frequencies contained in the data.
- Separation of external and internal contributions with the formula

$$
\varepsilon^m_n(\omega) = \frac{v^m_n(\omega)}{1 + Q_n(\omega)},
$$

which follows from the definition of $v^m_n$ and eq. (2.31).

- Inverse Fourier transform, yielding time series $\varepsilon^m_n(t)$.

A more consistent method involves the solution of the system of linear equations (2.17). It was e.g. applied by Olsen & Kuvshinov (2004) and Koch & Kuvshinov (2015). This method, however, is only applicable if there are no gaps in the data, since the time spectra $B(\omega)$ can only be computed if the time series $B(t)$ are complete. In a different context, we found that both methods yield very similar source models.

The above algorithm was applied to 16 years of observatory hourly means (1997–2012). We chose to recover 9 low-degree SHE coefficients $\varepsilon^m_n$ ($n \leq 3$, $|m| \leq 1$).
Indications for a Complex Source

Figure 3.4: Power spectral density of the external coefficients $\varepsilon_{m}^{n}$, which were derived from 16 years of observatory data. Here, the power spectral density is defined as $P(\varepsilon_{m}^{n}(\omega)) = |\varepsilon_{m}^{n}(\omega)|^2$.

choice does not have any physical basis; it was merely made to mimic a complex source. Note also that the recovered coefficients constitute a mix of signals of magnetospheric origin (related to magnetic storms) and of ionospheric origin (daily $Sq$ variations and seasonal cycle). For the computation of synthetic $C$-responses, we used subsets of 4.5 years of the recovered coefficient time series (July 1998 – December 2002), which are depicted in Figure 3.3.

Power spectra of the estimated coefficients are shown in Figure 3.4. Clear peaks are visible at 1 day and its harmonics, reflecting the daily $Sq$ variations – with, as expected, most energy in coefficient $\varepsilon_{1}^{0}$ (cf. Appendix B). Further distinct peaks are apparent at 1 year (and its second harmonic), with most energy in coefficient $\varepsilon_{0}^{2}$. The seasonal variations are also well visible in the time series (Figure 3.3). Both daily and yearly variations are of ionospheric origin and are known to be due to a complicated source. We are, however, interested in periods between 1 day and 100 days, in which magnetic variations are mostly of magnetospheric origin. In this period range, coefficient $\varepsilon_{0}^{1}$ has most energy, as apparent from both Figure 3.3 and Figure 3.4. The dominance of $\varepsilon_{0}^{1}$ increases with period; for periods $>10$ days, other coefficients seem to be negligible. This appearance will be tested in the following.

Given the $\mathbf{B}_{m}^{n}(r_{a},\omega_{j})$ and the time spectra of the $\varepsilon_{m}^{n}$, synthetic $C$-responses at sites of interest $r_{s}$ can be calculated in the following way:
Variability of C-Responses

- Spatial interpolation of the $B_n^m(r_a, \omega_j)$ to the sites of interest, yielding $B_n^m(r_s, \omega_j)$.
- Spectral interpolation of $B_n^m$ to the full set of frequencies contained in the data, yielding $B_n^m(r_s, \omega)$.
- Computation of magnetic field time spectra at site $r_s$ with eq. (2.17).
- Inverse Fourier transformation, yielding time series $B(r_s, t)$.
- Estimation of C-responses from time series of $B_r$ and $B_\theta$ with the Z/H-method, cf. eq. (2.36), using the data processing algorithm outlined in Section 2.5.4.

We generated synthetic datasets for each of the following four cases:

(a) Induction due to a simplified source (only coefficient $\varepsilon_1^0$) in the 1-D model (i.e. the profile shown in the right part of Figure 3.2 without the surface shell).

(b) Induction due to a simplified source (only coefficient $\varepsilon_1^0$) in the 3-D model. With this case we study the influence of the “ocean effect”.

(c) Induction due to a complex source (described by nonzero coefficients $\varepsilon_n^m, n \leq 3, |m| \leq 1$) in the 1-D model. With this case we study the influence of the “source effect”.

(d) Induction due to a complex source in the 3-D model. This case contains both ocean effect and source effect.

Figure 3.5 presents, next to the observed C-responses already shown in Figure 3.1, the estimated C-responses for the simulated cases (b)–(d), as well as squared coherencies between $Z$ and $X$. We only show results for the 77 mid-latITUDE observatories of Figure 3.1. Outside this latitude range, the estimation of C-responses with the Z/H-method becomes unstable, i.e. already minor violations of the assumptions can lead to large errors. This becomes apparent when analysing eq. (2.36): At the equator ($\vartheta = 90^\circ$), a vanishing $Z$ must compensate for $\tan \vartheta$ approaching infinity, while at the poles ($\vartheta = 0^\circ$, resp. $180^\circ$), a vanishing $X$ must compensate for $\tan \vartheta$ approaching zero.

Figure 3.5b corresponds to case (b) and shows results obtained by simulating induction due to $\varepsilon_1^0$ in the given 3-D model. It thus presents the variability of C-responses due to the ocean effect. The variability is very large for short periods, spanning more than 1000 km at a period of 2 days. As expected, it decreases with increasing period, since longer periods sample deeper regions of the Earth and are thus less affected by heterogeneities in the top layer. The variability of C-responses due to the ocean effect is discussed in detail by Semenov & Kuvshinov (2012). The coherency is equal to one, because $p = 1$ is fulfilled and there is no noise in the synthetic data.
Figure 3.5: Variability of observed (a) and modelled (b)–(d) C-responses for the locations of 77 observatories at geomagnetic latitudes between $\pm 10^\circ$ and $\pm 55^\circ$. (b) Variability due to the ocean effect. (c) Variability due to a complex source. (d) Variability due to ocean and source effect. The black lines in all plots denote, as a reference, the globally uniform C-response corresponding to the 1-D model that has been excited by $\varepsilon_0^1$.

Figure 3.5c, corresponding to case (c), shows results obtained by simulating induction due to the full set of spherical harmonic sources in the corresponding 1-D model. It thus presents the variability of the responses due to source structures other than $Y_1^0$. The real part of the responses (Re $C$) seems to be slightly more affected than the imaginary part (Im $C$). A variability in Re $C$ of about 500 km is apparent for virtually the entire period range. For periods $>10$ days, the variability of Re $C$ due to source effects becomes dominant over the variability due to the ocean effect. For Im $C$, the source effect variability dominates over the ocean effect variability only at periods $>40$ days. It is interesting to note that the variability due to a complex source is almost independent of period, although the dominance of $\varepsilon_1^0$ increases with period (Figure 3.4). We do not have an obvious explanation for this result.

Figure 3.5d, corresponding to case (d), shows results obtained by simulating induction due to the full set of spherical harmonic sources in the 3-D model. With this simulation, we want to mimic the situation on the Earth. The synthetic $C$-responses show a large variability, explaining a major part of the variability in the observed $C$-responses (Figure 3.5a). The low coherencies indicate that the output variable $Z$ cannot fully be
described by the input variable $X$ and thus confirms that $p \neq 1$. This is an example of correlated noise due to undescribed sources (e.g. Egbert & Booker, 1989). The coherencies of the modelling results are, however, still substantially larger than those of the observed $C$-responses, indicating that there are even more sources of noise than those derived by us.

Spatial patterns of both source and ocean effect can be analysed by plotting global maps of $C$-responses, as presented in Figure 3.6. We show the real and the imaginary part for three selected periods (2.0 days, 13.6 days and 91.3 days). The panels of Figure 3.6 correspond to the cases (a)–(d) presented above. As a reference, Figure 3.6a shows the $C$-responses computed in a 1-D model that was excited by $\varepsilon_1^0$. As expected, the responses

Figure 3.6: Maps of modelled $C$-responses (in km) for periods of 2.0 days, 13.6 days and 91.3 days, respectively. Top: real part, bottom: imaginary part of $C$. (a) 1-D model, excited by $\varepsilon_1^0$. (b) 3-D model, excited by $\varepsilon_1^0$ (showing the ocean effect). (c) 1-D model, excited by the full set of $\varepsilon_m^n$ (showing the source effect). (d) 3-D model, excited by the full set of $\varepsilon_m^n$ (showing ocean and source effects). The solid black lines indicate geomagnetic latitudes of $\pm 10^\circ$ and $\pm 55^\circ$, respectively. Observed responses at observatory locations are added as coloured dots to panel (d).
are the same everywhere on the globe. Figure 3.6b presents C-responses corresponding to induction due to the same source ($\varepsilon_1^0$) in a 3-D model. The remaining columns show C-responses corresponding to induction due to the full set of source terms in a 1-D model (c) and a 3-D model (d), respectively.

The effect of a complex source structure is presented in Figure 3.6c. It is most clearly seen at the period of 91.3 days. As expected and already discussed, maximum anomalies in the C-responses are detected close to the magnetic pole and the magnetic equator. But anomalous C-responses are also very pronounced in mid-latitudes. For example, Im C shows a strong source effect in the Indian Ocean. Another prominent feature follows the geometry of the geomagnetic equator. The effect can be traced up to geomagnetic latitudes of ±20°, which in particular means that C-responses at many mid-latitude observatories (for example Honolulu) are likely influenced by the source complexity.

Figure 3.6d also shows the estimated C-responses at observatory locations as coloured dots. Modellings and estimates are in good agreement at a period of 2.0 days, but deviate strongly at 91.3 days. This is likely due to the large uncertainties of C-response estimates at long periods.

A comparison of the results presented in Figures 3.6b, 3.6c and 3.6d confirms that the ocean effect is the dominant source of variability for short periods, while the source effect dominates at long periods. The imaginary part at long periods is more affected by the ocean effect than the real part. Ocean effect and source effect together can explain a large proportion of the variability in observatory C-responses. Differences between observed and computed responses might be due to erroneous data, more complicated source structures (e.g. the auroral electrojet, cf. Semenov & Kuvshinov, 2012), and deep 3-D conductivity heterogeneities.

3.2 Alternative responses for observatory data

The Z/H-method yields a handy scalar transfer function, but in case of a source that is not exclusively described by $Y_1^0$, this transfer function is heavily contaminated by coherent noise. The array transfer functions $T_n^m$, $U_n^m$ and $V_n^m$ pose an alternative that can handle a complex source structure. We will now investigate their performance by applying the concept to 16 years of observatory data (1997–2012). The application requires time series of external coefficients $\varepsilon_n^m$. For $n \leq 3$ and $|m| \leq 1$, these coefficients have already been derived with the algorithm outlined in the previous section (cf. Figures 3.3 and 3.4).

From time series of $\varepsilon_n^m$, X, Y and Z, we estimated, according to eqs (2.38)–(2.44), the proposed transfer functions $T_n^m$, $U_n^m$ and $V_n^m$ for selected observatories. To this purpose, we used the multivariate time series analysis algorithm outlined in Section 2.5. As a reference, we also estimated C-responses with the Z/H-method.
Alternative responses for observatory data

3.2.1 Transfer functions for the Hermanus observatory

In Figure 3.7, we present estimates of $C$ and $T_m^n$ for the observatory Hermanus (HER, South Africa, geomagnetic latitude $34°\text{S}$). As expected, $C$ and $T_1^0$ are similar in shape. This similarity confirms that $\varepsilon_1^0$ is the dominant inducing coefficient. However, $T_m^n$ of higher $n$ and $|m|$ are non-zero and show distinct structures (especially at short periods), e.g. $T_3^0$, $T_2^{-1}$ and $T_2^1$. The uncertainties of these responses increase at periods $>30$ days, which is probably due to the limited length of the time series. In solid lines, we show modelled transfer functions corresponding to the conductivity model of Figure 3.2. For many $T_m^n$, there is a good correspondence between estimates and modellings, at least concerning the general trend. Differences might be due to noise in the data, inaccuracies

Figure 3.7: Transfer functions estimated for the observatory Hermanus (HER, South Africa) at a geomagnetic latitude of $34°\text{S}$. The bottom left panel shows $C$-responses. The bottom right panel shows squared coherencies for $C$ and multiple squared coherencies for the alternative transfer functions $T_m^n$, $U_m^n$ and $V_m^n$. The further panels show the transfer functions $T_m^n$ ($n \leq 3$, $|m| \leq 1$). For all responses, the real part is presented in blue, the imaginary part in red. The 90% confidence interval is indicated for each estimate. Modelled transfer functions, corresponding to the conductivity model shown in Figure 3.2, are marked by solid lines.
in the estimated source coefficients, but also due to structures not present in our simplified conductivity model. The latter is probably the reason for the differences between modelled and estimated $T_0$ at periods $<5$ days.

Estimates of $U^m_n$ for HER are presented in Figure 3.8. $U^0_1$, corresponding to induction by $\varepsilon^0_1$, is the best-resolved element, indicated by small confidence limits. The estimated $U^0_1$ also agrees well with the model prediction. Several other elements show distinct structures and reasonable agreement with the model predictions, such as, for instance, $U^0_3$.

The estimates of $V^m_n$ are presented in Figure 3.9. There is no element among the $V^m_n$ with particularly good resolution, since there is no dominant source explaining variations in $Y$. Reasonable agreement with the model predictions is only achieved for few elements, such as $V^{-1}_2$. The model predictions for $V^0_n$ are very close to zero, since a field described by $Y^0_n$ has no $Y$-component. The non-zero estimates of $V^0_n$ are thus clear artefacts.

We want to note again that both $U^m_n$ and $V^m_n$ are not very sensitive to induction. However, analysing their coherencies can help to understand the source structure. Squared coherencies $\text{coh}^2(C)$ and multiple squared coherencies $\text{coh}^2_{\text{mult}}(T^m_n)$, $\text{coh}^2_{\text{mult}}(U^m_n)$ and $\text{coh}^2_{\text{mult}}(V^m_n)$ are presented in the bottom right panel of Figure 3.7. The plot clearly shows that for all periods, $\text{coh}^2_{\text{mult}}(T^m_n) > \text{coh}^2(C)$. This means that the addition of a small number of source terms substantially increases the coherency and thus decreases
the bias of the estimated responses by correlated noise (in agreement with the results of Olsen, 1998).

Squared coherencies for the $V_n^m$ are relatively small; indeed, $\text{coh}_{\text{mult}}^2(V_n^m) < \text{coh}^2(C)$ for all periods. The low coherencies primarily indicate that variations of $Y$ at HER cannot be explained by low-degree spherical harmonic sources alone. In contrast, $\text{coh}_{\text{mult}}^2(U_n^m)$ are very large and approach 1 with increasing period. Variations in $X$ at HER are thus well explained by low-degree spherical harmonic sources. Note that, when deriving the $\varepsilon_n^m$ by a spherical harmonic analysis (SHA) of the horizontal components of $B$, we excluded data from HER to avoid any circularity in our analysis. Tests showed that this has only very minor effects on the resulting transfer functions and coherencies. The effect might be larger for more isolated observatories (e.g. Honolulu).

We do not show ordinary coherencies for individual $T_n^m$, $U_n^m$ and $V_n^m$, describing the proportion of $Z$, $X$ or $Y$, respectively, that can be described by the individual inputs $\varepsilon_n^m$. The ordinary coherency for $T_0^0$ is very similar to that of the $C$-response. The coherencies for other $T_n^m$ are small (generally below 0.2), but non-zero and thus contribute to $\text{coh}_{\text{mult}}^2$. The ordinary coherency for $U_0^0$ approaches unity for periods longer than 5 days. In contrast to $Z$, variations in $X$ are thus dominated by a large-scale symmetric ring current. Coherencies for other $U_n^m$ are low. Among the $V_n^m$, $V_{-1}^2$ and $V_{1}^2$ show the highest ordinary coherencies (ranging between 0.2 and 0.4, depending on period).

Figure 3.9: Transfer functions $V_n^m$ estimated for the observatory Hermanus (HER, South Africa). See also caption of Figure 3.7.
3.2.2 Analysis of coherencies

The same investigations as for Hermanus can be done for any magnetic observatory. We focus on presenting squared coherencies for further locations, as they contain the most interesting information. Figure 3.10 shows coherency plots for the observatories Kakioka (KAK, Japan), Fürstenfeldbruck (FUR, Germany), Irkutsk (IRT, Russia) and Addis Abeba (AAE, Ethiopia).

For the mid-latitude observatory KAK, the addition of source terms does not lead to a substantial increase in the coherencies, i.e. \( \text{coh}_{\text{mult}}^2(T_n^m) \approx \text{coh}^2(C) \) at all periods. For FUR and IRT, \( \text{coh}^2 \) however increases substantially when estimating the \( T_n^m \) instead of \( C \), especially at short periods. Remember that the estimation of \( C \)-responses with the \( Z/H \)-method becomes unstable towards high latitudes. The addition of source terms other than \( \varepsilon_0^1 \) seems to improve the situation. The low coherencies of \( C \) at FUR and IRT are, however, not only due to the way \( C \) is estimated. The measurements at both observatories are believed to be influenced by the polar electrojet (e.g. Fujii & Schultz, 2002; Semenov & Kuvshinov, 2012). The transfer functions of higher \( n \) and \(|m|\) might thus “catch” part of the noise arising from this source.

![Figure 3.10](image)

**Figure 3.10:** Squared coherencies for \( C \) (black) and multiple squared coherencies for \( T_n^m \) (magenta), \( U_n^m \) (orange) and \( V_n^m \) (green) at different geomagnetic observatories. Geomagnetic latitude is indicated.
Coherencies of $C$ are generally very low for AAE. This is due to the vanishing $Z$-component close to the geomagnetic equator, as discussed in Section 3.1. $\text{coh}^2_{\text{mult}}(T^m_n)$ are not much larger, indicating that the chosen subset of $\varepsilon^m_n$ can not explain the variations of $Z$ at AAE. For KAK, FUR and IRT, coherencies of $C$, $T^m_n$ and $U^m_n$ increase with period. We attribute this behaviour to a growing dominance of $\varepsilon^0_1$ at longer periods. This assumption is confirmed by the power spectra shown in Figure 3.4. The same argument holds for the decrease of $\text{coh}^2_{\text{mult}}(V^m_n)$ with increasing period, since a source described spatially by $Y_0^1$ does not contribute to variations in $Y$ unless conductivity heterogeneities are present.

Multiple squared coherencies of the $U^m_n$ are very high for all observatories analysed in here. This is even the case at AAE, where the other transfer functions fail. The high coherencies of $U^m_n$ are due to the fact that the $X$-component of magnetic variations only vanishes near the poles and is less sensitive to source structures of high $n$ than the $Z$-component, cf. eqs. (2.25)–(2.27).

3.2.3 Discussion

In this study, we assumed that the source can be described by 9 external SHE coefficients ($p = 9$). Compared to the usual assumption of $p = 1$, we observed a substantial increase in coherencies between input and output signals of the estimated transfer functions. The increase in coherencies was particularly pronounced at periods $< 10$ days and geomagnetic latitudes $> 40^\circ$, where the polar electrojet is believed to affect the measurements.

The choice of coefficients, however, was rather arbitrary and does not have a physical basis. The recovered coefficients constitute a mix of signals of magnetospheric origin and of ionospheric origin. The expansion by spherical harmonics does not allow for a separation of the signals from different sources. Indeed, there may be strong correlations between the various coefficient time series. In our case, correlation coefficients range between 0.01 and 0.4. A more appropriate source parametrization might be attainable by a decomposition of the magnetic data into empirical orthogonal functions (EOFs). This method, which yields mutually independent spatio-temporal modes that might have a physical meaning, was recently applied to magnetic data by Shore et al. (2015). Deriving a more suitable parametrization for our problem is a task that we will leave open for future studies.

Semenov & Kuvshinov (2012) inverted $C$-responses of the global network of geomagnetic observatories for 3-D mantle conductivity structure. The alternative transfer functions $T^m_n$ introduced in this study could be inverted in a similar fashion. If treated with care, $U^m_n$ (and potentially also $V^m_n$) might be useful in regions where coherencies of $T^m_n$ are small, particularly near the equator. While Semenov & Kuvshinov (2012) excluded observatories at low and high latitudes from their analysis, we could, with a
3.3 Alternative responses for cable data

Geomagnetic variations are known to induce currents in man-made conductors such as pipelines or power transmission grids. While these geomagnetically induced currents are commonly regarded as natural hazard (cf. Appendix C), measurements of the induced voltage can also be used to gain knowledge about subsurface conductivity structure.

A network of abandoned submarine telecommunication cables is laid out in the North Pacific (Figure 3.11). Voltage data from these cables were used by Lizarralde et al. (1995), Koyama (2001), Utada et al. (2003), Kuvshinov et al. (2005), Koyama et al. (2006) and Shimizu et al. (2010a,b) to image 1-D and 3-D conductivity structure of the mantle in this region. With the assumption of a laterally homogeneous electric field, the
Alternative responses for cable data

Figure 3.12: Transfer functions $\Xi$ (bottom left panel) and $K_{nm}$, estimated for the cable TPC-1 (North Pacific). The bottom right panel shows squared coherencies. See also caption of Figure 3.7.

authors of these studies first synthesized time series of $E_{\theta}$ and $E_{\varphi}$ from the measured voltage $U$. The horizontal components of the electric field were then related to those of the magnetic field, measured at a nearby observatory, to derive the impedance.

This method is evidently cumbersome and approximate by nature. Moreover, all of these studies were based on the $P_{1}^{0}$-assumption. The problem can be treated in a much more elegant and consistent way by using the new transfer functions $K_{nm}$, which directly relate the voltage $U$ to the source coefficients $\varepsilon_{nm}$ (Section 2.4.2).

Voltage data from the cables shown in Figure 3.11 are available for the 1990s. For a test study, I took three years of data (January 1998 – December 2000) from cable TPC-1, laid out between Guam and the Philippine island Luzón (Figure 3.11). This cable extends over more than 2500 km and is almost parallel to the geomagnetic equator. By relating the voltage $U$ to time series of $\varepsilon_{nm}$, which were derived from observatory data (Section 3.1.2), I estimated $K_{nm}$ for $n \leq 3$, $|m| \leq 1$. For comparison, I also estimated a
scalar transfer function $\Xi$ relating $U$ to $B_\phi$, the latter being measured at the Kakioka geomagnetic observatory. This transfer function is nothing but a scaling of the scalar impedance.

The estimated $\Xi$ and $K_m^n$ are presented in Figure 3.12. As expected, $\Xi$ and $K_0^0$ are very similar in shape. Both transfer functions are very well recovered and show small uncertainties. $K_m^n$ of higher degrees and orders are badly recovered and would certainly not prove useful in an inversion. However, they seem to catch part of the noise in the data. This is apparent from the coherency plot (bottom right panel). For periods $<10$ days, $\text{coh}_\text{mult}^2(K_m^n) > 0.9$. The difference to $\text{coh}^2(\Xi)$ is particularly pronounced for the shortest periods. Coherencies of both transfer functions then drop to 0.75 at a period of 20 days. Due to the moderate quality of the voltage data and gaps in the time series, I could not estimate $K_m^n$ at longer periods.

The results confirm the applicability of the new transfer functions $K_m^n$ to voltage data in abandoned submarine telecommunication cables. They also confirm the superiority to impedances, which are estimated from voltage data and magnetic data from a nearby observatory. Investigations of data from further cables and longer time series would be necessary to assess the usefulness of these transfer functions and to understand the implications for an inversion.
Chapter 4

The *Swarm* Satellite Mission

4.1 Outline and objectives of the mission

*Swarm*, a constellation mission comprising three identical satellites to study the dynamics of the Earth’s magnetic field and its interactions with the Earth system (Friis-Christensen *et al.*, 2006) was launched in November 2013 from Plesetsk (Russia) by the European Space Agency (ESA). Two of the satellites (*Swarm* A and B) fly side-by-side at an altitude of 460 km, while the third (*Swarm* C) orbits the Earth at an altitude of 530 km. The latter is supposed to separate from the lower two over time to improve the coverage (Figure 4.1). The objective of the *Swarm* mission is to provide the best ever survey of the geomagnetic field and its temporal evolution, in order to gain new insights into the Earth system by improving the understanding of the Earth’s interior and environment.

![Figure 4.1: Expected development of the Swarm constellation. With time, Swarm C separates in local time from Swarm A and B, reaching an angular distance of approximately 90° after 4 years. Image: ESA.](image-url)
Each of the three *Swarm* satellites makes high-precision and high-resolution measurements of the strength, direction and variation of the magnetic field, complemented by precise navigation, accelerometer, plasma and electric field measurements. *Swarm* simultaneously obtains a space-time characterisation of both the internal field sources in the Earth and the ionospheric-magnetospheric current systems. The research objectives assigned to the mission are: (a) studies of core dynamics, geodynamo processes, and core-mantle interaction; (b) mapping of the lithospheric magnetisation and its geological interpretation; (c) determination of the 3-D electrical conductivity of the mantle; and (d) investigation of electric currents flowing in the magnetosphere and ionosphere.

In order to achieve the scientifically challenging research objectives, the *Swarm* “Satellite Constellation Application and Research Facility” (SCARF) was established. The purpose of SCARF is to derive commonly used scientific models and quantities and make them available to the scientific community at large. SCARF comprises a joint effort between six European partners, namely DTU (Lyngby/DK), TU Delft (Delft/NL), BGS (Edinburgh/UK), ETH (Zürich/CH), GFZ (Potsdam/D) and IPGP (Paris/F) with contributions from CUP (Prague/CZ), NOAA (Boulder/USA) and GSFC/NASA (Greenbelt/USA). The team behind SCARF has designed and implemented algorithms to derive advanced models of the geomagnetic field describing sources in the core, lithosphere, ionosphere and magnetosphere, models of the electrical conductivity of Earth’s mantle and time series of thermospheric wind and density at the positions of the *Swarm* satellites. The various processing chains of SCARF were thoroughly tested during the development phase of the *Swarm* mission.

The text above in large parts followed the paper of Olsen *et al.* (2013). In the following, I will focus on those activities of SCARF relevant for the determination of the electrical conductivity structure of Earth’s mantle (research objective (c)). The corresponding processing chains were developed at ETH and CUP, the former as part of my PhD. The algorithms that invert for 1-D and 3-D conductivity structure of the mantle will be presented in Chapters 5 and 6, respectively.

### 4.2 The *Swarm* SCARF test data set

In order to test the functionality and robustness of the processing chains, the SCARF generated synthetic magnetic data from models that were afterwards meant to be recovered. For the processing chains dealing with EM induction, these test data consisted of time series of SHE coefficients $\varepsilon^m_n$ and $\iota^i_k$, representing inducing and induced parts of the magnetic variation due to a synthetic magnetospheric source.

The 3-D conductivity model to be recovered, hereinafter referred to as “target model”, is shown in Figure 4.2. It consists of a thin surface shell of laterally varying conductance and a layered model, which contains different conductivity anomalies, underneath. The
Figure 4.2: Target conductivity model in S/m. Note that the conductivity of the top layer has been obtained by scaling the surface conductance map (Figure 3.2) to a thickness of 10 km.

shell conductance is obtained by considering contributions both from seawater and sediments; it was already introduced in Section 3.1 and shown in Figure 3.2. The surface shell is scaled to a thickness of 10 km.

Three local conductors of 0.04 S/m, representing possible mantle plumes and subduction zones, are embedded in a resistive layer of 0.004 S/m that extends from 10 km to 400 km. A deep-seated large-scale structure with conductivity of 1 S/m, describing a hypothetical regional conductor beneath the Pacific plate, is embedded in a layer of 0.04 S/m that extends from 400 km to 700 km. At depths between 700 km and the core-mantle boundary at 2900 km, the target model consists of a uniform conductor of 2 S/m. Each spherical sub-layer is discretized laterally in $180 \times 90$ cells of $2^\circ \times 2^\circ$. The aim of this model is not to mimic the “true” world, but to provide a test model for the retrieval algorithms.

Hourly mean time series of external coefficients $\varepsilon^m_n$ in a geomagnetic dipole coordinate system ($n \leq 3, |m| \leq 1$) were obtained by analysis of 4.5 years of observatory data (July 1998 – December 2002). The generation of these time series, which are depicted in Figure 3.3, was already discussed in Section 3.1.

The procedure to derive time series of internal coefficients $\iota^l_k$ in large parts follows the general scheme described in Olsen & Kuvshinov (2004) and Kuvshinov & Olsen (2005). It consists of the following steps:

- Fourier transformation of the external coefficients $\varepsilon^m_n$.
- Simulation of EM induction by spherical harmonic sources $Y^m_n$ ($n \leq 3, |m| \leq 1$) for a set of logarithmically spaced frequencies $\omega_j$, using a numerical solution
(Kuvshinov, 2008) based on a contracting integral equation approach (Pankratov et al., 1995). This yields $B_{mn}^r(r, \omega_j)$.

- For each frequency $\omega_j$, recovery of $Q_{km}^{lm}$ by spherical harmonic analysis of the simulated $B_{n,r}^{mn}$ ($k, l \leq 15$). This calculation involves eq. (6.44), which will be introduced in Section 6.2.3.

- Spline interpolation of $Q_{km}^{lm}$ to all frequencies contained in the data.

- Calculation of the time spectra of internal coefficients $\iota_k^l$ using eq. (2.37).

- Inverse Fourier transformation of the recovered $\iota_k^l$.

The coefficient time series obtained with the procedure outlined above constitute a noise-free input for the inversion. These noise-free data will be used to test the data processing algorithm in Section 6.5.2. In practice, however, the coefficient time series first have to be derived from raw magnetic data. In context of the Swarm mission, this task will be accomplished by the Comprehensive Inversion (CI; Sabaka et al., 2002; Sabaka & Olsen, 2006; Sabaka et al., 2013). The CI aims at separating magnetic contributions from various sources (core, lithosphere, ionosphere, and magnetosphere) in the form of corresponding SHE coefficients. In order to simulate the full processing of Swarm data more realistically, the $\varepsilon_{n}^{m}$ and $\iota_{k}^{l}$ are thus used to predict the magnetospheric field at orbit altitudes and observatory locations (with a sampling frequency of 1 Hz). Adding the contributions due to different sources (core, lithosphere and ionosphere), which were prepared by different partners of the SCARF, and a small amount of white noise yields complete synthetic Swarm data.

The external and internal SHE coefficients recovered from these data by the CI constitute the SCARF test data set for the induction-related processing chains. Time series of $\varepsilon_{1}^{0}$ and $\iota_{1}^{0}$ are recovered with a sampling rate of 1.5 hours; coefficients of higher degree and order ($n \leq 3$, $|m| \leq 1$, $k \leq 5$, $|l| \leq 5$) with a sampling rate of 6 hours. All time series comprise 4.5 years. The generation of the full test data set is described more extensively in Olsen et al. (2013).
Chapter 5

1-D Inversion for Mantle Conductivity Structure

5.1 Introduction

The recovery of 1-D conductivity-depth profiles of Earth’s mantle is an old geophysical problem that has been revisited many times over the past century. A summary of past studies was given in Section 1.2. The Swarm multi-satellite mission (Chapter 4) recently prompted the development of a new method to recover 1-D conductivity structure, which takes into account 3-D effects arising from the known distribution of oceans and continents. The development of algorithms, their validation in the context of SCARF, and their later application to real data was summarized in two publications by Püthe & Kuvshinov (2013a) and Püthe et al. (2015b). The text in this chapter in large parts follows these papers.

In the following, I will first outline the iterative 1-D inversion scheme and demonstrate the validation of its functionality with the SCARF test data set (Section 4.2). I will then describe the application of the scheme to ten years (September 2000 to August 2010) of magnetic measurements from the satellites Ørsted, CHAMP, and SAC-C, and the global network of geomagnetic observatories, in addition to eight months (December 2013 to July 2014) of data from the three Swarm satellites and the geomagnetic observatories. This is the largest dataset ever used for a 1-D mantle conductivity study. The use of both satellite and observatory data combines the strengths of both data origins.

A 3-D correction scheme for induction in the oceans was presented before by Kuvshinov & Olsen (2006). We extended their methodology and in parallel developed an alternative, more consistent approach to correct for the ocean effect. Geophysical inverse problems suffer from non-uniqueness. As a consequence, analysis of model resolution and accuracy is crucial, but rarely addressed in EM induction studies. In this chapter, I will describe how we derived 1-D mantle conductivity models using both deterministic and
probabilistic methods, and show that both approaches can be used to gain knowledge about model uncertainties.

5.2 An iterative 1-D inversion

Figure 5.1 presents an algorithm to invert EM data for the 1-D distribution of electrical conductivity in the mantle. Its complicated, iterative structure is due to the applied correction for the ocean effect. The inversion scheme requires time series of $\varepsilon_0^i$ and $\iota_0^i$ as inputs. These SHE coefficients describe induction due to a magnetospheric ring current in a spherically layered conductivity model. A transfer function relating $\varepsilon_0^i$ and $\iota_0^i$ is the scalar $Q$-response $Q_{i}^{obs}(\omega)$, which was introduced in eq. (2.31). The $Q$-response is estimated for $N_\omega$ frequencies with the time series analysis algorithm presented in
Section 2.5 and subsequently converted into the global $C$-response,

$$C^{\text{obs}}(\omega) = \frac{a}{2} \left(1 - \frac{2Q^{\text{obs}}_1(\omega)}{1 + Q^{\text{obs}}_1(\omega)}\right), \quad (5.1)$$

as shown by Schmucker (1987). The corresponding uncertainties are converted with the formula

$$\delta C^{\text{obs}}(\omega) = \frac{3a}{2} \frac{1}{|1 + Q^{\text{obs}}_1(\omega)|^2} \delta Q^{\text{obs}}_1(\omega), \quad (5.2)$$

which follows from the error propagation law.

Within each iteration of the inversion scheme, synthetic global responses $C^{1-D}(\omega)$ and $C^{3-D}(\omega)$ are computed, which correspond to trial 1-D and 3-D models of Earth’s conductivity structure, respectively. The 1-D model represents the conductivity structure recovered in the previous iteration of the inversion. The 3-D model is nothing but the 1-D model plus a laterally heterogeneous shell representing the surface conductance map (Figure 3.2). The calculation of synthetic $C$-responses for a X-D model, where X-D refers to either 1-D or 3-D, involves three steps:

- Simulation of EM induction by a unit amplitude ring current source for the $N_\omega$ frequencies of interest, using a numerical solution (Kuvshinov, 2008) based on a contracting integral equation approach (Pankratov et al., 1995). This yields time spectra $B^{X-D}(r_a, \omega)$.

- Recovery of the transfer function $Q^{X-D}_1(\omega)$ by spherical harmonic analysis of the simulated $B^{X-D}_r$. This calculation involves eq. (6.44), which will be introduced in Section 6.2.3.

- Conversion of $Q^{X-D}_1(\omega)$ to $C^{X-D}(\omega)$ using eq. (5.1).

The synthetic responses $C^{1-D}(\omega)$ and $C^{3-D}(\omega)$ are needed to correct the observed responses $C^{\text{obs}}(\omega)$ for the ocean effect (cf. Figure 5.1). In the original implementation of the algorithm, the correction formula read

$$C^{\text{corr}}(\omega) = C^{\text{obs}}(\omega) + C^{1-D}(\omega) - C^{3-D}(\omega). \quad (5.3)$$

The logic of this heuristic correction is as follows: If the 3-D conductivity model coincides with Earth’s true conductivity structure, $C^{3-D}(\omega)$ and $C^{\text{obs}}(\omega)$ cancel out, and $C^{\text{corr}}(\omega)$ is then simply given by $C^{1-D}(\omega)$. Eq. (5.3) was used to correct observed $C$-responses when validating the algorithm, cf. Section 5.3.

When applying the algorithm to real data (cf. Section 5.4), however, we used the modified formula

$$\text{Re } C^{\text{corr}}(\omega) = \text{Re } C^{\text{obs}}(\omega) \frac{\text{Re } C^{1-D}(\omega)}{\text{Re } C^{3-D}(\omega)}, \quad (5.4)$$
5.2 Demonstration of the convergence of $C^{\text{obs}}(\omega)$ and $C^{3-D}(\omega)$ within five iterations of the inversion scheme. Note that the series with positive values represent Re $C$, those with negative values Im $C$.

\[ \text{Im } C^{\text{corr}}(\omega) = \text{Im } C^{\text{obs}}(\omega) \cdot \text{Im } C^{1-D}(\omega) / \text{Im } C^{3-D}(\omega). \] (5.5)

This multiplicative scheme implies a relative correction of the estimated $C$-responses, which yields more reliable results than the absolute, additive correction given by eq. (5.3). A separate treatment of Re $C$ and Im $C$ is necessary because a combined correction would be biased towards the real part, which has larger amplitudes.

Convergence of the iterative scheme is reached if

\[ \text{RMS} = \sqrt{\frac{1}{N^2} \sum_{\omega} \left| \frac{C^{\text{corr}}(\omega) - C^{1-D}(\omega)}{\delta C^{\text{obs}}(\omega)} \right|^2} \leq \epsilon. \] (5.6)

If, on the other hand, RMS $> \epsilon$, the corrected $C$-responses are inverted for a new 1-D conductivity model, and a new iteration is initiated (cf. Figure 5.1). For the inversion itself, the deterministic algorithm, which will be outlined in more detail in Section 5.5.1, is employed.

5.3 Validation of the inversion scheme

The iterative algorithm presented in Figure 5.1 is validated with time series of $\varepsilon_1^0$ and $\iota_1^0$ from the SCARF test data set. The goal of the exercise is thus to recover the background...
Validation of the inversion scheme

conductivity structure of the SCARF target model shown in Figure 4.2. Note that the target model contains the surface conductance map, which demands a correction of the data for induction in the oceans.

\( C \)-responses are estimated at 23 logarithmically spaced periods between 14 hours and 83 days. We invert the \( C \)-responses to recover 1-D mantle conductivity at depths between 10 km and the core-mantle boundary at 2890 km. The inversion domain is stratified into 44 layers with thicknesses of 50 km (at depths below 1500 km) and 100 km (at depths greater than 1500 km), respectively. As initial (starting) model, a uniform mantle with conductivity of 1 S/m is prescribed.

The inversion scheme converges after 5 iterations. Figure 5.2 shows the convergence of the \( C \)-responses. A good agreement between modelled and estimated responses in the final iteration validates the correction scheme.

The recovered conductivity model in comparison to the (laterally averaged) target model is shown in Figure 5.3. Lateral averaged conductivity here denotes the arithmetic mean of the conductivity of all cells in the respective layer. The results indicate that the inversion scheme is able to recover mantle conductivity at all depths. Although the initial model is very different from the target model, the conductivity distribution of the final model agrees well with that of the latter. Due to the applied smoothing, the recovered model does not comprise the large jumps in conductivity that are apparent in the target model at depths of 400 km and 700 km.
5.4 Processing of real satellite and observatory data

5.4.1 Selection of the data

We processed more than 10 years of magnetic satellite and observatory data, dating from two periods separated in time. The period from September 2000 to August 2010 will hereinafter be denoted as “CHAMP phase”, while that from December 2013 to July 2014 will be denoted as “Swarm phase”. Both names refer to the satellites providing vector data for the indicated period.

Hourly mean vector data from observatories were available for the entire CHAMP phase; their number ranged between 111 and 132. Ørsted vector data were only available from September 2000 to December 2005, while scalar data could be retrieved (with considerable gaps) until the end of the CHAMP phase. SAC-C provided scalar data from January 2001 to December 2004. All satellite data were resampled to minute resolution. Due to the different sampling rates, the amount of observatory data and satellite data are comparable. This is also the case for the Swarm phase, although the number of observatories providing data (dropping over time from 80 to a minimum of 43) is considerably smaller than for the CHAMP phase. Figure 5.4 displays the data availability during both phases.

The raw data were processed as follows. First, we removed core and crustal field as predicted by the CHAOS-4 magnetic field model (Olsen et al., 2014). Obvious outliers and baseline jumps were, after careful inspection, removed manually. If necessary,
remaining slow variations in the observatory data were removed by fitting low-degree polynomials to the time series. No such correction was applied to satellite data.

In order to reduce the influence of ionospheric currents (Sq system and polar electrojets), we only used night-time data (defined here by local-time between 19:00 and 05:00) and avoided latitudes $>55^\circ$. The remaining magnetic field variations are assumed to be due to a large-scale magnetospheric source that consists mainly of a ring current around the geomagnetic equator. With the assumption of a 1-D conductivity distribution, the spatial structure of the magnetic field due to such a source can be described by the single spherical harmonic $Y_1^0 = \cos \vartheta$. Its temporal evolution is characterized by the external coefficient $\varepsilon_1^0$ and its induced counterpart $\iota_1^0$. The magnetic potential $V$ (eqs 2.19–2.20) reduces to

$$V(\mathbf{r}, t) = a \left\{ \varepsilon_1^0(t) \left( \frac{r}{a} \right) + \iota_1^0(t) \left( \frac{a}{r} \right)^2 \right\} \cos \vartheta. \quad (5.7)$$

We fit the magnetic field variations with these coefficients in the time-domain in bins of 1 hour. Note that the procedure does not contradict the finding of a complex magnetospheric source, which was demonstrated in Chapter 3. By using eq. (5.7), we merely extract those parts of the magnetic variations that are due to a symmetric ring current and discard the variations due to other source components. In practice, allowing for more coefficients did not improve the results, but rather destabilized the processing. An alternative parametrization of the time-dependency with cubic splines, as applied by Kuvshinov & Olsen (2006), did not change the results significantly.

### 5.4.2 Estimation and correction of transfer functions

$C$-responses were estimated from time series of $\varepsilon_1^0$ and $\iota_1^0$ as described in Section 5.2. This was first done separately for each of the two phases. For the CHAMP phase, we estimated $C$-responses at 27 periods between 1.5 days and 150 days. This is the period range in which ring-current activity is known to be the dominant source of magnetic variations (e.g. Schmucker, 1985). Outside this range, the magnetospheric ring current is not the dominant source, which is why extensions to shorter and longer periods were avoided. For the Swarm phase, we were restricted to periods up to 25 days due to the shortness of the available time series. The results are presented in Figure 5.5a.

$C$-responses estimated for the CHAMP and Swarm phase agree fairly well for all frequencies. This is remarkable, considering the limited amount of data available in the Swarm phase. Even if uncertainties are clearly larger for the Swarm phase than for the CHAMP phase, reliable estimates of $C$-responses for periods up to 25 days are attainable from only 8 months of satellite and observatory data. When data from both phases are combined, the resulting $C$-responses only differ insignificantly from those obtained for the CHAMP phase. Squared coherencies exceed 0.9 throughout, justifying the use of
Figure 5.5: a) Estimated (uncorrected) $C$-responses in this study in comparison to those obtained by Kuvshinov & Olsen (2006). b) $C$-responses corrected for induction in the oceans; solid lines indicate $C$-response predictions corresponding to the recovered conductivity models (Figure 5.8). Top panels show squared coherencies.

eq. (5.7). The real part of $C$, which is a measure of the penetration depth, increases monotonically from 700 km to 1600 km.

We compare our results to those of Kuvshinov & Olsen (2006), who conducted a similar study based on five years (2001-2005) of satellite magnetic data. Overall, results from the two studies are observed to agree fairly well. Our $C$-responses, however, are smoother, show smaller uncertainties, and higher coherencies. This is most probably due to the larger dataset used in this study. Additionally, Re $C$ is consistently found to be larger than that determined by Kuvshinov & Olsen. This is explained as follows: When fitting the magnetic data with coefficients $\varepsilon_1$ and $\iota_0$, the authors added a small damping parameter to stabilize the solution and obtain continuous coefficient time series in spite of gap-bearing raw data. This damping, however, slightly biased the estimated $C$-responses towards smaller amplitudes. In contrast to Kuvshinov & Olsen, we use observatory data in addition to satellite data. As a result, a stable estimation of the coefficients is possible for each instant, obviating the requirement for damping.

From here on, we work with $C$-responses estimated from data from both phases. These (observed) responses $C^{\text{obs}}(\omega)$ are corrected for the ocean effect with the method described in Section 5.2, using eqs (5.4)–(5.5). Corrected $C$-responses $C^{\text{corr}}(\omega)$ are shown in Figure 5.5b and compared to those obtained by Kuvshinov & Olsen (2006), who used a different correction scheme. The ocean effect is clearly visible in both the real and imaginary part at periods $<10$ days. Re $C^{\text{corr}}$ remains almost constant at 850-900 km for periods up to 10 days. This implies a thick, highly resistive layer underneath the surface shell. The effect of the correction is slightly more pronounced than in the results of Kuvshinov & Olsen; the differences (in the real part) therefore increase for periods $<10$ days. This is likely a result of the different correction scheme. The numerical values of observed and corrected $C$-responses, uncertainties, and squared coherencies are provided in Table 5.1.
Table 5.1: Observed and corrected $C$-responses with uncertainties (in km) and squared coherencies as functions of period (in seconds).

<table>
<thead>
<tr>
<th>Period</th>
<th>Re $C_{\text{obs}}$</th>
<th>Im $C_{\text{obs}}$</th>
<th>Re $C_{\text{corr}}$</th>
<th>Im $C_{\text{corr}}$</th>
<th>$\delta C_{\text{obs}}$</th>
<th>coh$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>129600</td>
<td>692.3</td>
<td>-277.9</td>
<td>872.2</td>
<td>-132.3</td>
<td>43.5</td>
<td>0.93</td>
</tr>
<tr>
<td>154800</td>
<td>723.5</td>
<td>-232.5</td>
<td>870.7</td>
<td>-111.3</td>
<td>40.8</td>
<td>0.95</td>
</tr>
<tr>
<td>183600</td>
<td>748.4</td>
<td>-209.8</td>
<td>868.7</td>
<td>-102.6</td>
<td>37.5</td>
<td>0.96</td>
</tr>
<tr>
<td>219600</td>
<td>773.0</td>
<td>-179.2</td>
<td>870.3</td>
<td>-90.9</td>
<td>36.5</td>
<td>0.96</td>
</tr>
<tr>
<td>262800</td>
<td>781.8</td>
<td>-156.4</td>
<td>859.3</td>
<td>-83.4</td>
<td>35.4</td>
<td>0.97</td>
</tr>
<tr>
<td>313200</td>
<td>798.6</td>
<td>-135.4</td>
<td>861.7</td>
<td>-76.2</td>
<td>35.2</td>
<td>0.97</td>
</tr>
<tr>
<td>370800</td>
<td>822.9</td>
<td>-134.3</td>
<td>875.9</td>
<td>-80.2</td>
<td>41.9</td>
<td>0.97</td>
</tr>
<tr>
<td>439200</td>
<td>836.6</td>
<td>-144.6</td>
<td>881.0</td>
<td>-91.7</td>
<td>45.7</td>
<td>0.97</td>
</tr>
<tr>
<td>522000</td>
<td>847.1</td>
<td>-152.9</td>
<td>884.4</td>
<td>-102.9</td>
<td>43.1</td>
<td>0.97</td>
</tr>
<tr>
<td>619200</td>
<td>853.4</td>
<td>-179.0</td>
<td>885.1</td>
<td>-127.6</td>
<td>51.3</td>
<td>0.97</td>
</tr>
<tr>
<td>738000</td>
<td>877.2</td>
<td>-192.2</td>
<td>905.0</td>
<td>-144.6</td>
<td>46.0</td>
<td>0.98</td>
</tr>
<tr>
<td>878400</td>
<td>890.1</td>
<td>-223.7</td>
<td>914.6</td>
<td>-176.6</td>
<td>42.3</td>
<td>0.98</td>
</tr>
<tr>
<td>1044000</td>
<td>917.4</td>
<td>-248.9</td>
<td>939.4</td>
<td>-204.8</td>
<td>48.6</td>
<td>0.97</td>
</tr>
<tr>
<td>1242000</td>
<td>921.7</td>
<td>-256.3</td>
<td>941.4</td>
<td>-218.6</td>
<td>59.2</td>
<td>0.97</td>
</tr>
<tr>
<td>1476000</td>
<td>942.6</td>
<td>-278.3</td>
<td>960.5</td>
<td>-244.5</td>
<td>63.0</td>
<td>0.97</td>
</tr>
<tr>
<td>1756800</td>
<td>989.2</td>
<td>-302.3</td>
<td>1006.1</td>
<td>-272.2</td>
<td>45.4</td>
<td>0.98</td>
</tr>
<tr>
<td>2088000</td>
<td>1031.3</td>
<td>-326.7</td>
<td>1047.2</td>
<td>-300.0</td>
<td>54.5</td>
<td>0.98</td>
</tr>
<tr>
<td>2484000</td>
<td>1052.9</td>
<td>-365.4</td>
<td>1067.6</td>
<td>-340.1</td>
<td>68.3</td>
<td>0.97</td>
</tr>
<tr>
<td>2955600</td>
<td>1071.8</td>
<td>-367.6</td>
<td>1085.4</td>
<td>-347.4</td>
<td>89.1</td>
<td>0.96</td>
</tr>
<tr>
<td>3513600</td>
<td>1120.4</td>
<td>-337.3</td>
<td>1133.3</td>
<td>-322.1</td>
<td>121.1</td>
<td>0.94</td>
</tr>
<tr>
<td>4179600</td>
<td>1160.2</td>
<td>-314.3</td>
<td>1172.4</td>
<td>-302.7</td>
<td>164.2</td>
<td>0.92</td>
</tr>
<tr>
<td>4971600</td>
<td>1239.1</td>
<td>-329.3</td>
<td>1250.9</td>
<td>-319.3</td>
<td>202.5</td>
<td>0.91</td>
</tr>
<tr>
<td>5911200</td>
<td>1269.4</td>
<td>-397.2</td>
<td>1280.4</td>
<td>-387.2</td>
<td>211.8</td>
<td>0.91</td>
</tr>
<tr>
<td>7030800</td>
<td>1357.4</td>
<td>-453.0</td>
<td>1368.2</td>
<td>-443.6</td>
<td>160.1</td>
<td>0.93</td>
</tr>
<tr>
<td>8362800</td>
<td>1428.5</td>
<td>-518.3</td>
<td>1438.8</td>
<td>-509.2</td>
<td>141.8</td>
<td>0.94</td>
</tr>
<tr>
<td>9946800</td>
<td>1574.9</td>
<td>-525.7</td>
<td>1585.2</td>
<td>-517.8</td>
<td>182.3</td>
<td>0.91</td>
</tr>
<tr>
<td>11829600</td>
<td>1602.6</td>
<td>-562.4</td>
<td>1612.0</td>
<td>-554.9</td>
<td>194.3</td>
<td>0.92</td>
</tr>
</tbody>
</table>

5.5 Deterministic inversion

5.5.1 1-D inversion: concept

Deterministic inversion seeks a single model $\mathbf{m}$ that minimizes the misfit between data and model predictions given additional constraints. It can be formulated as a minimization problem, in which the objective function $\phi$ is defined as

$$\phi(\mathbf{m}, \lambda) = \phi_d(\mathbf{m}) + \lambda \phi_m(\mathbf{m}),$$  \hspace{1cm} (5.8)

where $\phi_d$ is data misfit and $\lambda$ and $\phi_m$ are regularization parameter and regularization term, respectively. The model vector $\mathbf{m}$ consists of a discrete parametrization of the radial conductivity structure.
We formulate the data misfit as
\[ \phi_d = \frac{1}{N_\omega} \sum_\omega |C^{\text{pred}}(m, \omega) - C^{\text{obs}}(\omega)|^2 / \delta C^{\text{obs}}(\omega)^2, \] (5.9)
where \( C^{\text{obs}}(\omega) \) are estimated \( C \)-responses (potentially corrected for the ocean effect), \( \delta C^{\text{obs}}(\omega) \) are corresponding uncertainties, and \( C^{\text{pred}}(\omega) \) are modelled (predicted) \( C \)-responses. The regularization term \( \phi_m \) in our implementation penalizes jumps in conductivity between adjacent layers.

Descent methods (e.g. Nocedal & Wright, 2006) make use of the gradient \( \nabla \phi \) (and often also of the Hessian \( H(\phi) \)) to systematically move through the model space until a point is reached where \( \phi \) is minimum. Here, we apply the full Newton method, in which the model is updated as
\[ m_{k+1} = m_k - \alpha_k H^{-1}(\phi_k) \nabla \phi_k, \] (5.10)
where \( \alpha_k \) determines the step length in an inexact line-search (e.g. Nocedal & Wright, 2006). We compute model predictions \( C^{\text{pred}}(\omega) \), gradient, and Hessian of the data misfit \( \phi_d \) analytically as outlined in Appendix A.1.

Let us assume that \( \phi \) has a minimum at \( m_0 \). Since the gradient of \( \phi \) vanishes at \( m_0 \), a second-order polynomial approximation reads
\[ \phi(m_0 + \Delta m) \approx \phi(m_0) + \frac{1}{2} \Delta m^\top H(\phi(m_0)) \Delta m, \] (5.11)
with \( \Delta m \) being a perturbation of \( m_0 \). Let us define
\[ \Delta \phi = \phi(m_0 + \Delta m) - \phi(m_0) \] (5.12)
as a maximum permissible perturbation of \( \phi \). For simplicity, we allow \( C^{\text{pred}}(\omega) \) to deviate from \( C^{\text{obs}}(\omega) \) within uncertainties \( \delta C^{\text{obs}}(\omega) \). According to eq. (5.9), this yields \( \Delta \phi = 1 \) (if the regularization term is ignored). Eq. (5.11) can be rewritten as
\[ \Delta \phi = \frac{1}{2} \Delta m^\top H(\phi(m_0)) \Delta m. \] (5.13)
In case of a diagonal Hessian, this is easily solved for maximum perturbations of a model parameter \( m_j \):
\[ \Delta m_j = \sqrt{\frac{2 \Delta \phi}{H(\phi(m_0))_{jj}}}. \] (5.14)
In case of a non-diagonal Hessian, a more sophisticated relation can be derived (Pankratov & Kuvshinov, 2015), and a proxy for $\Delta m_j$ is given by

$$\Delta m_j = \sqrt{2\Delta \phi H(\phi(m_0))^{-1}}. \quad (5.15)$$

Whether diagonal or non-diagonal, the perturbations $\Delta m_j$ can be interpreted as estimates of model uncertainties. In the present context, these estimates only approximate the true model uncertainties. First, the use of a second-order polynomial implies a linearisation of a non-linear inverse problem around the minimum of the objective function. Second, the choice of $\Delta \phi = 1$ is heuristic, and there might be good reasons for other choices. Finally, the applied regularization has generated large covariances between model parameters, such that the bounds for the conductivity in a specific layer necessarily depend on the conductivity in all other layers. Nevertheless, the perturbations $\Delta m_j$ yield valuable information about relative uncertainties and thus about the resolution of the recovered model at different depths.

### 5.5.2 1-D inversion: implementation

The model is parametrized using $N = 40$ spherical layers in depth between Earth’s surface and the core-mantle boundary (CMB) located at a depth of 2890 km. A very good conductor is prescribed for the core. The thickness of the layers is generally fixed to 50 km at depths $<1000$ km and to 100 km underneath. Minor modifications of this rule permit layer boundaries at the main seismic discontinuities in the mid-mantle, located at depths of 410 km, 520 km, and 660 km, respectively.

We invert the corrected $C$-responses for several values of $\lambda$ and manually pick the final results from an L-curve relating $\phi_d$ and $\phi_m$ (Hansen, 1992), shown in Figure 5.6. In practice, we choose the “simplest” model, i.e., the model with smallest $\phi_m$, with the constraint $\phi_d < 1$.

![Figure 5.6: L-curve relating misfit term $\phi_d$ and regularization term $\phi_m$. The results shown in Figure 5.8 correspond to point 3, at which both $\phi_d$ and $\phi_m$ are minimized.](image-url)
The inverse Hessian at the point of convergence $m_0$ is shown in Figure 5.7. The matrix is diagonally-dominant, but contains significant energy in off-diagonal elements, implying correlations between the individual model parameters. These are particularly pronounced at depths $<400$ km and $>1600$ km, indicating that the solution at these depths might be more constrained by the regularization than by the data. We apply eq. (5.15) to calculate model uncertainties $\Delta m_j$.

Figure 5.8 shows the recovered 1-D model with its uncertainties determined by analysis of the inverse Hessian. Also shown is the conductivity profile recovered from uncorrected $C$-responses and the result of Kuvshinov & Olsen (2006). The recovered model is characterized by a highly resistive zone in the top 400 km, with a minimum value of $2 \times 10^{-3}$ S/m just beneath the surface shell. Conductivity increases steadily to a depth of 900 km, reaching a maximum of 2 S/m. The model then shows a distinct kink; at greater depths, conductivity is almost constant, varying between 1 S/m and 2 S/m down to the CMB. The correction for the ocean effect has a great influence on the results in the top 600 km. As expected, the corrected $C$-responses correspond to a considerably more resistive conductivity model. This model is also significantly more resistive than that recovered by Kuvshinov & Olsen (2006) to a depth of 800 km. Numerical values of the recovered conductivity model are provided in Table 5.2.

The uncertainty estimates form an hourglass-shaped structure. Smallest uncertainties are observed at depths between 800 km and 1200 km in line with the structure of the inverse Hessian (Figure 5.7). At depths $<400$ km and $>1600$ km, conductivity is poorly constrained.
5.5.3 Quasi-1-D inversion

In the previous sections, we showed how to correct the estimated responses for 3-D effects due to induction in the oceans by an iterative approach, and how to invert the corrected responses for 1-D conductivity structure. Although this approach has proven successful, a more natural and consistent treatment of 3-D effects is given by inverting the (uncorrected) responses directly in a 3-D environment.

We modified an existing modular 3-D inversion code (cf. Section 6.3) to invert for 1-D structure in the presence of a heterogeneous surface shell. For consistency with the existing implementation, the modified code does not invert $C$-responses, but the corresponding $Q$-responses (cf. eq. 5.1). In a 3-D environment, model predictions, gradient and Hessian of the data misfit cannot be computed analytically as in the 1-D case. The gradient is computed with finite differences, which requires $N$ additional forward
Table 5.2: Conductivity models obtained in the deterministic 1-D inversion. Depth (to the top of the respective layer) in km, and conductivity in S/m. Model $\sigma_1$ is obtained with the iterative correction scheme (red curve in Figure 5.8), model $\sigma_2$ is obtained with the direct quasi-1-D inversion (yellow curve in Figure 5.8).

<table>
<thead>
<tr>
<th>Depth</th>
<th>Model $\sigma_1$</th>
<th>Model $\sigma_2$</th>
<th>Depth</th>
<th>Model $\sigma_1$</th>
<th>Model $\sigma_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.814e-03</td>
<td>N/A</td>
<td>950</td>
<td>2.344e+00</td>
<td>1.873e+00</td>
</tr>
<tr>
<td>10</td>
<td>1.829e-03</td>
<td>5.703e-04</td>
<td>1000</td>
<td>1.815e+00</td>
<td>1.563e+00</td>
</tr>
<tr>
<td>60</td>
<td>1.916e-03</td>
<td>6.311e-04</td>
<td>1100</td>
<td>1.401e+00</td>
<td>1.379e+00</td>
</tr>
<tr>
<td>110</td>
<td>2.085e-03</td>
<td>7.587e-04</td>
<td>1200</td>
<td>1.232e+00</td>
<td>1.339e+00</td>
</tr>
<tr>
<td>160</td>
<td>2.348e-03</td>
<td>9.747e-04</td>
<td>1300</td>
<td>1.206e+00</td>
<td>1.387e+00</td>
</tr>
<tr>
<td>210</td>
<td>2.737e-03</td>
<td>1.319e-03</td>
<td>1400</td>
<td>1.269e+00</td>
<td>1.491e+00</td>
</tr>
<tr>
<td>260</td>
<td>3.304e-03</td>
<td>1.867e-03</td>
<td>1500</td>
<td>1.388e+00</td>
<td>1.619e+00</td>
</tr>
<tr>
<td>310</td>
<td>4.136e-03</td>
<td>2.741e-03</td>
<td>1600</td>
<td>1.542e+00</td>
<td>1.751e+00</td>
</tr>
<tr>
<td>360</td>
<td>5.378e-03</td>
<td>4.176e-03</td>
<td>1700</td>
<td>1.710e+00</td>
<td>1.871e+00</td>
</tr>
<tr>
<td>410</td>
<td>7.290e-03</td>
<td>6.577e-03</td>
<td>1800</td>
<td>1.874e+00</td>
<td>1.966e+00</td>
</tr>
<tr>
<td>460</td>
<td>1.034e-02</td>
<td>1.076e-02</td>
<td>1900</td>
<td>2.019e+00</td>
<td>2.039e+00</td>
</tr>
<tr>
<td>520</td>
<td>1.559e-02</td>
<td>1.848e-02</td>
<td>2000</td>
<td>2.136e+00</td>
<td>2.077e+00</td>
</tr>
<tr>
<td>560</td>
<td>2.460e-02</td>
<td>3.302e-02</td>
<td>2100</td>
<td>2.224e+00</td>
<td>2.099e+00</td>
</tr>
<tr>
<td>610</td>
<td>4.158e-02</td>
<td>6.269e-02</td>
<td>2200</td>
<td>2.284e+00</td>
<td>2.096e+00</td>
</tr>
<tr>
<td>660</td>
<td>7.604e-02</td>
<td>1.276e-01</td>
<td>2300</td>
<td>2.322e+00</td>
<td>2.087e+00</td>
</tr>
<tr>
<td>700</td>
<td>1.497e-01</td>
<td>2.737e-01</td>
<td>2400</td>
<td>2.344e+00</td>
<td>2.071e+00</td>
</tr>
<tr>
<td>750</td>
<td>3.248e-01</td>
<td>6.073e-01</td>
<td>2500</td>
<td>2.356e+00</td>
<td>2.059e+00</td>
</tr>
<tr>
<td>800</td>
<td>7.490e-01</td>
<td>1.235e+00</td>
<td>2600</td>
<td>2.360e+00</td>
<td>2.050e+00</td>
</tr>
<tr>
<td>850</td>
<td>1.596e+00</td>
<td>1.915e+00</td>
<td>2700</td>
<td>2.362e+00</td>
<td>2.047e+00</td>
</tr>
<tr>
<td>900</td>
<td>2.412e+00</td>
<td>2.106e+00</td>
<td>2800</td>
<td>2.362e+00</td>
<td>2.045e+00</td>
</tr>
</tbody>
</table>

computations per iteration. A quasi-Newton method (e.g. Nocedal & Wright, 2006) is employed to find the minimum of the objective function $\phi$. As in the 1-D case, $\phi$ includes a regularization term that minimizes jumps between adjacent layers.

We applied the modified 3-D inversion code to the uncorrected $Q$-responses. The results for an appropriate regularization parameter are shown in Figure 5.8 and tabulated in Table 5.2. At depths $>400$ km, the result agrees perfectly with that of the iterative 1-D inversion. At shallower depths, the result of the direct inversion is slightly more resistive, but well within uncertainties. The very good agreement of the results confirms the functionality of the iterative approach, which is computationally less expensive than the direct method. It also justifies the more pronounced effect of the correction compared to that of Kuvshinov & Olsen (2006), cf. Figure 5.5.

5.6 Probabilistic inversion

5.6.1 Definitions

In contrast to deterministic inversion, probabilistic or Bayesian inversion (e.g. Tarantola, 2005) does not seek a single model that explains data. Instead, it explores the parameter
space and generates a multitude of models that can be analysed statistically.

Central to the Bayesian approach to inverse problems is the use of probability density functions (pdfs) to describe any piece of information entering the problem. We define a prior pdf $\rho(m)$, which contains information about the model that is independent of data, a likelihood function $L(m)$ measuring the probability density of a model given data, and a posterior pdf $\Sigma(m)$, which is given by

$$\Sigma(m) = \kappa \rho(m) L(m),$$

where $\kappa$ is a proportionality factor ensuring that the integral of $\Sigma(m)$ over the entire model space equals 1. Integrating $\Sigma(m)$ over a part of the model space corresponds to the probability that the true model $m^*$ lies within that part, given data and prior information. Assuming

$$L(m) = \exp(-\phi_d(m))$$

and

$$\rho(m) = \exp(-\lambda \phi_m(m)),$$

a maximization of $\Sigma$ becomes equivalent to a minimization of $\phi$ in the deterministic inversion. The formulation of $\phi_d$, given by eq. (5.9), implies a Gaussian pdf for $L$.

### 5.6.2 Grid-based sampling

Grid-based sampling, also known as “exhaustive search”, is the most straightforward solution to probabilistic inverse problems. The full model space (except possibly for irrelevant parts) is binned by a multidimensional grid, and pdfs are computed for each grid point. Unfortunately, this method is computationally very expensive and generally only feasible in case of a small number of model parameters.

We divide the model domain into eight layers with thickness of 200 km each at depths between 0 km and 1600 km. The model is fixed at greater depths. For each layer, nine logarithmically spaced values for the conductivity are tested, ranging between $10^{-3}$ S/m and 10 S/m. This yields $9^8$ different combinations. For each combination, we compute the misfit $\phi_d$ as defined by eq. (5.9), a regularization term $\phi_m$ penalizing jumps in conductivity between adjacent layers and the posterior pdf $\Sigma(m)$ according to eqs (5.16)–(5.18) for different $\lambda$. Note that the computation of the misfit involves the corrected $C$-responses $C^{corr}(\omega)$.

Following the argumentation of Tarantola (2005) for strictly positive parameters such as conductivity, we can claim that each of our models represents an equally large part of the model space. The probability of such a part containing $m^*$ is therefore just a scaling of $\Sigma(m)$. We scale $\kappa$ such that $\sum_k \Sigma(m_k) = 1$. The results are shown in Figure 5.9 for six different regularization parameters $\lambda$. 


For $\lambda = 0$ (top left panel), a lot of models agree well with data, as indicated by the various shades of grey in each layer. Only the layer extending from 800 km to 1000 km seems to be well constrained. If increasing $\lambda$, the number of acceptable models decreases, and a preferred structure forms in the parameter space. This structure consists of a resistive upper mantle (0–400 km), increasing conductivity in and beneath the transition zone (400–800 km) and a good conductor underneath. For $\lambda = 30$ (bottom left panel), only a single model with considerable probability remains. This model has great similarity with the result of the deterministic inversion (Figure 5.8). Increasing $\lambda$ further yields smoother models with higher conductivity in the upper and middle mantle.
### 5.6.3 Monte Carlo sampling

While grid-based sampling is supposed to explore the full parameter space, Monte Carlo methods are tailored to explicitly sample those parts of it where $\Sigma(m)$ is large. This saves computational cost, which can be invested in a finer parametrization of the model. We use the Metropolis-Hastings algorithm (Metropolis et al., 1953; Hastings, 1970), which was shown to be particularly efficient in sampling the posterior pdf. It can be described as follows (Mosegaard & Tarantola, 1995):

Given a function $K(m)$, which samples the prior pdf iteratively, and a uniformly distributed random number $\alpha$ drawn from the interval $[0, 1]$, the model is updated as

$$m_{k+1} = \begin{cases} K(m_k) & \text{if } \alpha \leq \min\left(1, \frac{L(K(m_k))}{L(m_k)}\right), \\ m_k & \text{else,} \end{cases} \quad (5.19)$$

with $L(m)$ defined as in eq. (5.17). This algorithm generates successive samples of the posterior pdf without explicitly calculating $\Sigma(m)$. The sampling density is proportional to the probability density, i.e. low-probability areas of the model space are sampled less excessively.

The critical aspect in the implementation of the Metropolis-Hastings algorithm is the function $K(m)$, which is supposed to generate successive samples of the prior pdf. The constraints imposed upon the model in deterministic inversion (Section 5.5) are not easily applicable in Monte Carlo methods. Based on laboratory measurements of anhydrous mantle mineral conductivities, Khan et al. (2011) assumed conductivity to be a non-decreasing function of depth. This strong constraint, however, yielded unrealistically small model uncertainties (not shown here for brevity). We therefore opted for the following constraints:

1. Conductivity must not vary by more than one order of magnitude between adjacent layers,
2. Conductivity has to lie in the range $[10^{-5} \text{ S/m}; 10^{3} \text{ S/m}]$.

We use the same model parametrization as for the deterministic inversion, in which the $i$-th model parameter relates to the conductivity of the $i$-th layer as $m_i = \log_{10}(\sigma_i/\sigma_0)$, with $\sigma_0 = 1 \text{ S/m}$. This yields an equivalent first constraint for $m$ and boundary values $m_{\text{min}}$ and $m_{\text{max}}$. The number of model parameters to be perturbed in an iteration according to the above constraints was adjusted to yield an overall acceptance rate of 40%.

$10^6$ models were sampled in total. In Figure 5.8, we present 400 near-independent samples of the posterior pdf, obtained by retaining only one sample every 1000 iterations. The collection of sampled models agrees well with the result of the deterministic
inversion. The spread of the models is minimum at a depth of 1000 km and increases both at shallower and greater depths, in agreement with the uncertainty estimates of the deterministic inversion. The results of the Monte Carlo inversion, however, do not spread symmetrically around the result of the deterministic inversion. This is particularly the case in the top 800 km, where the Monte Carlo results tend to smaller conductivities.

In line with Mosegaard & Tarantola (1995), we do not compute measures such as a mean model and covariances, since these would rely on assumptions about the posterior pdf, e.g. the assumption that the pdf is Gaussian. We think that the pdf is best characterized by the distribution of the samples themselves.

5.7 Discussion

Deterministic inversion is computationally cheap and therefore most often the preferred solution in large geophysical inverse problems. Comparison of our result to that of Kuvshinov & Olsen (2006) shows large differences in the top 800 km, where our model is significantly more resistive. The model of Kuvshinov & Olsen is generally smoother, which is most probably due to stronger regularization. The fact that the models partially differ by more than an order of magnitude, however, is most likely due to data-related issues:

1. The real part of our $C$-responses is larger at all periods, which is due to the fact that Kuvshinov & Olsen included a damping parameter when processing the raw data.

2. Kuvshinov & Olsen estimated $C$-responses at periods $< 1$ day and therefore sampled shallower depths.

3. The effect of the correction for induction in the oceans is slightly more pronounced in our study (cf. Figure 5.5) due to different correction schemes.

In contrast to Kuvshinov & Olsen, we provide model uncertainties, estimated from the inverse Hessian of the objective function. These uncertainties should rather be interpreted qualitatively than quantitatively, because their estimation is based on several approximations (cf. Section 5.5). Nevertheless, they provide good indications of the resolution and show that our data are most sensitive to conductivity at depths between 800 km and 1200 km. The most prominent feature of our results, the marked kink at a depth of 900 km, lies in this well-resolved depth range and thus might represent real structure.

Probabilistic approaches to inverse problems offer an alternative, generally more consistent framework for analysing the reliability of a recovered model. The probability maps obtained in grid-based sampling unfortunately did not prove very useful to this
purpose. From a certain amount of regularization onwards, the solution converged to a single model. A more informative map might be achievable with a finer parametrization, but that is computationally prohibitive.

The results of an independent Monte Carlo study, which relied on different prior information, agree well with those of the deterministic inversion. In particular, the marked kink at a depth of 900 km is also visible in the Monte Carlo results. The recovered models, however, tend to smaller conductivities in the upper mantle and show more structure in the lower mantle. This might indicate that the prior constraints used in the deterministic inversion are slightly stronger than those used in the probabilistic inversion. The Monte Carlo results also confirm the depth-dependency of the uncertainties obtained in the deterministic inversion. Only in the top 600 km, the upper bound of these uncertainties appears too large.

The results of both deterministic and probabilistic inversion exhibit a subtle decrease of conductivity at depths $>900$ km. Since a similar feature was also observed in the results of the test studies (Figure 5.3), it might rather be a numerical artefact than real structure. The uncertainty estimates in Figure 5.8 clearly show that the data can be explained by a model in which conductivity is a non-decreasing function of depth.

### 5.8 Preliminary interpretation of mantle conductivity

To interpret the inverted conductivity profile (Figure 5.8), we construct laboratory-based conductivity profiles as a function of mantle composition, temperature, pressure, and water content. We combine laboratory measurements of mineral conductivity with a self-consistently computed mineralogical model of the Earth’s mantle using Gibbs free-energy minimization following the approach outlined in Khan & Shankland (2012). For present purposes, we assume a chemically homogeneous and adiabatic mantle made of pyrolite. The bulk electrical conductivity profiles so computed are shown in Figure 5.10 for different values of mantle water content (here restricted to be present in the minerals olivine (ol), orthopyroxene, wadsleyite (wads), and ringwoodite) and self-consistently computed mantle adiabats. Input temperature for the latter is defined as the temperature at the location where the mantle adiabat intersects the conductive geotherm at 150 km depth. For more details on constructing laboratory-based conductivity profiles, we refer the reader to Khan & Shankland (2012).

The discontinuities associated with mineral phase transformations at 410, 520, and 660 km depth are clearly present in the laboratory-based conductivity profiles, but absent in the field-derived profile. The inability of EM fields to sense discontinuities results directly from their diffusive nature. Conductivities found here in the upper mantle appear to be well-estimated by an upper mantle water content of 0.001 wt% and a mantle temperature of 1200°C at 150 km depth in line with earlier observations (e.g.
Figure 5.10: 1-D conductivity profiles estimated in this study (blue line) and computed using laboratory-based conductivity data for various mantle water contents and temperatures. Ol and wads refer to major upper mantle and transition-zone minerals olivine and wadsleyite, respectively. $T_{ad}$ is the temperature at the location where the mantle adiabat intersects the conductive geotherm at 150 km depth. For the computations related to variations in water content (black lines) we assumed a mantle adiabat of 1300°C with an intersection depth of 100 km, whereas for the mantle adiabats (grey lines) we fixed water content to 0.001 wt% (ol) and 0.01 wt% (wads). $\sigma_0=1$ S/m.

Karato, 2011; Khan & Shankland, 2012; Yoshino & Katsura, 2013). In the absence of conductivity measurements of hydrous lower mantle minerals, the kink in the lower at around 900 km depth either requires higher temperatures or the presence of material of higher conductivity such as that associated with ponding of melt in and below the transition zone. Recent geophysical studies suggest ponding of melt at the top of the lower mantle as a means of explaining some anomalous features. For example, in a regional 3-D EM study Koyama et al. (2014) found a strong a conductivity anomaly underneath the south-eastern part of Australia at the bottom of the transition-zone that appears to require the presence of melt. Schmandt et al. (2014), using P-to-S conversions (receiver functions), likewise observed what appears to be evidence for melt below the transition-zone underneath the North American continent. Locally large conductivity anomalies
in the topmost lower mantle might be related to carbonate melts, which have been observed experimentally to increase conductivity significantly beyond what is possible with hydrous olivine (e.g., Gaillard et al., 2008; Yoshino et al., 2012). As discussed by e.g., Litasov (2011) melting in CO$_2$-containing systems can produce carbonate melts in these regions of the mantle.
Chapter 6

3-D Inversion for Mantle Conductivity Structure

6.1 Introduction

Mapping 3-D structure of electrical conductivity in Earth’s mantle is one of the primary scientific objectives for the Swarm multi-satellite geomagnetic mission (Chapter 4). Global 3-D mantle conductivity models were derived before by Kelbert et al. (2009) and Semenov & Kuvshinov (2012). These studies were based on C-responses, derived with the Z/H-method from data from the global network of geomagnetic observatories. Although differing in details, the recovered global 3-D images reveal a substantial level of lateral heterogeneity in the mantle at depths between 410 and 1600 km. Conductivity in the results varies laterally by more than an order of magnitude between resistive and conductive regions.

Bearing in mind that geomagnetic observatories are sparsely and irregularly distributed with large gaps in oceanic regions and the southern hemisphere, an interpretation of the 3-D inversion results in many regions requires extreme care. A lack of observations precludes any conclusive inferences about conductivity distributions in these regions. In spite of continuing efforts to improve the coverage by long-term measurements in those regions (Shimizu & Utada, 1999; Chulliat et al., 2009; Korte et al., 2009; Matzka et al., 2009, among others), reliable images of 3-D variations of mantle conductivity in oceanic regions and as a whole in the southern hemisphere can hardly be obtained at present or in the foreseeable future with the use of ground-based data alone. Moreover, the use of C-responses derived with the Z/H-method is problematic in case of a complex source structure, as elaborated in Chapter 3. For the mentioned reasons, the 3-D models presented by Kelbert et al. (2009) and Semenov & Kuvshinov (2012) hardly contain reliable information about lateral variations in conductivity.

The Swarm mission has prompted the development of methodologies for recovering 3-D electrical conductivity variations from space. Early concepts and model studies
were summarized in the report by Kuvshinov et al. (2010). A rigorous time-domain approach was described by Velímský (2013). Frequency-domain approaches, based on time spectra of induced coefficients $\iota_k^l$ and matrix $Q$-responses, were elaborated by Püthe & Kuvshinov (2013b, 2014). The text in this chapter in large parts follows the two latter papers. Modifications of the general concept to invert the new ground- and sea-based transfer functions introduced in Section 2.4.2 are discussed alongside.

6.2 Mathematical formulation

6.2.1 General concept

The inverse problem of conductivity recovery is formulated as an optimization problem. We aim at minimizing an objective function $\phi(m, \lambda)$ given by

$$\phi(m, \lambda) = \phi_d(m) + \lambda \phi_m(m), \quad (6.1)$$

where $\phi_d$ is data misfit and $\lambda$ and $\phi_m$ are regularization parameter and regularization term, respectively. Note that eq. (6.1) is identical to eq. (5.8), which was used in the deterministic inversion for 1-D mantle conductivity structure. For the recovery of 3-D conductivity structure, we stick to the deterministic formulation – the alternative, probabilistic inversion methods presented in Section 5.6 are to date not applicable due to computational limitations.

The data misfit $\phi_d(m)$ is conventionally written as

$$\phi_d(m) = \|F(m) - d\|^2 C_d^{-1} [F(m) - d], \quad (6.2)$$

where $d$ is the data vector, in our case usually composed of $N_d$ observed (estimated) transfer functions, and $m$ is the model vector, composed of the $N_m$ model parameters, which describe conductivity structure of Earth’s mantle. $F$ is the functional solving the forward problem, i.e. predicting the model responses for a given $m$, and $C_d$ is the data covariance matrix.

Covariances between individual transfer functions are generally hard to estimate reliably. $C_d$ is therefore often assumed to be diagonal, i.e. to contain only the variances of the estimated transfer functions, which can be estimated with the data processing algorithm outlined in Section 2.5. With the assumption of a diagonal covariance matrix, we can rewrite eq. (6.2) as

$$\phi_d(m) = \sum_{i=1}^{N_d} \frac{|F_i(m) - d_i|^2}{(\delta d_i)^2}. \quad (6.3)$$
In this representation, $\phi_d(m)$ is the weighted sum of the squared differences between observed and predicted (modelled) transfer functions, with the uncertainties $\delta d_i$ serving as weights. Here and in the following, the term “uncertainties” generally refers to the estimated confidence intervals.

The regularization term $\phi_m(m)$ is conventionally written as

$$
\phi_m(m) = m^\top C_m^{-1} m, \tag{6.4}
$$

where $C_m$ is the model covariance matrix. It is often more convenient not to define $C_m$, but a regularization matrix $W$, such that $W^\top W = C_m^{-1}$. With this definition, we can rewrite eq. (6.4) as

$$
\phi_m(m) = (Wm)^\top (Wm). \tag{6.5}
$$

$W$ is supposed to smooth the solution, its form depends on the desired level of smoothness and the parametrization of the model. Regularization will be discussed more thoroughly in Section 6.3.3.

Due to the non-linearity of 3-D EM inverse problems, iterative descent methods (e.g. Nocedal & Wright, 2006) are typically the methods of choice. These methods require a computation of the gradient of the penalty function $\phi$ with respect to the model parameters, i.e.

$$
\nabla \phi = \left( \frac{\partial \phi}{\partial m_1}, \frac{\partial \phi}{\partial m_2}, \ldots, \frac{\partial \phi}{\partial m_{N_m}} \right)^\top. \tag{6.6}
$$

While the gradient of the regularization term is easily calculated analytically and given by

$$
\nabla \phi_m(m) = 2W^\top Wm, \tag{6.7}
$$

the calculation of the data misfit gradient is more challenging. Let us take the derivative of $\phi_d$ as defined in eq. (6.3) with respect to model parameter $m_k$. This yields

$$
\frac{\partial \phi_d}{\partial m_k} = 2\text{Re} \sum_{i=1}^{N_d} \frac{[F_i(m) - d_i]^* \frac{\partial F_i(m)}{\partial m_k}}{(\delta d_i)^2}, \tag{6.8}
$$

where the upper asterisk * stands for complex conjugate. The above representation arises from taking the derivative of the squared norm of a complex-valued function $z(m)$ (Pankratov & Kuvshinov, 2010),

$$
\frac{\partial}{\partial m} |z(m)|^2 = \frac{\partial}{\partial m} (zz^*) = \frac{\partial z}{\partial m} z^* + z \frac{\partial z^*}{\partial m} = \frac{\partial z}{\partial m} z^* + \left( z^* \frac{\partial z}{\partial m} \right)^* = 2\text{Re} \left( z^* \frac{\partial z}{\partial m} \right), \tag{6.9}
$$

The last term in eq. (6.8) is the partial derivative of the function $F_i(m)$ with respect to the model parameter $m_k$. The partial derivatives of $F(m)$ are also known as sensitivities, as they reflect the change of a given response when perturbing a given model parameter.
The sensitivities are assembled in the *Jacobian* $J(m)$. It seems straightforward to derive $J$ by means of numerical differentiation, using a formula like

$$J_{ik} = \frac{\partial F_i(m)}{\partial m_k} \approx \frac{F_i(m_1, \ldots, m_k + \Delta m_k, \ldots, m_{N_m}) - F_i(m_1, \ldots, m_k, \ldots, m_{N_m})}{\Delta m_k}.$$  (6.10)

But this method requires extremely high computational loads, as it involves $N_m$ (per frequency and source configuration) additional solutions of the forward problem. On top, the solution is approximate by nature, as $\Delta m_k$ is finite. A much more efficient and elegant way to rigorously calculate the gradient of the misfit is provided by an adjoint approach (e.g. Dorn *et al.*, 1999).

The adjoint approach does not rely on an explicit determination of $J$, and it allows the calculation of the misfit gradient for the price of only a few additional forward calculations, which rely on a specific (adjoint) source. Each inverse problem setting requires the finding of explicit formulas for the adjoint source. We will now first outline the general concept, following the derivation by Pankratov & Kuvshinov (2010), and thereafter derive formulas for specific settings. For convenience, we will in the following sections work with the total differential of the data misfit instead of partial derivatives. We therefore rewrite eq. (6.8) as

$$d\phi_d = 2\text{Re} \sum_{i=1}^{N_d} \left[ F_i(m) - d_i \right]^* \frac{\partial}{\partial d_i^2} dF_i(m).$$  (6.11)

Explicit derivatives with respect to the model parameters $m_k$ depend on the parametrization of the inversion domain and will be discussed in Section 6.3.2.

### 6.2.2 Adjoint approach

Let us start by re-writing Maxwell’s equations (2.12) and (2.13),

$$\frac{1}{\mu_0} \nabla \times \mathbf{B}_p = \sigma \mathbf{E}_p + \mathbf{j}_p, \quad (6.12)$$
$$\nabla \times \mathbf{E}_p = i\omega \mathbf{B}_p, \quad (6.13)$$

where $\mathbf{j}_p$ is an extraneous current with a given polarization $p$. $\mathbf{E}_p = \mathcal{G}^{cj}(\mathbf{j}_p)$ and $\mathbf{B}_p = \mathcal{G}^{bj}(\mathbf{j}_p)$ are the electric and magnetic fields excited by this source, respectively. $\mathcal{G}^{cj}$ and $\mathcal{G}^{bj}$ are here defined as operators that solve Maxwell’s equations (6.12)–(6.13) for a given current source. We will also need the solution of a modified set of Maxwell’s equations,

$$\frac{1}{\mu_0} \nabla \times \mathbf{B}_q = \sigma \mathbf{E}_q, \quad (6.14)$$
$$\nabla \times \mathbf{E}_q = i\omega \mathbf{B}_q + \mu_0 \mathbf{h}_q, \quad (6.15)$$
where \( h_q \) is a “magnetic source” term with a given polarization \( q \). \( E_q = G^{eh}(h_q) \) is the electric field solution of this modified set of Maxwell’s equations. Pankratov & Kuvshinov (2010) showed that this formulation can be converted into the more common representation of Maxwell’s equations with a current source, given by eqs (6.12)–(6.13). Eqs (6.14)–(6.15) are, however, convenient for the adjoint approach, as will become clear later. An important property of the operators \( G^{ej} \), \( G^{eh} \) and \( G^{bj} \) are their reciprocity relations (Pankratov & Kuvshinov, 2010):

\[
\langle G^{ej}(a), b \rangle = \langle a, G^{ej}(b) \rangle, \quad (6.16)
\]

\[
\langle G^{eh}(a), b \rangle = \langle a, G^{bj}(b) \rangle, \quad (6.17)
\]

where

\[
\langle a, b \rangle = \int_{\mathbb{R}^3} a(r) \cdot b(r) \, dv \quad (6.18)
\]

denotes a complex-valued bilinear scalar product.

Let us now consider eqs (6.12)–(6.13) in an Earth’s model with infinitesimally changed conductivity \( \sigma + d\sigma \), yielding electric and magnetic fields \( E_p + dE_p \) and \( B_p + dB_p \), respectively:

\[
\begin{align*}
\frac{1}{\mu_0} \nabla \times (B_p + dB_p) &= (\sigma + d\sigma)(E_p + dE_p) + j_p, \quad (6.19) \\
\nabla \times (E_p + dE_p) &= i\omega(B_p + dB_p). \quad (6.20)
\end{align*}
\]

Now subtract eqs (6.12)–(6.13) from eqs (6.19)–(6.20):

\[
\begin{align*}
\frac{1}{\mu_0} \nabla \times dB_p &= (\sigma + d\sigma)dE_p + d\sigma E_p, \quad (6.21) \\
\nabla \times dE_p &= i\omega dB_p. \quad (6.22)
\end{align*}
\]

Using the operators defined above, we can rewrite eq. (6.21) as

\[
\frac{1}{\mu_0} \nabla \times dB_p = \sigma dE_p + d\sigma G^{ej}(j_p). \quad (6.23)
\]

Note that we neglected the second-order quantity \( d\sigma dE_p \). Eqs (6.22)–(6.23) constitute a set of Maxwell’s equations for the infinitesimal fields \( dE \) and \( dB \) excited by the “source” \( d\sigma G^{ej}(j_p) \). With the operators defined above,

\[
\begin{align*}
\quad dE_p &= G^{ej}(d\sigma G^{ej}(j_p)), \quad (6.24) \\
\quad dB_p &= G^{bj}(d\sigma G^{ej}(j_p)). \quad (6.25)
\end{align*}
\]
Let $F_i$ be any of the model responses calculated by $F(m)$ at any frequency and for site $r_i$. The total differential of $F_i$ is given by
\[
d F_i = \sum_p \left( \frac{\partial F_i}{\partial E_p} dE_p + \frac{\partial F_i}{\partial B_p} dB_p \right).
\] (6.26)

The partial derivatives of $F_i$ with respect to $E$ and $B$ are usually easily evaluated analytically. The actual formulation depends on the considered transfer functions; some examples will be discussed in Section 6.2.3. Note the sum over polarizations $p$, which reflects the fact that measured fields can be decomposed into fields due to different source polarizations, cf. eq. (2.14). Inserting eqs (6.24)–(6.25) into eq. (6.26) yields
\[
d F_i = \sum_p \left( \frac{\partial F_i}{\partial E_p} G^{ej}(r_i) d\sigma G^{ej}(j_p) + \frac{\partial F_i}{\partial B_p} G^{bj}(r_i) d\sigma G^{ej}(j_p) \right).\] (6.27)

For the following calculations, remember an important property of Dirac’s delta function, which reads
\[
\int_{\mathbb{R}^3} f(r') \delta(r - r') dv' = f(r).\] (6.28)

With eq. (6.28) and the reciprocity relations (6.16)–(6.17), eq. (6.27) can be rewritten as
\[
d F_i = \sum_p \left( G^{ej}(r_i) \left( \frac{\partial F_i}{\partial E_p} \delta(r - r_i) \right), d\sigma G^{ej}(j_p) \right) + \left( G^{eh}(r_i) \frac{\partial F_i}{\partial B_p} \delta(r - r_i), d\sigma G^{ej}(j_p) \right),\] (6.29)
or, by defining $G^e(j, h) = G^{ej}(j) + G^{eh}(h),$
\[
d F_i = \sum_p \left( G^e \left( \frac{\partial F_i}{\partial E_p}, \frac{\partial F_i}{\partial B_p} \right) \delta(r - r_i), d\sigma G^{ej}(j_p) \right).\] (6.30)

To compute $dF_i$, we thus have to solve Maxwell’s equations not only for the extraneous current sources $j_p$, but also for an additional, fictitious source, which consists of an EM point source at the measurement site.

Now remember that $F_i$ was defined as one specific model response at a specific frequency and at site $r_i$, while we are eventually interested in the gradient of the data misfit $\nabla \phi_d$. Thanks to the linearity of the operators $G^{ej}$ and $G^{eh}$, an insertion of eq. (6.30) into eq (6.11) yields the simple formula
\[
d \phi_d = 2\text{Re} \sum_\omega \sum_p \left( G^e \left( A^e_p, A^h_p \right), d\sigma G^{ej}(j_p) \right),\] (6.31)
where $A^e_p(r, \omega)$ and $A^h_p(r, \omega)$ are electric and magnetic adjoint sources, respectively. For a general derivation of eq. (6.31), and a general representation of $A^e_p$ and $A^h_p$, we refer to Pankratov & Kuvshinov, 2010. The adjoint sources will be derived for some examples.
in Section 6.2.3. Eq. (6.31) shows the essence of the adjoint approach: Only one (per frequency $\omega$ and polarization $p$) additional solution of the forward problem is required to compute the data misfit gradient $\nabla \phi_d$.

The derivations so far did not contain any assumptions about the parametrization in a numerical application. Let us now assume that the model domain consists of cells with piecewise constant conductivity $\sigma_k$. Such a parametrization is e.g. used by the forward solver $x3dg$ (Kuvshinov, 2008; Kuvshinov & Semenov, 2012), which we use to simulate induction in a 3-D Earth model. In this case, the integral over $\mathbb{R}^3$ inherent to eq. (6.31) can be split into integrals over the individual cells, such that

$$\frac{\partial \phi_d}{\partial \sigma_k} = 2 \text{Re} \sum_{\omega} \sum_{p} \int_{V_k} \left( E_p^{(j)} (r, \omega) \cdot E_p^{(A)}(r, \omega) \right) dv,$$

(6.32)

where $V_k$ is the volume of the cell comprised by $\sigma_k$, superscript $(j)$ indicates the current source $J_p$, and superscript $(A)$ indicates the adjoint source. The derivative of $\phi_d$ with respect to the model parameter $m_j$ is dependent on the parametrization of the inversion domain and follows from eq. (6.32) with the chain rule. Examples will be discussed in Section 6.3.2.

### 6.2.3 Application to new transfer functions

The concept elaborated in the previous section will now be applied to some of the transfer functions introduced in Section 2.4.2. In particular, we will derive adjoint sources for the $Q$-matrix $Q_{lm}^{kn}$, for the ground-based responses $T_m^m$, and for the cable responses $K_m^m$. On top of that, we will derive the adjoint source for time spectra of induced coefficients $\iota^l_k$.

**Induced coefficients**  If the EM data are described by induced coefficients estimated for a set of frequencies, the misfit (6.3) can be written as

$$\phi_d (m) = \sum_\omega \sum_{k,l} \left| \iota^l_k (m) - \iota^l_k \right|^2 \delta \iota^l_k \left( \omega \right)^2.$$

(6.33)

Here and in the following, superscript “pred” denotes modelled (predicted) data, whereas superscript “obs” denotes observed data. The $\iota^l_k \text{pred}$ are conveniently derived from the radial component of the magnetic field. At Earth’s surface,

$$B_r (r_a, \omega) = B_r^{\text{ext}} (r_a, \omega) + \sum_{k,l} (k + 1) \iota^l_k (\omega) Y^l_k (\theta, \varphi),$$

(6.34)
which follows directly from eq. (2.22). By making use of the orthogonality of the spherical harmonics $Y^l_k$, we can solve this for $t^l_k$,

$$
t^l_{k,\text{pred}}(\omega) = \frac{1}{(k + 1)\|Y^l_k\|^2} \int_S (B_r(r_a, \omega) - B^\text{ext}_r(r_a, \omega)) Y^l_k(\vartheta, \varphi) d\Omega. \quad (6.35)
$$

Here, $d\Omega = \sin \vartheta d\vartheta d\varphi$, and $\|Y^l_k\|^2$ is the squared norm of the spherical harmonic $Y^l_k$.

Note that $B^\text{ext}_r$ depends only on the external current source $j^\text{ext}$. $B_r$, however, also depends on Earth’s conductivity structure (and thus on $m$).

Taking the differential of eq. (6.35) yields

$$
dt^l_{k,\text{pred}}(\omega) = \frac{1}{(k + 1)\|Y^l_k\|^2} \int_S dB_r(r_a, \omega) Y^l_k(\vartheta, \varphi) e_r(r) \delta(r - a) \quad (6.36)
$$

This result is in line with the general formula (6.26); note, however, the absence of a sum over source polarizations. By inserting eq. (6.36) into eq. (6.30) we obtain

$$
d\phi_d(m) = 2\text{Re} \sum_{\omega} \sum_{k,l} \left[ t^l_{k,\text{pred}}(\omega, m) - t^l_{k,\text{obs}}(\omega) \right]^* \delta t^l_{k,\text{obs}}(\omega)^2 dt^l_{k,\text{pred}}(\omega, m). \quad (6.39)
$$

By inserting eq. (6.37), changing the order of summation and integration and making use of the linearity of the operator $G^{ch}$, this can be simplified to

$$
d\phi_d(m) = 2\text{Re} \sum_{\omega} \left\langle G^{ch}(A), d\sigma G^{-}\langle j^{\text{ext}} \rangle \right\rangle. \quad (6.40)
$$

$A(r, \omega)$ is the adjoint source, given by

$$
A(r, \omega) = \sum_{k,l} \left[ t^l_{k,\text{pred}}(\omega, m) - t^l_{k,\text{obs}}(\omega) \right]^* \delta t^l_{k,\text{obs}}(\omega)^2 h^l_k(r). \quad (6.41)
$$
Eq. (6.40) is equivalent to the general formula (6.31). Note that the sum over source polarizations $p$ drops out, since the formulation is not based on transfer functions, but on time spectra of observables.

**$Q$-matrix** The derivations for the $Q$-matrix are very similar. The data misfit is given by

$$\phi_d(\mathbf{m}) = \sum_\omega \sum_{k,l} \sum_{n,m} \frac{\left| Q_{kn}^{lm,\text{pred}}(\omega, \mathbf{m}) - Q_{kn}^{lm,\text{obs}}(\omega) \right|^2}{\delta Q_{kn}^{lm,\text{obs}}(\omega)^2}. \quad (6.42)$$

In line with eq. (2.17), let us denote the magnetic field due to a unit amplitude spherical harmonic source $Y_n^m$ with $B_n^m$. With the definition of the $Q$-matrix (2.37), we can write a relation similar to eq. (6.34),

$$B_{n,r}^m(\mathbf{r}_a, \omega) = B_{n,r}^{m,\text{ext}}(\mathbf{r}_a, \omega) + \sum_{k,l} (k + 1) Q_{kn}^{lm}(\omega) Y_k^l(\vartheta, \varphi). \quad (6.43)$$

The predicted responses $Q_{kn}^{lm,\text{pred}}$ are derived by making use of the orthogonality of the spherical harmonics,

$$Q_{kn}^{lm,\text{pred}}(\omega) = \frac{1}{(k + 1) \| Y_k^l \|^2} \int_S \left( B_{n,r}^m(\mathbf{r}_a, \omega) - B_{n,r}^{m,\text{ext}}(\mathbf{r}_a, \omega) \right) Y_k^l(\vartheta, \varphi) d\Omega, \quad (6.44)$$

and the differential is given by

$$dQ_{kn}^{lm,\text{pred}}(\omega) = \frac{1}{(k + 1) \| Y_k^l \|^2} \int_S dB_{n,r}^m(\mathbf{r}_a, \omega) Y_k^l(\vartheta, \varphi) d\Omega. \quad (6.45)$$

In analogy to eq. (6.25),

$$dB_n^m = G^{bj} \left( d\sigma G^{cj}(j_n^m) \right). \quad (6.46)$$

As above for the induced coefficients, the surface integral in eq. (6.45) can be transformed into a volume integral. The resulting formula reads

$$dQ_{kn}^{lm,\text{pred}}(\omega) = \left\langle G^{ek}(\mathbf{h}_k^l), d\sigma G^{cj}(j_n^m) \right\rangle, \quad (6.47)$$

with $\mathbf{h}_k^l$ defined as in eq. (6.38).

The gradient of the data misfit $\phi_d$ is derived from eq. (6.42),

$$d\phi_d(\mathbf{m}) = 2 \text{Re} \sum_\omega \sum_{k,l} \sum_{n,m} \left[ Q_{kn}^{lm,\text{pred}}(\omega, \mathbf{m}) - Q_{kn}^{lm,\text{obs}}(\omega) \right]^* dQ_{kn}^{lm,\text{pred}}(\omega, \mathbf{m}). \quad (6.48)$$

This equation is very similar to the corresponding formula for induced coefficients, eq. (6.39). Note, however, the sum over $n$ and $m$, which corresponds to different source polarizations.
polarizations. The adjoint formulation is given by

$$d\phi_d(m) = 2\text{Re} \sum_\omega \sum_{n,m} \left< G^{ch}(A_n^m), d\sigma G^{cj}(j_n^m) \right>, \quad (6.49)$$

with the adjoint source

$$A_n^m(r, \omega) = \sum_{k,l} \left[ Q_{kn}^{lm,\text{pred}}(\omega, m) - Q_{kn}^{lm,\text{obs}}(\omega) \right] \delta Q_{kn}^{lm,\text{obs}}(\omega)^2 h^l_k(r). \quad (6.50)$$

**Ground-based responses** The derivation for the ground-based responses $T_n^m$ is very simple. The data misfit $\phi_d(m)$ can be written as

$$\phi_d(m) = \sum_\omega \sum_{n,m} \sum_{s \in \text{sites}} \left| T_n^m (r_s, \omega, m) - T_n^m (r_s, \omega, m) \right|^2 \delta T_n^m (r_s, \omega)^2, \quad (6.51)$$

and its differential is given by

$$d\phi_d(m) = 2\text{Re} \sum_\omega \sum_{n,m} \sum_{s \in \text{sites}} \left[ T_n^m (r_s, \omega, m) - T_n^m (r_s, \omega, m) \right]^* \frac{\delta T_n^m (r_s, \omega)^2}{\delta T_n^m (r_s, \omega)^2} dT_n^m (r_s, \omega, m). \quad (6.52)$$

Now remember from its definition (2.38) that $T_n^m = -B_{nr}^m$. Direct application of eq. (6.30) hence yields

$$dT_n^m (r_s, \omega) = \left< G^{ch} (-e_r \delta(r - r_s)), d\sigma G^{cj}(j_n^m) \right> \quad (6.53)$$

The fictitious source is thus a radial magnetic dipole with unit amplitude at the measurement site. The adjoint formulation is given by that for the $Q$-matrix, eq. (6.49), and the corresponding source reads

$$A_n^m(r, \omega) = - \sum_{s \in \text{sites}} \left[ T_n^m (r_s, \omega, m) - T_n^m (r_s, \omega, m) \right]^* e_r \delta(r - r_s). \quad (6.54)$$

For the transfer functions $U_n^m$ and $V_n^m$ (cf. Section 2.4.2), which relate the horizontal components of $B$ with the source coefficients $\varepsilon_n^m$, the derivation is analogous. The adjoint source, however, consists of horizontal magnetic dipoles at the measurement sites.

**Cable responses** The formulation of the data misfit for cable responses $K_n^m$ is analogous to that for the ground-based responses,

$$\phi_d(m) = \sum_\omega \sum_{n,m} \sum_{c \in \text{cables}} \left| K_n^m (c, \omega, m) - K_n^m (c, \omega, m) \right|^2 \delta K_n^m (c, \omega)^2, \quad (6.55)$$
where \( c \) is an index for the cables along which a voltage \( U(c) \) is measured, cf. Section 2.4.2. Combining eqs (2.45)–(2.46) with the spherical harmonic representation of the electric field (2.18) yields an expression for \( K_{n}^{m} \),

\[
K_{n}^{m,\text{pred}}(c, \omega) = -\int_{c} E_{n}^{m}(r, \omega) \, dr. \tag{6.56}
\]

Its differential is simply given by

\[
dK_{n}^{m,\text{pred}}(c, \omega) = -\int_{c} dE_{n}^{m}(r, \omega) \, dr. \tag{6.57}
\]

In analogy to eq. (6.24),

\[
dE_{n}^{m} = G_{ej} \left( d\sigma \mathcal{G}_{ej}(j_{n}^{m}) \right). \tag{6.58}
\]

The line integral is converted into a volume integral by means of

\[
dK_{n}^{m,\text{pred}}(c, \omega) = \langle G_{ej}(-b_{c}(r)), d\sigma \mathcal{G}_{ej}(j_{n}^{m}) \rangle, \tag{6.59}
\]

where \( b_{c}(r) \) is a function that only takes nonzero values along cable \( c \). Note that, in contrast to all other formulations considered so far, the calculation of \( dK_{n}^{m,\text{pred}} \) only involves the operator \( G_{ej} \) (and not \( G_{eh} \)).

The differential of the data misfit is given by

\[
d\phi_{d}(m) = 2\text{Re} \sum_{\omega} \sum_{n,m} \sum_{c \in \text{cables}} \frac{K_{n}^{m,\text{pred}}(c, \omega, m) - K_{n}^{m,\text{obs}}(c, \omega)}{\delta K_{n}^{m,\text{obs}}(c, \omega)^{2}} dK_{n}^{m,\text{pred}}(c, \omega, m). \tag{6.60}
\]

The adjoint formulation reads

\[
d\phi_{d}(m) = 2\text{Re} \sum_{\omega} \sum_{n,m} \langle G_{ej}(A_{n}^{m}), d\sigma \mathcal{G}_{ej}(j_{n}^{m}) \rangle. \tag{6.61}
\]

In contrast to eq. (6.49), the adjoint source \( A_{n}^{m} \) is processed by operator \( \mathcal{G}_{ej} \). This source is given by

\[
A_{n}^{m}(r, \omega) = -\sum_{c \in \text{cables}} \frac{K_{n}^{m,\text{pred}}(c, \omega, m) - K_{n}^{m,\text{obs}}(c, \omega)}{\delta K_{n}^{m,\text{obs}}(c, \omega)^{2}} b_{c}(r). \tag{6.62}
\]

Left to derive is a meaningful representation for the function \( b_{c}(r) \). To this purpose, imagine that the electric field is computed numerically on a regular spherical grid. The
Numerical implementation

87

integral in eq. (6.56) is then replaced by a sum, i.e.

\[
K^{m,\text{pred}}(c, \omega) = -\sum_i E_{m,\vartheta}^n(r_i, \omega) r_i \Delta \vartheta_i(c) + E_{m,\varphi}^n(r_i, \omega) r_i \sin \vartheta_i \Delta \varphi_i(c)
\]

\[
= -\sum_i E_{m,\vartheta}^n(r_i, \omega)b_{\vartheta,i}(c) + E_{m,\varphi}^n(r_i, \omega)b_{\varphi,i}(c),
\]

(6.63)

where index \(i\) runs over all cells that are crossed by cable \(c\). The factors \(b_{\vartheta,i}(c)\) and \(b_{\varphi,i}(c)\) parametrize the cable, i.e. they represent the arc lengths of cable \(c\) in cell \(i\) in \(\vartheta\)- and \(\varphi\)-direction, respectively. The adjoint source \(A^m_n\) can then be represented as

\[
A^m_n(r_i, \omega) = -\sum_{c \in \text{cables}} \frac{\left[K^{m,\text{pred}}(c, \omega, m) - K^{m,\text{obs}}(c, \omega)\right]^*}{\delta K^{m,\text{obs}}(c, \omega)^2} \left[\mathbf{e}_\vartheta b_{\vartheta,i}(c) + \mathbf{e}_\varphi b_{\varphi,i}(c)\right],
\]

(6.64)

where \(\mathbf{e}_\vartheta\) and \(\mathbf{e}_\varphi\) are unit vectors in \(\vartheta\)- and \(\varphi\)-direction, respectively. The adjoint source hence consists of horizontal electric line currents, which flow along the considered cables.

6.3 Numerical implementation

The concept elaborated in the previous section was implemented in a numerical 3-D inversion code. In this section, I will describe some details of the implementation, concerning the solution of the forward problem, the discretization of forward and inverse domain, the regularization, and the optimization scheme.

6.3.1 Forward computations

The forward problem of simulating the magnetic (and electric) field at Earth’s surface for a given (extraneous or adjoint) source and a given conductivity model is solved by a contracting integral equation approach. The approach was developed by Pankratov et al. (1995); its numerical implementation was described by Kuvshinov (2008). An extensive description of its application to inverse problems is given in the paper by Kuvshinov & Semenov (2012).

For forward computations, the 3-D conductivity structure is discretized on a regular spherical grid, consisting of \(n_r \times n_\vartheta \times n_\varphi\) cells. The conductivity within each elementary volume cell is constant, thus satisfying the condition imposed by eq. (6.32). The 3-D structure is embedded in a 1-D background structure.

The most expensive part of the forward solution in terms of computational cost is the calculation of the Green’s tensors. However, the Green’s tensors are actually independent of the 3-D model (Kuvshinov & Semenov, 2012). To make the inversion algorithm more efficient, we thus isolated their computation from the rest of the forward calculations, such that it does not need to be repeated in each iteration of the inversion.
scheme. A parallelization with respect to frequencies $\omega$ and source polarizations $p$ has been implemented for a further acceleration of the calculations.

### 6.3.2 Parametrization of the inversion domain

The inversion domain is divided into $N_r$ layers of possibly variable thicknesses. $N_r$ is not necessarily equal to $n_r$ (i.e. the number of laterally heterogeneous layers relevant for forward modelling), as we might only be interested in recovering the distribution of conductivity in specific layers. However, the layer boundaries coincide with those of the forward modelling domain.

A natural parametrization assigns one model parameter to each cell of the forward domain. To prevent negative conductivities, $m_k = \log_{10} \sigma_k$ is a convenient choice. The use of the logarithm in inversions for strictly positive quantities such as electrical conductivity was also suggested by Tarantola (2005).

A similar parametrization, which we hereinafter denote as “block parametrization”, was used by Kuvshinov & Semenov (2012) and Koch & Kuvshinov (2013), and is implemented in the inversion algorithm. In block parametrization, the model parameters relate to the conductivities as

$$m_k = \frac{\log_{10} \sigma_k - c_b}{c_a}, \quad (6.65)$$

where $c_a > 0$ and $c_b > 0$ are chosen such that $m_k \in [-1, 1]$ based on assumptions about minimum and maximum conductivities in the mantle. To reduce the number of model parameters and hence include a natural regularization in the parametrization, there is a possibility to merge several cells of the forward domain (within one layer). The number of model parameters $N_m$ is given by $N_m = N_r \times n_\vartheta \times n_\varphi / M^2$, where $M$ is the number of cells to be merged in $\vartheta$- and $\varphi$-direction.

If inverting global data such as the $Q$-matrix, which is based on a spherical harmonic representation of both external and induced signals, the block parametrization might, however, not be the optimum choice. It seems more natural to also parametrize the model domain in terms of spherical harmonics, as previously done by e.g. Kelbert et al. (2008). Within each layer, conductivity is thus defined as a finite sum of spherical harmonics up to a cut-off degree $L$. The number of model parameters is then given by $N_m = N_r \times (L + 1)^2$.

The conductivity of each cell is first normalized as in eq. (6.65),

$$s(r_i, \vartheta_i, \varphi_i) = \frac{\log_{10} \sigma(r_i, \vartheta_i, \varphi_i) - c_b}{c_a}. \quad (6.66)$$

Solving eq. (6.66) for $\sigma$ yields

$$\sigma(r_i, \vartheta_i, \varphi_i) = 10^{s(r_i, \vartheta_i, \varphi_i) c_a + c_b}. \quad (6.67)$$
We then expand $s$ for each layer by spherical harmonics,

$$
s(r_i, \vartheta_i, \varphi_i) = g_0^0(r_i) + \sum_{l=1}^{L} g_l^0(r_i) P_l^0(\cos \vartheta_i) + \sum_{l=1}^{L} \sum_{m=1}^{l} \left[ g_l^m(r_i) \cos(m \varphi_i) + h_l^m(r_i) \sin(m \varphi_i) \right] P_l^m(\cos \vartheta_i), \quad (6.68)
$$

where $l$ and $m$ are degree and order of the spherical harmonics, respectively, and the $P_l^m$ are Schmidt quasi-normalized associated Legendre polynomials. The model vector $\bf{m}$ is accordingly composed of the coefficients of the SHE,

$$
\bf{m} = \left[ g_0^0(r_1), g_1^0(r_1), \ldots, g_L^0(r_1), g_0^1(r_1), g_1^1(r_1), \ldots, g_L^1(r_1), h_L^0(r_1), \ldots, g_0^L(r_N), g_1^L(r_N), \ldots, g_L^L(r_N), h_L^L(r_N) \right]^\top. \quad (6.69)
$$

Its constituents can be derived from eq. (6.68) by making use of the orthogonality of the spherical harmonics, i.e.

$$
g_l^m(r_i) = \frac{1}{\|P_l^m\|^2} \int s(r_i, \vartheta, \varphi) P_l^m(\cos \vartheta) \cos(m \varphi) d\Omega, \quad (6.70)
$$

$$
h_l^m(r_i) = \frac{1}{\|P_l^m\|^2} \int s(r_i, \vartheta, \varphi) P_l^m(\cos \vartheta) \sin(m \varphi) d\Omega, \quad (6.71)
$$

where $\|P_l^m\|^2$ is the squared norm of the associated Legendre polynomial $P_l^m$.

In Section 6.2.2, we presented a formula (eq. 6.32) to compute the partial derivative of the data misfit $\phi_d$ with respect to the conductivity of the $k$-th cell of the forward modelling domain, $\sigma_k$. The partial derivative with respect to model parameter $m_j$ follows with the chain rule, i.e.

$$
\frac{\partial \phi_d}{\partial m_j} = \sum_k \frac{\partial \phi_d}{\partial \sigma_k} \frac{\partial \sigma_k}{\partial m_j}. \quad (6.72)
$$

For block parametrization, the factor $\frac{\partial \sigma_k}{\partial m_j}$ follows from eq. (6.65),

$$
\frac{\partial \sigma_k}{\partial m_j} = \ln(10)c_a \sigma_k \delta_{jk}, \quad (6.73)
$$

where $\delta_{jk}$ is Kronecker’s delta. For the spherical harmonic parametrization introduced above, this term is calculated as

$$
\frac{\partial \sigma_k}{\partial m_j} = \frac{\partial \sigma_k}{\partial s_k} \frac{\partial s_k}{\partial m_j}, \quad (6.74)
$$

$$
\frac{\partial \sigma_k}{\partial s_k} = \ln(10)c_a 10^{s_k c_a + c_k}, \quad (6.75)
$$

$$
\frac{\partial s_k}{\partial m_j} = \begin{cases} \cos(m_j \varphi_k) & \text{for } \cos(m_j \varphi_k) > 0, \\ \sin(m_j \varphi_k) & \text{for } \cos(m_j \varphi_k) < 0 \end{cases} P_l^m(\cos \vartheta_k). \quad (6.76)
$$
Figure 6.1: Effect of the different parametrizations in a test 3-D inversion. a) Target model, b)-d) block parametrization (b) no merging, c) merging of 2 × 2 cells, d) merging of 3 × 3 cells), e)-f) spherical harmonic parametrization (e) $L = 10$, f) $L = 20$). More information in the text.

Note that $m_j$ on the left-hand side of eq. (6.76) denotes a model parameter, while on the right-hand side, it denotes the order of the spherical harmonic for this model parameter.

Figure 6.1 shows the results of test 3-D inversions performed with different model parametrizations. All results were obtained by inverting synthetic coefficients $\iota_l k$ for $k \leq 7, |l| \leq 7$ at 10 periods between 2 and 60 days. These coefficients had been generated by simulating induction due to a simple ring current source ($P^0_l$) in a target conductivity model that contains a single heterogeneous layer at a depth of 670–1000 km, shown in Figure 6.1a. No regularization was applied in any of the inversions.

The results confirm that the spherical harmonic parametrization yields the smoothest model. Merging might stabilize the inversion numerically, but does not reduce the number of artefacts in the solution. High cut-off degrees $L$ in the spherical harmonic parametrization permit a more accurate recovery of 3-D conductivity structure, if the data contain the necessary information.

6.3.3 Regularization

As mentioned in Section 6.2.1, we stabilize the solution of our inversion with a regularization term $\phi_m$. The regularization matrix $W$ serves as smoothing operator, i.e. it
prevents jumps in conductivity. In case of block parametrization, \( W \) is a finite difference approximation of the gradient operator.

A parametrization with spherical harmonics automatically yields a smooth solution. Due to the finite cut-off degree \( L \), an additional natural regularization is included in the parametrization. Further smoothing can be implemented by down-weighting coefficients of high degree \( l \). In the original implementation, this was performed by multiplication with a factor \( l^\beta \), where \( \beta > 0 \) is chosen independently from the bulk regularization parameter \( \lambda \). Tests have shown that a variation of \( \beta \) is essentially equivalent to a variation of \( \lambda \); thus fixing \( \beta \) to a moderate value, e.g. \( \beta = 0.3 \), avoids a two-dimensional exploration of the regularization parameter space. This regularization scheme is similar to the scheme previously presented by Kelbert et al. (2008), who however defined the inverse of \( W \).

In the current implementation, smoothing is performed by multiplication with a factor \( l(l+1) \). This was shown to correspond to gradient regularization (Velímský, personal communication) and prevents the choice of an additional, independent parameter.

Radial smoothing, i.e. regularization across layer boundaries, was originally implemented by a finite difference approximation of the vertical gradient (acting on the respective spherical harmonic coefficients). However, more recent tests revealed that radial smoothing is not necessary in case of a small number of layers, say \( N_r \leq 8 \). Since we never inverted for more layers, radial smoothing is omitted in the current implementation.

An inversion is usually started with strong regularization. After convergence, the value of the regularization parameter \( \lambda \) is decreased, and the results obtained with the previous \( \lambda \) are used as starting model. This gradual adaptation of the amount of regularization constrains the solution to be close to the global minimum in every stage of the iterative inversion. It hence facilitates convergence and avoids stepping into local minima. The final result is picked from a trade-off curve (L-curve, cf. Hansen, 1992).

### 6.3.4 Optimization methods

The objective function \( \phi \) introduced in eq. (6.1) is minimized with a descent method. Within each iteration, the model vector \( m \) is updated as

\[
m_{k+1} = m_k - \alpha_k p_k,
\]

where \( \alpha_k > 0 \) and \( p_k \) are the step length and the searching direction, respectively, in the \( k \)-th iteration. The scheme is iterated until \( m \) remains constant, which indicates that a minimum of \( \phi \) has been reached.

In Newton’s method and its variants, \( p \) is obtained by a matrix-vector product of the inverse Hessian with the gradient of the objective function, i.e.

\[
p_k = H^{-1}(\phi_k) \nabla \phi_k.
\]
Figure 6.2: Recovery of a 1-layer chequerboard target model (a) from ideal, noise-free synthetic data, using different parametrizations of the model domain and different optimization schemes. Middle row (b-d): block parametrization, bottom row (e-g): spherical harmonic parametrization. First column (b & e): QN, second column (c & f): LMQN, third column (d & g): NLCG. Colours denote electrical conductivity in logarithmic units.

An exact calculation of the Hessian is computationally prohibitive for most 3-D problems, even if making use of an adjoint approach (Pankratov & Kuvshinov, 2015). For this reason, it is common practice to approximate the Hessian. Quasi-Newton (QN) methods, for example, compute an approximation of $H(\phi)$ (or its inverse) from the model vectors and gradients of previous iterations. The bottleneck in standard QN methods is the memory requirement ($H$ is an $N_m \times N_m$-matrix) and the calculation of the matrix-vector product. For inverse problems with a very large number of model parameters, the computational effort can be enormous. Limited-memory quasi-Newton (LMQN) methods offer a solution to this problem, since they never compute the full Hessian, but only its product with $\nabla \phi$.

A different widely used optimization method is the non-linear conjugate gradients (NLCG) technique. NLCG does not require a computation of the Hessian, but derives $p$ from previous searching directions. We implemented full (standard) QN, LMQN and NLCG in the 3-D inversion code. For QN (and for LMQN), we used the Broyden-Fletcher-Goldfarb-Shanno (BFGS) formula; for NLCG, we used the Polak-Ribière formula. The implementation of all methods follows Nocedal & Wright (2006).
Numerical implementation

Table 6.1: Performance of the different optimization schemes in block parametrization on a regular $5^\circ \times 5^\circ$ grid ($N_m = 2592$). From left to right: number of iterations to reach convergence, average number of forward calls per iteration, average time to compute the searching direction $p$. Note that the total time (last column) includes all processing steps and in particular the solution of the forward problem.

<table>
<thead>
<tr>
<th>Optimization scheme</th>
<th>Iterations</th>
<th>Fw calls/iter</th>
<th>Time for $p$ (s)</th>
<th>Total time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Limited memory quasi-Newton</td>
<td>30</td>
<td>1.20</td>
<td>0.0</td>
<td>265</td>
</tr>
<tr>
<td>Full (standard) quasi-Newton</td>
<td>27</td>
<td>1.04</td>
<td>270.0</td>
<td>8602</td>
</tr>
<tr>
<td>Non-linear conjugate gradients</td>
<td>32</td>
<td>2.97</td>
<td>0.0</td>
<td>828</td>
</tr>
</tbody>
</table>

Table 6.2: Performance of the different optimization schemes in spherical harmonic parametrization with a cut-off degree 7 ($N_m = 64$). See caption of Table 6.1 for more details.

<table>
<thead>
<tr>
<th>Optimization scheme</th>
<th>Iterations</th>
<th>Fw calls/iter</th>
<th>Time for $p$ (s)</th>
<th>Total time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Limited memory quasi-Newton</td>
<td>12</td>
<td>1.25</td>
<td>0.0</td>
<td>154</td>
</tr>
<tr>
<td>Full (standard) quasi-Newton</td>
<td>20</td>
<td>1.10</td>
<td>1.5</td>
<td>167</td>
</tr>
<tr>
<td>Non-linear conjugate gradients</td>
<td>20</td>
<td>2.90</td>
<td>0.0</td>
<td>461</td>
</tr>
</tbody>
</table>

To compare the performance of the three methods, we first generated synthetic data (coefficients $i_{kl}$ at a set of frequencies) by simulating induction due to a ring current source ($P_{01}^0$) in a simple conductivity model. The model has a single laterally heterogeneous layer at a depth of 400–600 km with chequered conductivity structure (shown in Figure 6.2a), which is embedded in a 1-D background model. We then recovered this model from the data, using the two different parametrizations described in Section 6.3.2 and the three mentioned optimization methods. Figure 6.2 shows the results of these tests. For a given parametrization, the recovered models are fairly similar, which confirms a correct implementation of the methods and shows that all of them are able to recover the conductivity structure. The differences between the results obtained with different parametrizations are much more pronounced, showing once again their respective strengths and limitations discussed above.

Table 6.1 summarizes the performance of the different optimization schemes for block parametrization ($N_m = 2592$). To reach convergence, the QN method requires slightly fewer iterations than both LMQN and NLCG. Both quasi-Newton methods are clearly superior to the NLCG method when regarding the number of forward calls per iteration, with slight advantages for the full QN method. Quasi-Newton methods automatically generate steps of optimal length, and the line search algorithm is only rarely used. This is different for NLCG, which requires a sophisticated line search algorithm and various iterations to find a suitable step length. The time to compute the searching direction $p$ is negligible to other computational loads in LMQN and NLCG, but becomes dominant in full QN. This is apparent when regarding the total time needed to reach convergence.
NLCG and LMQN clearly outperform full QN. LMQN is still significantly faster than NLCG due to the smaller number of iterations and forward calls – in this set-up, one solution of the forward problem takes about 8 seconds.

The situation changes when parametrizing the model domain with spherical harmonics ($N_m = 64$), cf. Table 6.2. The much smaller number of model parameters significantly reduces the time to compute $p$ with the full QN method. Due to the smaller number of forward calls, it clearly outperforms NLCG and becomes comparable to LMQN.

The results of the tests show that all three implemented optimization methods are workable and appropriate to solve the 3-D problem of conductivity recovery. Since the LMQN method needs least resources while providing equivalent results, it was employed for most of the computations presented in the forthcoming sections.

The step length $\alpha_k$ is computed by an inexact line search. In our case, $\alpha$ is chosen to fulfil the Wolfe conditions:

1. Sufficient decrease condition

   $$\phi(\alpha^*) < \phi(0) - c_1 \alpha^*, \quad (6.79)$$

   where $\alpha^*$ is a trial value for $\alpha$ and $c_1$ is a (usually very small) positive parameter. This condition makes sure that the objective function actually decreases, i.e. that we move towards a minimum.

2. Curvature condition

   $$\left| \frac{\partial \phi}{\partial \alpha} \right|_{\alpha=\alpha^*} < c_2 \left| \frac{\partial \phi}{\partial \alpha} \right|_{\alpha=0}, \quad (6.80)$$

Figure 6.3: Illustration of the Wolfe conditions in an inexact line search. Only trial step lengths $\alpha^*$ in intervals 1 and 2 are accepted. In the widely shaded intervals, the curvature condition is not fulfilled. In the densely shaded interval, the sufficient decrease condition is not fulfilled.
where \( c_2 \) is a positive parameter, \( 0 < c_2 < 1 \). This condition makes sure that our model update is not too close to the model of the previous iteration. Note that \( \partial \phi / \partial \alpha < 0 \) for \( \alpha = 0 \).

An illustration of the Wolfe conditions is given in Figure 6.3. The numerical implementation of the line search algorithm follows Nocedal & Wright (2006).

### 6.3.5 A modular global 3-D inversion code

In collaboration with Stephan Koch, I developed a modular global 3-D inversion code in FORTRAN-90. It is based on an original non-modular code, written in FORTRAN-77, which was devised to invert satellite-based \( C \)-responses and time spectra of induced coefficients (Kuvshinov et al., 2010). Modifications were developed by Kuvshinov & Semenov (2012) and Koch & Kuvshinov (2013) to invert observatory \( C \)-responses and time spectra of the magnetic field, respectively.

The new modular version employs various model parametrizations and optimization schemes, and it can be used both on the full sphere and on a belt of limited latitude. Moreover, it unites the separate versions used before for different problem settings. The code can now handle the following types of data:

- Observatory \( C \)-responses,
- Time spectra of \( B \) at observatory locations,
- Ground-based responses \( T_n^m, U_n^m \) and \( V_n^m \),
- Time spectra of induced coefficients \( \iota_k^l \),
- \( Q \)-matrix,
- Cable responses \( K_n^m \).

Data type, model parametrization, optimization scheme and many other parameters, such as the value of the regularization parameter \( \lambda \), can be defined in a separate parameter file. Further options are easily implemented thanks to the modular structure. The code is documented in a user manual.

A separate version of the code solves the 1-D problem of conductivity recovery in a 3-D environment by inverting scalar \( Q \)-responses (cf. Section 5.5.3). In this problem, the 1-D background structure is updated in each iteration of the inversion scheme. The calculation of Green’s tensors hence cannot be separated from the rest of the forward computations and has to be repeated after each update of the model.
6.4 Tests and resolution studies

This section is dedicated to testing the performance of the inversion algorithm and investigating the resolution that can be achieved with different types of ideal data.

6.4.1 Resolution study with matrix $Q$-responses

Inspired by similar works by Kelbert et al., 2008 and Koch & Kuvshinov, 2013, we performed a resolution study with the $Q$-matrix. To this purpose, we generated eight different synthetic data sets, each of them consisting of matrix $Q$-responses (for $n \leq 3, |m| \leq 1, k \leq 15, |l| \leq 15$) at 11 logarithmically spaced periods between 2 days and 30 days. These responses were computed by simulating induction in eight different conductivity models, differing in the depth of a laterally heterogeneous layer, which is embedded in a 1-D background structure (Figure 6.4). The depth ranges of this anomalous layer are 10–100 km, 100–250 km, 250–410 km, 410–520 km, 520–670 km, 670–900 km, 900–1200 km, and 1200–1600 km, respectively. The heterogeneous layer has a chequered conductivity structure, with minimum and maximum conductivities of $\sigma_b/\sqrt{10}$ and $\sigma_b\sqrt{10}$, respectively, where $\sigma_b$ denotes the background conductivity of the respective layer. The surface conductance map (cf. Figure 3.2) comprises the top 10 km.

Each data set is now separately inverted in order to recover the heterogeneous layer at the respective depth. The inversion is initiated with the background 1-D model. The inversion domain is stratified into the eight layers described above, and the conductivity structure of each layer is described by spherical harmonics up to degree $L = 15$ (cf. Section 6.3.2). No regularization is applied. The surface conductance map is fixed during inversion. For forward modelling, each layer (including the surface shell) is discretized in $72 \times 36$ cells with a size of $5^\circ \times 5^\circ$.

The inversion results are presented in Figure 6.5. The colouring scheme is normalized to $\log_{10}(\sigma/\sigma_b)$; values different from zero thus indicate anomalous structures. Each

![Figure 6.4: Left: Reference chequerboard conductivity structure of the anomalous layer used in the resolution studies. Conductivity is described as $\log_{10}(\sigma/\sigma_b)$, where $\sigma_b$ is the background conductivity of the respective layer. Right: 1-D background conductivity structure $\sigma_b$ in the top 1600 km.](image)
Figure 6.5: Results of the resolution study. Each column corresponds to an individual inversion, which aims at recovering the conductivity structure of an anomalous layer buried in the depth range indicated at the top of the respective column. The depth of the resolved layers is indicated on the right. Conductivity is plotted as $\log_{10} (\sigma / \sigma_b)$, where $\sigma_b$ is the background conductivity of the respective layer (cf. Figure 6.4).

column corresponds to a different inversion, i.e. column $i$ corresponds to the inversion of the $i$-th data set, which itself corresponds to an anomaly in the $i$-th layer. Perfect resolution at all depths would thus be indicated by chequered structure in the diagonal of the $8 \times 8$-matrix and zeros elsewhere.

The results reveal that 3-D mantle conductivity structure can – with the given data – only be recovered at depths greater than 100 km. Best resolution is achieved at depths from 500 km to 900 km, but anomalous structures can be detected in the entire depth range from 100 km down to 1600 km. In all inversion runs, the conductivity structure of the laterally heterogeneous layer is smeared to the adjacent layers. This is due to the finite (and actually sparse) set of involved frequencies. The relatively poor recovery of the (comparably thin) layer extending from 410 km to 520 km might be due to the same reason. Note in this context that the vertical resolution is governed by the frequency range, while the lateral resolution is governed by the number of rows in the $Q$-matrix, i.e. by the cut-off degree for internal coefficients, $N_\ell$. When using a modified data set with 14 periods between 2 days and 60 days, the resolution at depths $>1200$ km increases (results not shown). Note that the depth resolution depends on the chosen background conductivity structure; it might thus be slightly different for real data in the same period range.
6.4.2 Test inversions of ground- and sea-based responses

To validate the correct implementation and investigate the suitability for 3-D inversions, we performed test inversions of the ground-based transfer functions $T_{m}^{n}$, $U_{n}^{m}$ and $V_{n}^{m}$, and of the cable responses $K_{n}^{m}$ (cf. Section 2.4.2). Test data were generated by simulating induction in the model already shown in Figure 6.2a. This model consists of a single laterally heterogeneous layer at a depth of 400–600 km with chequered conductivity structure, which is embedded in a 1-D background model. Induction was simulated for $p = 9$ spherical harmonic sources ($n \leq 3, |m| \leq 1$) and 21 logarithmically spaced periods between 2 days and 68 days.

The ground-based responses were synthesized for a regular grid of 2592 observatories with a spacing of $5^\circ$ in both directions, cf. Figure 6.6a. The cable responses were calculated for a regular grid of 180 cables, which is shown in Figure 6.6b.

Results of the inversions are presented in Figure 6.7. Inversion of $T_{n}^{m}$ (panel a) yields an almost perfect recovery of the target model; only the sharp edges of the chequered conductivity structure are not accurately reproduced. The inversion results for $U_{n}^{m}$ (panel b) are markedly worse. While conductive regions are, in general, well recovered, this is not the case for resistive regions. The opposite is true for the inversion of $V_{n}^{m}$ (panel c). The general chequered structure is well recovered, but the solution shows a lot of irregularities. Smoother results might be attainable by applying regularization. Finally, inverting $K_{n}^{m}$ (panel d) permits a very good recovery of the target conductivity structure. This is remarkable, considering that the spatial density of the data is much smaller than for the ground-based responses (Figure 6.6).
Figure 6.7: Results of test inversions of various ground- and sea-based transfer functions. a) $T_m^n$, b) $U_m^n$, c) $V_m^n$, d) $K_m^n$.

The various inversions converged in very different ways. While the misfit $\phi_d$ dropped by 63% in the inversion of the $T_m^n$, it only dropped by 30% in the inversion of the $V_m^n$ and by 10% in that of the $U_m^n$. This confirms that the latter transfer functions are not very sensitive to 3-D structures and therefore barely useful for inversion. Already small amounts of noise might make a recovery of the 3-D distribution of electrical conductivity impossible. In contrast, $\phi_d$ dropped by more than two orders of magnitude in the inversion for cable responses $K_m^n$. This confirms the high sensitivity of electric field data to conductivity anomalies, which is well-known from MT.

### 6.5 3-D inversion of the SCARF test data set

This section focuses on the 3-D inversion of the SCARF test data set, which was described in detail in Section 4.2. We first estimate matrix $Q$-responses from time series of $\varepsilon_m^n$ and $i^l_k$, which were derived from synthetic magnetic data by the CI. The estimated responses are subsequently inverted for 3-D conductivity structure, with the goal to recover the target conductivity model shown in Figure 4.2.
6.5.1 Some remarks on the period range

On the lower end, the period range of any kind of transfer function is limited by the Nyquist theorem. Since the time series of $\varepsilon_m^n$ and $\iota_k^l$ are provided by the CI with a sampling rate of 6 hours, the shortest period contained in the data is 12 hours. But for periods up to 24 hours, the ionospheric $Sq$ signals are the main cause for variations in the magnetic records. Since the CI cannot perfectly separate signals of ionospheric and magnetospheric origin, the noise level at these short periods is expected to be large. We thus only consider periods longer than 48 hours.

On the upper end, the period range is limited by the length of the time series. For a reliable least squares analysis, the number of events must significantly exceed the number of explanatory variables $p$. The SCARF test data set consists of 4.5 years of data, and since external coefficients are recovered for $n \leq 3$ and $|m| \leq 1$, $p = 9$. If we request the number of events to be at least $4p$ and use standard values for section length and overlap in the processing algorithm (Section 2.5), the maximum period is of about 30 days. As mentioned in Section 6.4, responses at longer periods would be fortunate in order to resolve conductivity structure at greater depths.

There are two ways to acquire long-period responses. First, the length of the time series scales linearly with the maximum period, thus more data would help out. Second, there is obviously a trade-off between an accurate description of the source (i.e. the number of explanatory terms $p$) and the maximum period of the estimated responses. By reducing $p$, e.g. only considering induction due to sources of degree $n = 1$, we can increase the ratio without altering the number of events. We however have to be aware that a neglected source has the effect of correlated noise, which biases the results (Egbert & Booker, 1989). We will get back to this idea in a different context in Section 6.5.3.

6.5.2 Estimation of the $Q$-matrix

The $Q$-matrix is estimated with the multivariate processing algorithm described in Section 2.5.2 for $n \leq 3$, $|m| \leq 1$, $k \leq 5$, $|l| \leq 5$, and 16 logarithmically spaced periods between 2 days and 28.5 days. $Q$ is hence a matrix with 35 rows and 9 columns. As a proof of concept and for comparison with later investigations, we first estimate $Q$ from noise-free test data, i.e. from the direct output of the procedure described in Section 4.2. The results are shown in Figure 6.8 and compared to theoretical predictions, obtained by simulating induction in the target model. For convenience, we never show the full $Q$-matrix, but only selected elements.

We first note that the magnitude of the responses in the top left element is two orders higher than in the remaining elements. This is due to the fact that this is a diagonal element of the $Q$-matrix, i.e. it describes the bulk conductivity and the 1-D structure, which dominate over the 3-D heterogeneities.
The theoretical prediction is recovered well for all elements, which validates the performance of our multivariate analysis algorithm. The correspondence between predicted and estimated responses however differs from element to element. Weaker correspondence is, as expected, always accompanied by larger uncertainties. The predicted responses are within the confidence limits for most estimates. Good recovery is observed for the elements corresponding to the source term $\varepsilon^0$ (second column). This is due to the strong signal of $\varepsilon^0_1$, i.e. its dominance in the data (cf. Figure 3.3). In the first row, the best-resolved element, however, is not the one describing excitation by $\varepsilon^0_1$, but the diagonal element $Q^{-1,1}_{1,1}$. This is clearly due to the fact that $\lambda^{-1}_1$ is mostly excited by the corresponding external coefficient $\varepsilon^{-1}_1$. Note in this context that not all rows of the $Q$-matrix have diagonal elements, since there are more rows than columns. For some features of the results – e.g. the substantial difference in quality between the recovery of $Q^{5,0}_{5,3}$ and $Q^{5,1}_{5,3}$ – we do not have an obvious explanation.

We now estimate the $Q$-matrix from the final SCARF test data set. This data set contains noise, since it is an output of the CI, which cannot perfectly separate signals of different origin, especially considering the sparse observations. Results obtained with the conventional approach (cf. Section 2.5.1) are presented in Figure 6.9. As a comparison, we also estimated the $Q$-matrix with the multi-frequency approach and an appropriate regularization parameter (cf. Section 2.5.2). The results are shown in Figure 6.10.
Let us first examine Figure 6.9. As expected, the agreement between predictions and estimates is dramatically worse than for noise-free test data, and uncertainties are significantly larger. However, the predictions are still mostly within the confidence limits.

In fact, most elements lack any useful information about subsurface conductivity structure, since the magnitudes of both estimates and confidence limits are about an order larger than the corresponding predictions (e.g. $Q_{3,3}^{-2,1}$, compare with the same element in Figure 6.8). Of the presented responses, only $Q_{1,1}^{-1,-1}$ (representing the 1-D structure) and $Q_{3,1}^{-2,0}$ (representing excitation by $\varepsilon_1^0$) are reliably resolved. This is representative for
the full $Q$-matrix, which we do not show for lack of space. Most of the well-recovered elements are either in the diagonal or correspond to excitation by $\varepsilon_0^1$.

The multi-frequency approach (Figure 6.10) enhances the recovery of the (already well recovered) diagonal element $Q_{1,1}^{-1}$. For most other elements, the offset between predictions and estimates is similar as in the results obtained with the conventional approach. However, uncertainties are partially dramatically reduced (e.g. for $Q_{3,3}^{2,1}$), such that for a lot of estimates, the confidence limits do not comprise the predictions. These seemingly well recovered responses might constitute a hazard for the inversion. For this reason, the $Q$-matrix estimated with the conventional approach is used for further investigations.

### 6.5.3 Inversion of the $Q$-matrix

The $Q$-matrix is inverted for conductivity at depths between 10 km and 1000 km. The surface conductance map describing the distribution of land and sea is scaled to a thickness of 10 km and fixed, i.e. we do not try to recover it, as its contribution to the induced field is assumed to be known. The conductivity at depths greater than 1000 km is fixed, too.

The inversion domain consists of five layers, each having a thickness of 200 km (except for the uppermost layer, which has a thickness of 190 km). This stratification intentionally does not coincide with the stratification of the target model (shown in Figure 4.2) in order to account for our limited knowledge of the stratification in Earth’s mantle.

For forward modelling, each laterally heterogeneous layer (including the thin surface shell) is discretized in $72 \times 36$ cells with a size of $5^\circ \times 5^\circ$. Since our data consist of matrix $Q$-responses that relate SHE coefficients up to degree $k = 5$, it seems reasonable to parametrize the inversion domain with spherical harmonics, and to choose a cut-off degree of $L = 5$ (cf. Section 6.3.2). The inverse problem is solved iteratively, hence an initial conductivity model is required. This model consists of the laterally heterogeneous surface shell and a 1-D section underneath, which has been derived from the data by our 1-D inversion algorithm (Section 5.3).

Results of the 3-D inversion are presented in Figure 6.11. Panel a) shows the conductivity structure recovered from an ideal $Q$-matrix, which was computed by simulating induction in the target model. Ideal responses were shown as solid lines in Figures 6.8-6.10. This inversion run was performed as a reference for further investigations; the results enable us to understand which resolution can be achieved with the considered data.

The target model (Figure 4.2) contains several small-scale anomalies in the upper mantle (10-400 km). These anomalies are not present in the inversion results, indicating that the resolution is limited to large-scale structures, i.e. structures of continental size. The broad shape of the large-scale anomaly beneath the Pacific plate is well recovered.
in the layer extending from 400 km to 600 km, but the structure lacks details. The layer extending from 600 km to 800 km samples contributions from two layers of the target model (note again the different stratifications). Its conductivity distribution appears very reasonable, since the background has an intermediate conductivity when compared to both layers of the target model, and the anomaly underneath the Pacific plate is clearly visible.

Figure 6.11b shows the results obtained by inverting the $Q$-matrix of Figure 6.9, which was estimated from the SCARF test data set with the conventional approach. The conductivity distribution in all layers is very similar to that of Figure 6.11a, which was recovered from ideal data. In particular, the large-scale anomaly beneath the Pacific plate is very well recovered and, if compared to panel a), only slightly distorted. A
few artefacts are perceptible in the results, in particular at great depths. However, considering that the data partially have very large uncertainties (cf. Figure 6.9), the target model is excellently recovered. An inversion of the $Q$-matrix estimated with the multi-frequency approach (Figure 6.10) yields very similar results (not shown). This proves the robustness of the inversion algorithm.

Let us now investigate which parts of the data actually contain information about subsurface conductivity structure, and which can be omitted without altering the inversion results. We have seen in the previous section that the best-resolved elements of the $Q$-matrix are the diagonal elements (describing bulk conductivity and 1-D structure), and those corresponding to induction by the dominant source term, $\varepsilon_{0,1}$. It thus seems reasonable to invert only the column of the $Q$-matrix containing the terms $Q_{k,0}^{l,0}$ (visually indicated in Figure 6.12a; note that, due to the chosen ordering of the coefficients, this is the second column of the $Q$-matrix). This column contains the diagonal term $Q_{0,0}^{0,0}$ and thus the necessary information on bulk conductivity and 1-D structure.

We have to distinguish between prior and posterior selection of the $Q$-matrix elements used for inversion. Posterior selection here signifies that we only use the desired column of the full $Q$-matrix estimated in Section 6.5.2 and shown in Figure 6.9. Prior selection, in contrast, signifies that we estimate a new $Q$-matrix, this time assuming that the source is exclusively described by $\varepsilon_{0,1}$. This reduces the multivariate analysis to a univariate analysis; the newly estimated $Q$-matrix thus only consists of one column.

Figure 6.11c shows the inversion results obtained by inverting this newly estimated $Q$-matrix (prior selection). The result clearly exhibits the effect of correlated noise. The
anomaly underneath the Pacific plate is still visible, but very badly resolved. On top, artefacts in the solution are dramatically enhanced. This proves the importance of the source coefficients of higher degrees and orders. It is also an indication of the errors that might be present in inversion results obtained with the assumption of $p = 1$.

In contrast, a posterior selection of transfer functions is not subject to additional assumptions about the source. Figure 6.13a shows the inversion result obtained by inverting the second column of the estimated full $Q$-matrix. The great similarity to Figure 6.11b justifies the assumption that the information on induction due to $\varepsilon_1^0$ is sufficient to recover the conductivity structure.

A final test concerns the difference between $Q$-matrix elements within the same column. We have already stated in the previous section that there are fundamental differences between $Q$-matrix rows with diagonal elements and such without diagonal elements.
In the latter, $\varepsilon^0$ is typically the dominant source for the internal coefficients $\iota^l_k$. In the former, however, the dominant source is the corresponding external coefficient of same degree and order, $\varepsilon^l_k$. Let us return to the data set obtained by posterior selection and divide it into two new, even smaller data sets. The first data set contains the 9 responses of rows with diagonal elements. The second data set contains the remaining 26 responses of rows without diagonal elements plus $Q_{0,0}^{1,0}$, which is needed to recover bulk conductivity and 1-D structure. The data sets are shown schematically in Figure 6.12.

The inversion results are presented in Figure 6.13 – panel b) showing the results obtained by inverting elements of $Q$-matrix rows with diagonal element, panel c) those of rows without diagonal element (plus $Q_{0,0}^{1,0}$). The results indicate that both subsets contain information about 3-D conductivity structure, but none of them contains the full information (compare with Figure 6.13a). In $Q$-matrix rows with diagonal elements (panel b), $\varepsilon^0_1$ is not the dominant source, but the signal describing induction due to $\varepsilon^0_1$ is above noise level. The layers extending from 400 km to 600 km and from 600 km to 800 km show an anomalous structure underneath the Pacific plate. Its poorly defined shape is due to the fact that we only invert $Q$-responses of low $k$ and $l$, which describe the coarse conductivity structure. The results in Figure 6.13c show more details about the shape of the anomaly, but miss part of the coarse structure. This is expected when inverting only $Q$-responses of high degrees and orders.

Both results obtained by inverting subsets of a specific column of the $Q$-matrix exhibit several artefacts. A closer look reveals that these artefacts are complementary to each other. A combination of both results will thus not only enhance the recovery of the conductivity anomaly beneath the Pacific plate, but also reduce the artefacts. This result indicates that we need the full column of the $Q$-matrix (here defined by $k \leq 5, |l| \leq 5$) in order to obtain reliable images of 3-D conductivity structure in Earth’s mantle.

### 6.5.4 Discussion

The present study is based on the SCARF test data set. Although this data set was supposed to mimic real magnetic data, at least the time-varying part of the synthesized magnetic field is strongly simplified. In particular, the magnetospheric source is described by a limited set of spherical harmonics ($p = 9$), which does not have any physical basis.

The spatial structure of the source was known when the CI separated synthetic magnetic data into its constituents, represented by SHE coefficient time series. There is correlated noise in the recovered coefficients, originating from different sampling rates (temporal leakage) and non-recovered internal/induced parts (spatial leakage). We however argue that the impact of this noise is small if compared to the impact of a non-described inducing source. Such a source is not present in the simplified data set.

Real data will contain a larger amount of correlated noise, e.g. due to field-aligned currents, magnetospheric sources of higher degree and order, or polar and equatorial
electrojets. In order to test the robustness of the algorithm to correlated noise, we reduced the number of sources prior to data analysis by assuming that the source can be described exclusively by its dominant term, $\epsilon_0^I$. The inversion results (Figure 6.11c) reveal that a recovery of 3-D mantle conductivity anomalies is hardly possible, since their shape is distorted, and the number of artefacts in the solution increases dramatically.

In this study, we distinguished between $Q$-matrix rows with and without diagonal element. The $Q$-matrix describing true Earth, however, does not have any rows without diagonal element. No matter how small a given magnetospheric source term $\epsilon_l^I$ might be, it will always be the dominant source for the corresponding internal coefficient $\iota_l^I$. Neglecting existing source terms (and thereby creating $Q$-matrix rows without diagonal elements) will thus add large portions of correlated noise to the estimated responses in the respective rows of the $Q$-matrix.

When translating these findings to real data, it is apparent that we can only trust the responses of $Q$-matrix rows with diagonal elements, since they will be comparably unaffected by correlated noise. If the CI can – from real data – recover the same number of magnetospheric source terms as in this test study ($p = 9$), the best resolution we can expect will thus rather resemble that of Figure 6.13b.

### 6.6 3-D analysis of real satellite and observatory data

Finally, the elaborated concept is applied to real magnetic data. We use 10 years of magnetic recordings from the satellites CHAMP, Ørsted and SAC-C, and from the global network of geomagnetic observatories, dating from September 2000 to August 2010. This corresponds to the “CHAMP phase” of the data set used in the 1-D inversion, cf. Figure 5.4. As for the 1-D analysis, we remove core and crustal field as predicted by the CHAOS-4 magnetic field model, we only use night-time data (defined here by local-time between 19:00 and 05:00) and avoid latitudes $>55^\circ$.

The remaining field variations are believed to be due to a magnetospheric source that can be described by low-degree spherical harmonics. As in the test studies, we confine ourselves to $p = 9$ coefficients $\epsilon_n^m$ with $n \leq 3, |m| \leq 1$. This choice does not have a physical basis; however, as observed in Section 3.2, a very large part of the magnetic measurements can be described by these sources. Allowing for more coefficients (e.g. 15 terms with $n \leq 3, |m| \leq 3$) did not improve the results.

As discussed in the previous section, the corresponding induced field is mostly described by the same spherical harmonics, i.e. coefficients $\iota_k^l$ with $k \leq 3, |l| \leq 1$. We fit the magnetic field variations with these coefficients in the time-domain in bins of 6 hours. Shorter bins of 3 hours did not improve the results, and an alternative parametrization of the time dependency with cubic splines (as in Kuvshinov & Olsen, 2006) didn’t yield an improvement either.
3-D analysis of real satellite and observatory data

Figure 6.14: Coefficient of determination $R^2$, measuring the proportion of the data that are described by nine low-degree spherical harmonics.

Figure 6.15: 3-D conductivity model compiled by Alekseev et al. (2015). Colours indicate electrical conductivity in units of S/m.

Figure 6.14 shows the coefficient of determination $R^2$ for each bin. $R^2$ here describes the proportion of the magnetic data that can be described by the 9 considered low-degree spherical harmonics. On average, $R^2 \approx 0.75$, but the variance is large. Hence, on average, about 25% of the measured magnetic variations are not captured by our parametrization. This might be due to source structures of smaller scales, but also due to fast variations of the magnetic field within one bin of 6 hours.
Figure 6.16: $Q$-matrix recovered from 10 years of satellite and observatory data. Blue and red dots denote the real and the imaginary part, respectively, of the individual responses. Confidence limits for a confidence level of 90% are indicated. Solid lines correspond to predictions from the conductivity model shown in Figure 6.15.

Matrix $Q$-responses are estimated at periods between 2 days and 55 days. We show the full $Q$-matrix, which is a $9 \times 9$-matrix, in Figures 6.16 and 6.17. The processing results are compared to model predictions. The latter are obtained by simulating induction in a 3-D conductivity model, which is shown in Figure 6.15. This model was recently compiled by Alekseev et al. (2015) and contains 3-D structures in the top 100 km. Apart from the surface conductance map, it includes known lateral variations in crustal thickness, hereby taking into account the differences between oceanic and continental lithosphere.
At depths >100 km, we use the 1-D conductivity model that we obtained by a 1-D inversion of the data, shown as a red line in Figure 5.8.

As expected, $Q_{1,1}^{0,0}$ (diagonal element in the second row) is the best-recovered element of the $Q$-matrix. This element shows the smallest uncertainties, and its estimates agree well with the model predictions. Some other diagonal elements ($Q_{1,1}^{1,-1}$, $Q_{1,1}^{1,1}$, $Q_{2,1}^{1,-1}$ and $Q_{2,2}^{1,1}$) are reasonably well recovered, at least for periods up to about 30 days. The corresponding rows of the $Q$-matrix also show the highest multiple coherencies (last column). The high coherencies are mostly due to the diagonal elements, which exhibit

Figure 6.17: $Q$-matrix recovered from 10 years of satellite and observatory data, continued. The last column presents multiple squared coherencies for the respective row of the $Q$-matrix (i.e. for the respective induced coefficient $i_k^j$).
the highest ordinary coherencies in the respective rows (not shown). This confirms again that a given coefficient $\epsilon_k^l$ is mostly induced by the corresponding external coefficient $\epsilon_k^l$.

As discussed before, the diagonal elements of the $Q$-matrix only describe bulk conductivity and 1-D structure. In the model studies (Section 6.5), the second column of the $Q$-matrix, corresponding to induction by $\epsilon_1^0$, showed the best-recovered off-diagonal elements. This is not the case for the $Q$-matrix estimated from real data. Although some transfer functions (e.g. $Q_{2,1}^{-1,0}$) are fairly smooth and thus seem to be well-recovered, a comparison with the model predictions reveals that the values are way too large. The information on 3-D conductivity structure is hence below noise level. We renounce an inversion of the data. The $Q$-matrix reveals that any lateral heterogeneity detected in an inversion would rather be an artefact than real structure.
Chapter 7

Conclusions

My PhD project was initiated to advance research in the area of global induction. In my studies, I aimed at developing new techniques for the analysis and the inversion of different types of EM data and, eventually, at providing new models of the distribution of electrical conductivity in Earth’s mantle.

As in many inverse problems, an accurate description of the source is crucial in EM induction research. The magnetospheric ring current is known to be the dominant source for induction processes at periods between 2 days and several months. Many historic and recent global induction studies indeed assume that the source consists of a large-scale symmetric ring current, which can be described by a single spherical harmonic (so-called $P^0$-assumption).

However, there has long been evidence for a more complex structure of the magnetospheric source. In model studies, we showed that the $P^0$-assumption is often not appropriate and leads to pronounced errors in the estimated transfer functions. If these transfer functions are inverted for 3-D conductivity structure, the errors might translate into fallacious conductivity anomalies in the mantle.

To overcome this problem, we introduced new transfer functions that can handle more complex source systems, and developed a multivariate data analysis tool to estimate these transfer functions from different types of EM data from ground, sea and space. By considering a moderate number of low-degree spherical harmonic source terms, we found markedly improved coherencies between input and output signals of the transfer functions for certain locations. But a significant proportion of the measured variations cannot be explained by the chosen terms, and a more adequate parametrization of the magnetospheric source is still not available.

The recovery of the radial (1-D) distribution of electrical conductivity in Earth’s mantle is an old geophysical problem. It can be solved as soon as one spherical harmonic source term and the corresponding induced signal are available. But for most existing studies, the reliability of the inversion results is – for two reasons – difficult to assess. First, most conventional studies do not account for induction in the highly conductive
Conclusions

This biases the results in the upper mantle, not to mention the pronounced 3-D effects that arise from the irregular distribution of land and sea. Second, model uncertainties are hardly ever addressed, which is why the informative value of the recovered models is unclear.

We estimated global $C$-responses from a vast amount of magnetic data from satellites and geomagnetic observatories. The responses were subsequently corrected for 3-D effects due to induction in the oceans by an iterative approach. We inverted the corrected $C$-responses for a 1-D electrical conductivity profile of Earth’s mantle.

The recovered model features a highly resistive upper mantle, increasing conductivity in and beneath the transition zone, a marked kink at a depth of 900 km, and high conductivities underneath. The results of a deterministic inversion were verified by a direct inversion of uncorrected responses in a 3-D environment (with fixed heterogeneous surface shell) and an independent probabilistic analysis. We showed that the resolution of the recovered model can be assessed within the framework of a deterministic inversion by making use of the inverse Hessian of the objective function. The uncertainty estimates reveal that the data are most sensitive to structures at depths between 800 km and 1200 km, whereas conductivity at depths $<400$ km and $>1600$ km is poorly constrained. The spread of the models obtained in the probabilistic study agrees with these findings.

The solution of the 3-D problem is far more complicated, because the induced signals arising from lateral heterogeneities in the mantle are very small. Their detection hence requires an accurate description of the source system, since already small amounts of coherent noise due to non-described sources can make an inversion intractable. To tackle this difficult problem, we developed the $Q$-matrix concept, which is to our knowledge the most consistent concept to treat the problem in the domain of spherical harmonics.

The concept was successfully implemented in a modular global 3-D inversion code, which is based on a fast integral equation forward solver and an efficient adjoint approach to compute the data misfit gradient. The inversion of a test data set, which was prepared during the development phase of the Swarm multi-satellite mission, proved successful. The results suggested that heterogeneous structures of continental size might be resolvable with data of the Swarm mission.

The application to a comparable set of ten years of real data from ground-based observatories and satellites, however, revealed that this appearance was deceiving. Not a single off-diagonal element of the $Q$-matrix was reliably recovered, rendering a 3-D inversion based on these data impossible. This difference to the test studies is explained by the insight that the test data set was oversimplified. The simulated magnetic data contained synthesized contributions of core field, crustal field, ionospheric field, and magnetospheric field. However, the ionospheric field did not include day-to-day variations of the $Sq$ system, and the magnetospheric field was described by a small, finite number of spherical harmonic terms. In reality, the series of magnetospheric source terms is
likely infinite, and we do not know which of these terms are relevant and which can be discarded. Moreover, the test data set did not include auroral currents, which are an important source at high latitudes and for periods up to several days. Finally, the processing of the data also neglects the fact that the magnetic field is not truly a potential field at satellite altitude due to field-aligned currents, which connect the ionospheric and magnetospheric current systems.

Since no 3-D model could be derived, the problem of uniqueness was not even touched. The 1-D analysis revealed that a large amount of models can fit the data within uncertainties. We can expect that the same will be true for the 3-D case. In particular, a reliable 3-D study must prove that lateral heterogeneities in the mantle are necessary to fit the data. I consider this as a great challenge for future studies.

Although the tools for data processing and inversion are available and functional, the recovery of a 3-D model of mantle conductivity failed in this study. The 3-D inversion hinges on a precise determination of the inducing sources. In my eyes, this task is currently out of reach due to the sparse distribution of geomagnetic observatories and the small number of satellites measuring the geomagnetic field. More efforts of the geomagnetic community are required to establish a much better coverage of worldwide geomagnetic observations in order to make the problem tractable one day.
Appendix A

Mathematical Derivations

A.1 Analytical computation of the gradient vector and the Hessian matrix for an inversion for 1-D mantle conductivity structure

Kuvshinov & Semenov (2012) discuss in the appendix of their paper the solution of Maxwell’s equations in a spherical 1-D model consisting of $N$ layers, in which conductivity $\sigma$ varies with radius $r$ as

$$\sigma(r) = \sigma_k \left( \frac{r_k}{r} \right)^2, \quad r_{k+1} < r < r_k,$$

(A.1)

where $r_1 = a$, $r_{N+1} = 0$ and $\sigma_k$ is an appropriate constant. Conductivity is thus a piecewise inverse quadratic function of depth. If the layers are thin, the variation of conductivity within a layer is small, thus $\sigma(r) \approx \sigma_k$ for $r_{k+1} < r < r_k$. Formulation (A.1), however, is mathematically easier to handle than a piecewise constant conductivity structure.

Kuvshinov & Semenov (2012) discuss the calculation of admittances $Y_k(\omega) = Y(\omega, r_k)$ in a spherical body with conductivity structure as given by eq. (A.1). Admittances can be calculated analytically with a recurrence formula, i.e. $Y_k = f(\sigma_k, Y_{k+1})$ and $Y_N = f(\sigma_N)$. Furthermore, the $C$-response is related to the admittance at Earth’s surface as

$$C(\omega) = -\frac{1}{i\omega\mu_0 Y_1(\omega)}.$$

(A.2)

The explicit recurrence formula, which is mathematically not complex, but cumbersome, is given in Appendix E of Kuvshinov & Semenov (2012).

Descent methods used in deterministic inversions require the computation of the gradient and Hessian of the data misfit, which in our case is given by eq. (5.9). The gradient $\nabla \phi_d$ contains the derivatives of the misfit $\phi_d$ with respect to the model parameters $m_k$,
which read

$$\frac{\partial \phi_d}{\partial m_k} = \frac{2}{N\omega} \text{Re} \sum_{\omega} \left[ \frac{C^{\text{pred}}(\omega, m) - C^{\text{obs}}(\omega)}{\delta C^{\text{obs}}(\omega)^2} \right] \cdot \frac{\partial C^{\text{pred}}(\omega, m)}{\partial m_k} \tag{A.3}$$

where superscript * stands for complex conjugation. $m_k$ is a function of the conductivities, which depends on the parametrization of the inversion domain. In our case, $m_k = \log_{10}(\sigma_k/\sigma_0)$, with $\sigma_0 = 1 \text{ S/m}$. We concentrate on calculating the derivatives of $C^{\text{pred}}$ with respect to $\sigma_k$; the derivatives with respect to $m_k$ follow with the chain rule.

Taking in mind the recurrence formula, we obtain

$$\frac{\partial C}{\partial \sigma_k} = \frac{\partial C}{\partial Y_1} \prod_{i=1}^{k-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_k}{\partial \sigma_k}, \tag{A.4}$$

where, from eq. (A.2),

$$\frac{\partial C}{\partial Y_1} = \frac{1}{i\omega\mu_0 Y_1(\omega)^2}. \tag{A.5}$$

The Hessian $H(\phi_d)$ contains the second derivatives of the misfit $\phi_d$ with respect to the model parameters. Its components follow from eq. (A.3),

$$\frac{\partial^2 \phi_d}{\partial m_k \partial m_l} = \frac{2}{N\omega} \text{Re} \sum_{\omega} \left[ \frac{[C^{\text{pred}}(\omega, m) - C^{\text{obs}}(\omega)]^* \cdot \partial^2 C^{\text{pred}}(\omega, m)}{\partial m_k \partial m_l} \right] \\
+ \frac{1}{\delta C^{\text{obs}}(\omega)^2} \left( \frac{\partial C^{\text{pred}}(\omega, m)}{\partial m_k} \right)^* \frac{\partial C^{\text{pred}}(\omega, m)}{\partial m_l} \right]. \tag{A.6}$$

This equation contains the second derivative of the $C$-response with respect to the model parameters $m_k$ and $m_l$. We again focus on the derivatives with respect to the conductivities. Taking the derivative of eq. (A.4) with respect to $\sigma_l$, we obtain

$$\frac{\partial^2 C}{\partial \sigma_k \partial \sigma_l} = \frac{\partial^2 C}{\partial Y_1^2} \prod_{i=1}^{l-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_l}{\partial \sigma_l} \prod_{i=l+1}^{k-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_k}{\partial \sigma_k} \\
+ \frac{\partial C}{\partial Y_1} \prod_{i=1}^{l-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial}{\partial \sigma_l} \left( \frac{\partial Y_l}{\partial Y_{l+1}} \right) \prod_{i=l+1}^{k-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_k}{\partial \sigma_k} \\
+ \sum_{j=1}^{l-1} \left[ \frac{\partial C}{\partial Y_1} \prod_{i=1}^{j-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial^2 Y_j}{\partial Y_{j+1}^2} \prod_{i=j+1}^{l-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_l}{\partial \sigma_l} \prod_{i=l+1}^{k-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_k}{\partial \sigma_k} \right]. \tag{A.7}$$
for off-diagonal elements of $H(\phi_d)$ (here assuming $l < k$; for $l > k$, indices must be switched). For diagonal elements, we obtain analogously

$$\frac{\partial^2 C}{\partial \sigma_k^2} = \frac{\partial^2 C}{\partial Y_1^2} \left( \prod_{i=1}^{k-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_k}{\partial \sigma_k} \right)^2 + \frac{\partial C}{\partial Y_1} \prod_{i=1}^{k-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial^2 Y_k}{\partial \sigma_k^2} + \sum_{j=1}^{k-1} \left[ \frac{\partial C}{\partial Y_1} \prod_{i=1}^{j-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial^2 Y_j}{\partial Y_{j+1}^2} \left( \prod_{i=j+1}^{k-1} \left( \frac{\partial Y_i}{\partial Y_{i+1}} \right) \frac{\partial Y_k}{\partial \sigma_k} \right)^2 \right]. \tag{A.8}$$

From eq. (A.2), we can deduce that

$$\frac{\partial^2 C}{\partial Y_1^2} = - \frac{2}{i \omega \mu_0 Y_1(\omega)^3}. \tag{A.9}$$

The computation of all other derivatives appearing in eqs (A.4), (A.7) and (A.8) requires the ingestion of the recurrence formula for $Y_k$ (Kuvshinov & Semenov, 2012) in the above equations.
Appendix B

Towards a new Parametrization of Global Magnetic Variations due to the \( Sq \) Current System: The Influence of Coordinates and Spherical Harmonic Analysis

B.1 Introduction

Schmucker (1999) analysed observatory magnetic data on quiet days with the goal of describing \( Sq \) variations by a spherical harmonic representation. In spite of otherwise encouraging results, he stated in Section 6 of his paper that “the overall representation of the global \( Sq \) field by spherical harmonics is poor, for \( Z \) worse than for \( X \) and \( Y \)”.

This study was initiated to investigate whether Schmucker’s pessimistic conclusion is due to some of the methods he applied. Schmucker separated external and induced contributions to the variations with Gauss’ potential method. This method does not require any prior information on the conductivity of the Earth and is known to provide an adequate separation of external and induced parts in case of a uniform coverage of observations. However, the distribution of magnetic observatories on Earth’s surface is very far from uniform (Figure 1.2). Koch & Kuvshinov (2013) introduced the \( S3D \) method, which makes use of a prior 3-D model of Earth’s conductivity structure and demonstrated that the \( S3D \) method clearly outperforms the Gauss method in case of the true, heterogeneous distribution of the data.

Further, Schmucker (1999) worked in a geographic coordinate system. The source region of \( Sq \) in the ionosphere, however, is so close to Earth’s surface that current systems with very high probability are influenced by the structure of Earth’s main field. That
is best described by a quasi-dipole coordinate system (Richmond, 1995), which is e.g. used to describe the ionospheric field and its induced counterpart in the Comprehensive Inversion (Sabaka et al., 2002).

In the following sections, I outline the various methods to parametrize the magnetic field due to \( S_q \) signals, and interpret the results with special emphasis on a rigorous analysis of uncertainties. This report summarizes the work performed during my research stay at DTU under the supervision of Nils Olsen in autumn 2014.

### B.2 Coordinate systems

The geographic (GG) coordinate system is a time-independent orthogonal spherical coordinate system with \( \vartheta = 0^\circ \) at the geographic North Pole. The geomagnetic dipole (GM) coordinate system is also orthogonal, but varies slowly with time as the main magnetic field changes. I use the GM dipole coordinate system corresponding to the main field of the epoch 2010 as described by the IGRF-11 model (Finlay et al., 2010), with the North geomagnetic pole situated at \( \vartheta^{GG} = 9.92^\circ, \varphi^{GG} = 287.78^\circ \). Spherical harmonics \( Y_m^n(\vartheta, \varphi) \) can be defined in either geographic or dipole coordinates, and can be rotated from one coordinate system to another by means of a rotation matrix \( R_n \). If \( Y_n \) is a vector containing the spherical harmonics of all orders of a given degree \( n \), then

\[
Y_n^{GM} = R_n Y_n^{GG}, \tag{B.1}
\]

\[
Y_n^{GG} = R_n^\top Y_n^{GM}, \tag{B.2}
\]

where superscript \( ^\top \) denotes matrix transpose. Note that the rotation of a given spherical harmonic \( Y_n^m \) to a different spherical coordinate system only adds energy to spherical harmonics of the same degree \( n \).

Many ionospheric phenomena are naturally organized with respect to the geometry of Earth’s magnetic field due to its influence on the motion of particles. It thus appears convenient to work in a coordinate system that is aligned with the magnetic field, such as the quasi-dipole (QD) coordinate system proposed by Richmond (1995). In this system, the dip equator has a colatitude of \( \vartheta^{QD} = 90^\circ \). The quasi-dipole coordinate system is not orthogonal, which inhibits closed-form solutions of Laplace’s equation. But at a specific radius \( r \), it is possible to expand a given quantity in quasi-dipole coordinates by spherical harmonics. Further, if \( Y \) is a vector containing spherical harmonics, it is possible to define a matrix \( D \), such that

\[
Y^{QD} = DY^{GM}. \tag{B.3}
\]

\( D \) maps energy from a given spherical harmonic \( Y_n^m \) to spherical harmonics \( Y_k^l \) of different orders and different degrees (note that I will use indices \( k \) and \( l \) for degree and order,
respectively, in QD coordinates). For this reason, both \( \mathbf{Y} \) and \( \mathbf{D} \) in theory must be of infinite dimension. This is, of course, not applicable in practice. But for a given \( Y^l_k \), tests have shown that choosing \( n_{\text{max}} \approx k + 10 \) is sufficient to reproduce all features of the desired spherical harmonic with sufficient accuracy.

Numerical codes converting coordinates between GG, GM and QD coordinate systems have been available for this study, as well as codes generating the rotation matrices \( \mathbf{R}_n \) and \( \mathbf{D} \). Thanks to the linearity of Maxwell’s equations, the matrices \( \mathbf{R}_n \) and \( \mathbf{D} \) can not only be used to rotate spherical harmonics (or their derivatives) from one coordinate system to another, but also the model responses \( B^m_n \), which are calculated in the GG coordinate system, in an analogous way. Note that in this study, the GM coordinate system is only used as intermediate step when converting spherical harmonics or model responses from the GG system to the QD system or vice versa.

### B.3 Data selection and processing

In the context of a study on 1-D mantle conductivity (Chapter 5), I had collected 10 years of hourly mean observatory magnetic data, ranging from September 2000 to August 2010. These raw data were processed as follows. First, I removed core and crustal field as predicted by the CHAOS-4 magnetic field model (Olsen et al., 2014). Obvious outliers and baseline jumps were, after careful inspection, removed manually. If necessary, remaining slow variations in the observatory data were removed by fitting low-degree polynomials to the time series.

The \( S_q \) variations are known to change from day to day, with season and solar activity. For the forthcoming analysis, I decided to pick a single quiet (undisturbed) equinoctial day from the time series. The choice fell on March 22, 2010. Since both the preceding and the successive day were also quiet, this date seemed particularly appropriate for my study. 120 observatories provided continuous measurements for the entire day. To avoid an influence of the electrojets, I excluded data from polar and equatorial regions, i.e. from geomagnetic latitudes \( >55^\circ \) and quasi-dipole latitudes \( <6^\circ \). 78 observatories remained.

From time series of hourly mean magnetic data, complex-valued time spectra are computed by a discrete Fourier transform. The information of 24 measurements in time is known to be contained in 12 spectra/harmonics (plus a baseline, which was removed beforehand). But how many of these spectra are necessary for an appropriate description of the smooth daily variation? To investigate this question, I compute the correlation between a measurement \( X \) and its calculated counterpart \( X^{\text{synth}} \). The coefficient of
Table B.1: Mean coefficients of determination $R^2$, measuring the correlations between measurements and predictions from a truncated Fourier synthesis of the first $p_{\text{max}}$ time harmonics.

<table>
<thead>
<tr>
<th>$p_{\text{max}}$</th>
<th>$R^2(B_r)$</th>
<th>$R^2(B_\theta)$</th>
<th>$R^2(B_\phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.279</td>
<td>0.343</td>
<td>0.273</td>
</tr>
<tr>
<td>2</td>
<td>0.631</td>
<td>0.715</td>
<td>0.696</td>
</tr>
<tr>
<td>3</td>
<td>0.863</td>
<td>0.877</td>
<td>0.917</td>
</tr>
<tr>
<td>4</td>
<td>0.940</td>
<td>0.945</td>
<td>0.970</td>
</tr>
<tr>
<td>6</td>
<td>0.972</td>
<td>0.975</td>
<td>0.988</td>
</tr>
<tr>
<td>8</td>
<td>0.986</td>
<td>0.987</td>
<td>0.993</td>
</tr>
</tbody>
</table>

determination $R^2(X)$ is defined as

$$R^2(X) = 1 - \frac{\sum_{i=1}^{N} |X_i - X_{\text{synth}}|^2}{\sum_{i=1}^{N} |X_i|^2},$$

where $X$ is any measurement ($B_r$, $B_\theta$ or $B_\phi$) at any observatory, and index $i$ runs over all $N = 24$ measurements taken on the considered day. $X_{\text{synth}}$ is obtained by a truncated Fourier synthesis of the first $p_{\text{max}}$ time spectra (here and in the following, $p$ is used to enumerate the time harmonics, i.e. $p = 1$ corresponds to a period of $T = 24$ h, etc).

Table B.1 presents means of $R^2$ (over all observatories) for all components and several choices for $p_{\text{max}}$. According to the results, more than 60% of the measurements are explained by the first two harmonics of $T = 24$ h and $T = 12$ h. If adding the next harmonics of $T = 8$ h and $T = 6$ h, more than 93% of the time-domain data are reproduced. With 6 harmonics, including those of $T = 4.8$ h and $T = 4$ h, even more than 97% of the data are explained. Differences between the individual field components are small, with a slight tendency to larger $R^2$ for the horizontal components.

I also investigated the effect of applying a trend correction to the time series before computing the spectra. Following the methodology of Schmucker (1999), this correction consists of replacing the first measurement $X(t_0)$ by $(X(t_0) + X(t_{24}))/2$, where $t_0$ is the time of the first measurement on the day of interest and $t_{24}$ is the time of the first measurement on the successive day. The values in Table B.1 increase slightly if such a trend correction is applied beforehand. The correction, however, also generates artificial kinks in the time series, which are due to different amplitudes of the magnetic field on successive days. This effect is maximum at observatories situated at longitudes close to 180°. Since the improvements in $R^2$ are relatively small, I therefore decided to use the spectra obtained without trend correction for my further analysis.
Spherical harmonic analysis

Schmucker (1999) and Koch & Kuvshinov (2013) used 6 time harmonics for their further investigations. From the results of Table B.1, this choice seems reasonable. I will, however, get back to this issue later in this report.

B.4 Spherical harmonic analysis

To derive coefficients $\varepsilon^m_n$ from observatory data, it is necessary to solve a linear system of equations, either given by eq. (2.17) or by eqs (2.25)–(2.27). In the latter case, they are calculated from $z^m_n$ and $v^m_n$ as

$$
\varepsilon^m_n(\omega) = \frac{(n+1)v^m_n(\omega) + z^m_n(\omega)}{2n + 1}.
$$

(B.5)

Using eqs (2.25)–(2.26) will be denoted as “Gauss method”, while using eq. (2.17) will be denoted as “S3D method”.

For the S3D method, model responses $B^m_n$ are required. I compute these responses with a numerical code (Kuvshinov, 2008) based on a contracting integral equation solver (Pankratov et al., 1995). The conductivity model coincides with that shown in Figure 3.2, where the heterogeneous top layer, which represents the distribution of oceans and continents, has a resolution of $2^\circ$.

My choice of spherical harmonic terms is emulated by the work of Schmucker (1999). It is easily shown that terms with $m = p$ are local-time terms, which describe waves moving westwards with the sun. To account for non-local-time effects, terms with $m < p$ and $m > p$ can be added. Further, it is known that terms with $n = m + 1$ dominate the spectrum. Following Schmucker (1999), the double sums in eqs (2.17) and (2.25)–(2.26) are therefore best dissolved as

$$
\sum_{n,m} = \sum_{m=p-L}^{p+L} \sum_{n=|m|}^{|m|+K-1},
$$

(B.6)

with parameters $K$ and $L$ chosen appropriately. The total number of spherical harmonic terms is then given by $M = K(1 + 2L)$, unless a term with $m = 0$ is present, in which case $M$ is reduced by one (to avoid magnetic monopoles). With $L = 1$ and $K = 4$ for all periods, $M = 12$ for $p \geq 2$ and $M = 11$ for $p = 1$. I will stick to these choices for the forthcoming analysis.

Note that $L$ and $K$ constrain the spherical harmonic terms used in the considered coordinate system – i.e., they constrain $n$ and $m$ if using a GG coordinate system, but $k$ and $l$ if using a QD coordinate system. With the present choices, $k_{\text{max}} = 10$. To make sure that spherical harmonics/responses with this degree are correctly reproduced in QD coordinates, corresponding spherical harmonics/responses are computed in GG coordinates up to $n_{\text{max}} = 30$. 
Towards a new Parametrization of the Sq Current System

With the different coordinate systems and separation methods introduced above in mind, there are 4 different options to estimate coefficients $\varepsilon_m^m$:

1. GG coordinate system, Gauss method
2. GG coordinate system, S3D method
3. QD coordinate system, Gauss method
4. QD coordinate system, S3D method

As elaborated above, I in this study do not try to recover $\varepsilon_n^m$ in a GM coordinate system. Both vertical and horizontal components of $B$ are necessary to estimate coefficients $\varepsilon_n^m$ if using the Gauss method. This is not the case for the S3D method, and I only use the horizontal components, since they are less affected by induction.

In each of the above cases 1–4, the system of linear equations is solved by a robust least squares method with Huber weights (e.g. Aster et al., 2005). Apart from estimating coefficients $\varepsilon_n^m$, an estimation of their uncertainties is crucial to understand how reliable the estimates are. Olsen (1991) compared four different methods for estimating uncertainties. However, all of these methods were based on the analysis of data from multiple equinoctial days, thus implicitly assuming that the magnetic field due to $Sq$ currents may exhibit statistical variations, but does not change systematically from day to day.

I prefer omitting such an assumption and analysing data from different days independently, which requires a different approach. The jackknife approach is an experimental method that has proven to yield reliable covariances in many data analysis problems. I apply this method as described by Chave & Thomson (1989) to estimate covariances of the coefficients $\varepsilon_n^m$ and then compute uncertainties $\delta\varepsilon_n^m$ by taking the square roots of the diagonal entries of the covariance matrix. Note that in case of the Gauss method, $\delta\varepsilon_n^m$ is not estimated directly, but derived from $\delta v_m^m$ and $\delta z_m^m$ according to eq. (B.5),

$$\delta\varepsilon_n^m(\omega) = \frac{(n + 1)\delta v_n^m(\omega) + \delta z_n^m(\omega)}{2n + 1}. \quad (B.7)$$

Table B.2 presents coefficients $\varepsilon_n^m$ and corresponding uncertainties $\delta\varepsilon_n^m$ for cases 1–4 and periods of 24 h, 12 h, 8 h and 6 h, i.e. $p = 1..4$. As expected, the largest amplitudes are observed for the well-known principal terms with $m = p$ and $n = m + 1$, i.e. the local-time terms $\varepsilon_1^2(24 \text{ h})$, $\varepsilon_2^3(12 \text{ h})$ etc. These terms seem to be well-constrained, as the corresponding errors only reach about 10% of the amplitudes of the estimates themselves. Moreover, very similar results are obtained with different separation methods (compare e.g. $\varepsilon_2^3(12 \text{ h})$ for cases 1 and 2). In contrast, low-order terms ($m < p$) with large amplitudes, such as $\varepsilon_0^0(24 \text{ h})$ or $\varepsilon_1^1(12 \text{ h})$, show large uncertainties (partially of the same magnitude as the estimates themselves) and can differ significantly if estimated with different methods (compare e.g. $\varepsilon_0^0(24 \text{ h})$ for cases 1 and 2). High-order terms ($m > p$)
Table B.2: Coefficients $\varepsilon^m_n$ (ℜ and ℑ denote the real and the imaginary part, respectively) and their uncertainties $\delta\varepsilon^m_n$ for 4 time harmonics ($p = 1.4$) and cases 1–4, estimated from observational magnetic data on the equinoctial day 2010/03/22.

<table>
<thead>
<tr>
<th>$T$ [h]</th>
<th>n</th>
<th>m</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>1</td>
<td>0</td>
<td>8.21</td>
<td>-2.65</td>
<td>15.66</td>
<td>-3.96</td>
</tr>
<tr>
<td>24</td>
<td>3</td>
<td>0</td>
<td>3.24</td>
<td>10.27</td>
<td>11.48</td>
<td>3.30</td>
</tr>
<tr>
<td>24</td>
<td>2</td>
<td>1</td>
<td>54.92</td>
<td>1.78</td>
<td>5.81</td>
<td>53.18</td>
</tr>
<tr>
<td>24</td>
<td>3</td>
<td>1</td>
<td>6.59</td>
<td>1.48</td>
<td>5.29</td>
<td>7.82</td>
</tr>
<tr>
<td>24</td>
<td>4</td>
<td>1</td>
<td>-17.27</td>
<td>-0.80</td>
<td>4.90</td>
<td>-18.49</td>
</tr>
<tr>
<td>24</td>
<td>2</td>
<td>2</td>
<td>-4.11</td>
<td>6.17</td>
<td>8.60</td>
<td>-1.71</td>
</tr>
<tr>
<td>24</td>
<td>3</td>
<td>2</td>
<td>0.13</td>
<td>2.47</td>
<td>4.10</td>
<td>-1.89</td>
</tr>
<tr>
<td>24</td>
<td>4</td>
<td>2</td>
<td>-2.68</td>
<td>-2.25</td>
<td>5.02</td>
<td>-3.39</td>
</tr>
<tr>
<td>24</td>
<td>5</td>
<td>2</td>
<td>3.46</td>
<td>2.61</td>
<td>3.96</td>
<td>5.02</td>
</tr>
</tbody>
</table>

For $\delta\varepsilon^m_n = 1$.
generally have relatively small amplitudes and uncertainties of similar magnitude as the estimates themselves, indicating that they are poorly constrained.

The uncertainties $\delta \varepsilon^m_n$ are markedly reduced if using the S3D method (case 2) instead of the Gauss method (case 1). The reduction on average reaches a factor 2 for $p = 1$ and $p = 2$ and somewhat less for higher time harmonics. This result is a clear recommendation for the S3D method. Note in this context that Olsen (1991) obtained smaller errors with the Gauss method than with a separation technique based on a prior 1-D model. This confirms the importance of 3-D effects. The relative errors (i.e. the magnitude of the errors in comparison to the estimates themselves) obtained in this study are, on average, far larger than those obtained by Olsen (1991). As elaborated above, the estimation of errors in Olsen (1991) was based on the assumption that there is no systematic day-to-day variability. Since there is no foundation for such an assumption, I believe that the error estimates obtained in this study are more realistic. Note that it is not possible to compare the absolute magnitudes of my estimates of $\varepsilon^m_n$ and those of Olsen (1991), since different normalizations were used in the Fourier transformations.

If using a quasi-dipole coordinate system (cases 3 and 4), the energy is concentrated in the same principal local-time terms, but due to the rotated and deformed coordinate system, the phase of the estimates may differ from that obtained in a geographic coordinate system (compare e.g. $\varepsilon^1_1$ (24 h) for cases 1 and 3). The error estimates are almost independent of the employed coordinate system and average out if analysing all harmonics in time and space.

To investigate how well the data are fit by the spherical harmonic expansions, I correlate estimated and synthesized time spectra of all observatories and compute coefficients of determination $R^2$ with a formula analogous to eq. (B.4). Here, “synthesized” time spectra denote spectra obtained from a spherical harmonic synthesis. $R^2$ for cases 1–4 are provided in Table B.3.

The first observation concerns the variation with period. For nearly all components and cases, $R^2$ are relatively stable for $p = 1..4$ and drop significantly for $p = 5, 6$. The latter time harmonics thus cannot adequately be described with the chosen spherical harmonic expansion. For a subsequent synthesis, it thus appears more appropriate to exclude these time harmonics. As seen in Table B.1, the first 4 harmonics still explain more than 93% of the temporal variation.

For none of the magnetic field components, the choice of a particular coordinate system or a particular separation method has a significant effect on $R^2$. Improvements at a specific period are compensated by setbacks at other periods. $R^2$ are generally higher for $B_\varphi$ than for $B_r$ and $B_\theta$. This might be due to the fact that $B_\varphi$ is barely affected by ring current activity, whereas it is strongly affected by $Sq$.

With the recovered coefficient time spectra and the spherical harmonics/modellings in hand, it is possible to synthesize the magnetic field not only at observatory locations, but
Table B.3: Coefficients of determination $R^2$, measuring the correlations between estimated and synthesized magnetic field time spectra for 6 time harmonics.

(a) Case 1: Gauss method, GG coordinates

<table>
<thead>
<tr>
<th>$T$ [h]</th>
<th>$R^2(B_r)$</th>
<th>$R^2(B_\theta)$</th>
<th>$R^2(B_\phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.0</td>
<td>0.73</td>
<td>0.72</td>
<td>0.80</td>
</tr>
<tr>
<td>12.0</td>
<td>0.72</td>
<td>0.68</td>
<td>0.94</td>
</tr>
<tr>
<td>8.0</td>
<td>0.76</td>
<td>0.56</td>
<td>0.92</td>
</tr>
<tr>
<td>6.0</td>
<td>0.81</td>
<td>0.44</td>
<td>0.86</td>
</tr>
<tr>
<td>4.8</td>
<td>0.38</td>
<td>0.31</td>
<td>0.66</td>
</tr>
<tr>
<td>4.0</td>
<td>0.35</td>
<td>0.33</td>
<td>0.51</td>
</tr>
</tbody>
</table>

(b) Case 2: S3D method, GG coordinates

<table>
<thead>
<tr>
<th>$T$ [h]</th>
<th>$R^2(B_r)$</th>
<th>$R^2(B_\theta)$</th>
<th>$R^2(B_\phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.0</td>
<td>0.64</td>
<td>0.72</td>
<td>0.80</td>
</tr>
<tr>
<td>12.0</td>
<td>0.80</td>
<td>0.67</td>
<td>0.94</td>
</tr>
<tr>
<td>8.0</td>
<td>0.80</td>
<td>0.59</td>
<td>0.92</td>
</tr>
<tr>
<td>6.0</td>
<td>0.72</td>
<td>0.46</td>
<td>0.85</td>
</tr>
<tr>
<td>4.8</td>
<td>0.28</td>
<td>0.32</td>
<td>0.65</td>
</tr>
<tr>
<td>4.0</td>
<td>0.28</td>
<td>0.32</td>
<td>0.48</td>
</tr>
</tbody>
</table>

(c) Case 3: Gauss method, QD coordinates

<table>
<thead>
<tr>
<th>$T$ [h]</th>
<th>$R^2(B_r)$</th>
<th>$R^2(B_\theta)$</th>
<th>$R^2(B_\phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.0</td>
<td>0.74</td>
<td>0.74</td>
<td>0.83</td>
</tr>
<tr>
<td>12.0</td>
<td>0.73</td>
<td>0.70</td>
<td>0.94</td>
</tr>
<tr>
<td>8.0</td>
<td>0.78</td>
<td>0.58</td>
<td>0.90</td>
</tr>
<tr>
<td>6.0</td>
<td>0.79</td>
<td>0.49</td>
<td>0.81</td>
</tr>
<tr>
<td>4.8</td>
<td>0.36</td>
<td>0.33</td>
<td>0.62</td>
</tr>
<tr>
<td>4.0</td>
<td>0.36</td>
<td>0.32</td>
<td>0.57</td>
</tr>
</tbody>
</table>

(d) Case 4: S3D method, QD coordinates

<table>
<thead>
<tr>
<th>$T$ [h]</th>
<th>$R^2(B_r)$</th>
<th>$R^2(B_\theta)$</th>
<th>$R^2(B_\phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.0</td>
<td>0.67</td>
<td>0.74</td>
<td>0.83</td>
</tr>
<tr>
<td>12.0</td>
<td>0.80</td>
<td>0.70</td>
<td>0.94</td>
</tr>
<tr>
<td>8.0</td>
<td>0.79</td>
<td>0.60</td>
<td>0.90</td>
</tr>
<tr>
<td>6.0</td>
<td>0.71</td>
<td>0.49</td>
<td>0.81</td>
</tr>
<tr>
<td>4.8</td>
<td>0.29</td>
<td>0.33</td>
<td>0.62</td>
</tr>
<tr>
<td>4.0</td>
<td>0.25</td>
<td>0.32</td>
<td>0.56</td>
</tr>
</tbody>
</table>

everywhere on Earth’s surface. For cases 1 and 3, which rely on the Gauss method, the magnetic field is calculated with the estimated $z_n^m$ and $v_n^m$ and the spherical harmonics $Y_n^m$. For cases 2 and 4, which rely on the S3D method, it is calculated with the estimated $\varepsilon_n^m$ and the modelings $B_n^m$. Figure B.1 shows the radial component for a period of $T = 24$ h and cases 1–4. Very different results are obtained with the Gauss method (panel 1) and the S3D method (panel 2). The latter show smaller-scale structures, which are due to induction in the heterogeneous top layer, and generally smaller amplitudes. In particular, the obvious artefact in the antarctic region in panel 1 is not present in panel 2.

If using the Gauss method in a quasi-dipole coordinate system (panel 3), results do not change markedly, and artefacts in regions that are not covered by observations rather increase. Combining the S3D method with quasi-dipole coordinates (panel 4) yields results that are clearly aligned with the dip equator. Equator-parallel stripes most probably result from the parametrization.

In contrast to the radial component, the synthesis of the $\theta$-component (Figure B.2) is mostly independent of the method used to separate external from internal contributions (panels 1 and 2). This confirms the information gained from Table B.3. The synthesized $B_\theta$ slightly depends on the coordinate system. If using quasi-dipole coordinates (panels 3 and 4), stripes parallel to the dip equator appear in the results.

It is striking to see that for all 4 cases, the largest amplitudes of the synthesized fields are observed in regions that are not covered by any data. For $B_\theta$, this is particularly apparent in the imaginary part, for which a strong negative anomaly extends over the
Towards a new Parametrization of the Sq Current System

Figure B.1: Synthesized spectra of the radial component $B_r$ (left: real part, right: imaginary part) for a period of $T = 24$ h and cases 1–4 (see text). Estimated spectra at observatory locations are plotted as coloured dots.

Pacific Ocean and South America. This anomaly, as well as others, is likely an artefact, arising from the poorly constrained spherical harmonic terms in Table B.2. In spite of the relatively small number of spherical harmonics (11) used to describe this time harmonic of the magnetic field, such artefacts appear in regions with poor data coverage due to the very heterogeneous distribution of magnetic observatories.

Olsen (1991) tackled this problem by applying regularization during the spherical harmonic analysis. He used a larger number of spherical harmonics to parametrize the magnetic field, but penalized terms of high degrees. This is the equivalent to first-order Tikhonov regularization in the wavenumber domain.
Schmucker (1999) used a different approach. He assigned weights to the observatories to simulate a more even global distribution. This approach appears more suitable in context of the present study, which seeks to parametrize the magnetic field with a moderate number of basis functions. I assign weights of 0.5 to observatories in Europe and East Asia, where the density of observatories is high, and weights of 1.0 to all others. The SHA is then performed with the weighted data. With regard to the previous results, I decided to employ the S3D method and use a GG coordinate system (case 2) for this experiment and all subsequent investigations.

The coefficients of determination are presented in Table B.4. If comparing to the
Table B.4: Coefficients of determination $R^2$ for case 2, with data weighted according to the observatory distribution.

<table>
<thead>
<tr>
<th>$T$ [h]</th>
<th>$R^2(B_r)$</th>
<th>$R^2(B_\beta)$</th>
<th>$R^2(B_\phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.0</td>
<td>0.68</td>
<td>0.74</td>
<td>0.83</td>
</tr>
<tr>
<td>12.0</td>
<td>0.81</td>
<td>0.64</td>
<td>0.95</td>
</tr>
<tr>
<td>8.0</td>
<td>0.80</td>
<td>0.56</td>
<td>0.93</td>
</tr>
<tr>
<td>6.0</td>
<td>0.71</td>
<td>0.46</td>
<td>0.88</td>
</tr>
</tbody>
</table>

results of the corresponding experiment without weights (Table B.3b), slightly larger $R^2$ are obtained on average. The differences are, however, small, and the maps of the synthesized magnetic field do not differ markedly from those in Figures B.1 and B.2.

B.5 Recovery of the source current

Like the magnetic field, the equivalent source current can be expanded in terms of spherical harmonics. The current function $\Psi$ is defined as (Olsen, 1991)

$$\Psi(r, \omega) = -\frac{a}{\mu_0} \sum_{n,m} \frac{2n + 1}{n + 1} \varepsilon_m^m(\omega) \left( \frac{r}{a} \right)^n Y_n^m(\theta, \varphi).$$  \hspace{1cm} (B.8)

The current density $j(r, \omega)$ is derived from $\Psi$ as

$$j = -e_r \times \nabla \Psi,$$  \hspace{1cm} (B.9)

where $e_r$ is the radial unit vector. The radius $r$ corresponds to the altitude of the current system; I set $r = a + 110$ km.

The synthesized evolution of the current function $\Psi$ in time is plotted in Figure B.3. To compute $\Psi$, I used coefficients $\varepsilon_m^m$ derived with the method of case 2. As expected,
the main features of $\Psi$ are two whirls, positive in the Northern hemisphere, negative in the Southern hemisphere, which move westwards with the Sun. The observation that the magnitude of the whirls increases towards 12 UTC and decreases later might be due to the good data coverage in Europe and southern Africa.

B.6 Analysis of day-to-day variability

The analysis carried out so far was based on data from a single quiet equinoctial day (March 22, 2010). Such a day is believed to be ideal for a spherical harmonic representation of the magnetic field due to ionospheric sources with a moderate number of terms (e.g. Schmucker, 1999). I tested this assumption by comparing the results obtained above to results obtained with the same method for other days. In Table B.5, I compare coefficients of determination $R^2$ for the basic period of $T = 24$ h and the quiet days 2009/09/23 (autumn equinox), 2009/12/30 (winter solstice), 2010/03/22 (spring equinox) and 2010/06/20 (summer solstice). All results were obtained with the S3D method in a GG coordinate system (case 2).

$R^2$ for the analysed days differ markedly. If averaging over all components, the best results are obtained for the summer solstice (2010/06/20), while the worst are obtained for the winter solstice (2009/12/30). This might be an effect of the globally uneven distribution of magnetic observatories. Due to the comparably good coverage north of the equator, enhanced signals in the northern hemisphere (as expected in the northern summer) are better captured than enhanced signals in the southern hemisphere (as expected in the northern winter). The differences, however, could also be due to random variations in the $Sq$ source system, and an analysis of further days from different seasons would be necessary to confirm the above interpretation. Note also that I only analysed quiet days; on disturbed days, the measurements are believed to be affected by magnetospheric signals in addition to the ionospheric signals, which requires different basis functions.

Table B.5: Coefficients of determination $R^2$ for a period of $T = 24$ h and quiet days of different seasons, obtained with the method of case 2.

<table>
<thead>
<tr>
<th>Date</th>
<th>$R^2(B_r)$</th>
<th>$R^2(B_\varphi)$</th>
<th>$R^2(B_\vartheta)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009/09/23</td>
<td>0.52</td>
<td>0.81</td>
<td>0.83</td>
</tr>
<tr>
<td>2009/12/30</td>
<td>0.42</td>
<td>0.72</td>
<td>0.63</td>
</tr>
<tr>
<td>2010/03/22</td>
<td>0.64</td>
<td>0.72</td>
<td>0.80</td>
</tr>
<tr>
<td>2010/06/20</td>
<td>0.69</td>
<td>0.79</td>
<td>0.85</td>
</tr>
</tbody>
</table>
A final test investigates how much the estimated time spectra of source coefficients \( \varepsilon_{\nu}^{\alpha}(\omega) \) themselves vary during the year. For this purpose, I analysed data from 13 relatively equally spaced quiet days between September 2009 and August 2010. Figures B.4 and B.5 present the results for periods of 24 h and 12 h, respectively.

The right panels of both figures show the variations of the absolute values of the dominant coefficients. For \( T = 24 \text{ h} \), these are \( \varepsilon_0^1 \), \( \varepsilon_1^1 \), and \( \varepsilon_2^1 \), while for \( T = 12 \text{ h} \), these are \( \varepsilon_1^1 \), \( \varepsilon_2^2 \), and \( \varepsilon_3^2 \). The absolute values differ markedly over the year. There does not seem to be a clear trend with season, except possibly for \( \varepsilon_2^2 (12 \text{ h}) \), which is stronger in summer than in winter. There does not seem to be a correlation with the \( F_{10,7} \) index either, which is commonly used as a measure for the intensity of the solar flux (e.g. Sabaka et al., 2004).
The left panels of Figures B.4 and B.5 present the same coefficients in the complex plane. There is again large variability for most coefficients. Interestingly, the coefficients with largest amplitudes ($\varepsilon_1^2(24 \text{ h})$ and $\varepsilon_3^2(12 \text{ h})$, respectively) show the smallest variability. This result might indicate that these dominant coefficients are determined with greater accuracy than the others, as already observed in Table B.2. However, for all coefficients, the observed variability clearly exceeds the estimated uncertainties. This shows that there is a significant day-to-day variability in the $Sq$ system that has to be taken into account when devising a parametrization.
Appendix C

Reproducing Electric Field Observations during Magnetic Storms by means of Rigorous 3-D Modelling and Distortion Matrix Co-estimation

C.1 Background

Electric fields induced in the conducting Earth by geomagnetic disturbances drive currents in power transmission grids, telecommunication lines or buried pipelines. These currents, known as Geomagnetically Induced Currents (GIC), are known to cause service disruptions (e.g. Daglis, 2004, and references therein). The effect is maximal at high latitudes due to the presence of strong polar electrojet currents (e.g. Viljanen & Pirjola, 1994; Pulkkinen et al., 2012). However, both observations and models show that massive GIC caused by intensifications of the magnetospheric ring current also pose a risk at low and mid-latitudes, where the majority of systems vulnerable to GIC are located (e.g. Kappenman, 2005).

A technique to model the geoelectric field induced by large-scale magnetospheric currents in a 3-D conductivity model of the Earth was presented by Püthe & Kuvshinov (2013c), based on a previous study by Olsen & Kuvshinov (2004). In that study, we used precomputed electromagnetic (EM) responses of the 3-D model and magnetic data from the global network of geomagnetic observatories to construct the magnetospheric source, described by spherical harmonic expansion (SHE) coefficients. A convolution of the source with the precomputed model responses yielded time series of electric and magnetic fields anywhere on the surface of the Earth.
The methodology of Püthe & Kuvshinov (2013c) is self-consistent, but depending on location, the presented results might still over- or underestimate the amplitudes of the actual electric field. This is due to galvanic effects, i.e. the build-up of electric charges along near-surface, small-scale conductivity contrasts or topographic inhomogeneities (e.g. Jiracek, 1990) that were not included in the model. Galvanic effects are well-known in the magnetotelluric (MT) community, where they are usually referred to as “static shift” (e.g. Simpson & Bahr, 2005; Berdichevsky & Dmitriev, 2008; Chave & Jones, 2012). This name reflects the frequency-independent shift of MT response functions (apparent resistivities) that the effect causes. MT responses are routinely corrected for the static shift by introducing a real-valued frequency-independent distortion matrix, which separates galvanic from (the usually desired) inductive effects (e.g. Groom & Bahr, 1992).

Little galvanic effects are expected on the bottom of oceanic basins due to the relatively homogeneous deposit of deep-sea sediments and the consequential layered structure. By analysing data from an ocean bottom MT survey in the Philippine Sea, we first validate the concept of Püthe & Kuvshinov (2013c). We then analyse electric field data at onshore geomagnetic observatories in Japan for 6 magnetic storms. By relating model predictions to the measurements, we estimate the distortion matrix for each observatory. Statistical inferences are drawn from a comparison of the results obtained for different storms. With help of the estimated distortion matrices, we finally show how our concept can be applied to real-time prediction of the electric field during magnetic storms.

The methods and results presented here were published as Püthe et al. (2014).

C.2 Methods

In this section, we first give an overview of the data used in the present study. We then briefly review the methodology presented in more detail by Püthe & Kuvshinov (2013c) before outlining the estimation of distortion matrices.

Table C.1: Overview of the magnetic data used in this study. The second column contains the peak Dst values for each storm. The last column contains the number of observatories from which data were used to construct the source field model.

<table>
<thead>
<tr>
<th>Storm</th>
<th>Dst</th>
<th>Start date/UTC</th>
<th>End date/UTC</th>
<th>obs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apr-2000</td>
<td>-288</td>
<td>00/04/03 14:00</td>
<td>00/04/13 14:00</td>
<td>56</td>
</tr>
<tr>
<td>Jul-2000</td>
<td>-301</td>
<td>00/07/12 18:00</td>
<td>00/07/22 18:00</td>
<td>65</td>
</tr>
<tr>
<td>Aug-2000</td>
<td>-235</td>
<td>00/08/09 00:00</td>
<td>00/08/19 00:00</td>
<td>63</td>
</tr>
<tr>
<td>Mar-2001</td>
<td>-387</td>
<td>01/03/28 00:00</td>
<td>01/04/07 00:00</td>
<td>63</td>
</tr>
<tr>
<td>Oct-2003</td>
<td>-388</td>
<td>03/10/26 12:00</td>
<td>03/11/05 12:00</td>
<td>70</td>
</tr>
<tr>
<td>Nov-2003</td>
<td>-422</td>
<td>03/11/17 00:00</td>
<td>03/11/27 00:00</td>
<td>72</td>
</tr>
</tbody>
</table>
Reproducing Electric Field Observations during Magnetic Storms

Figure C.1: E-field measurement sites. The three Japanese observatories provide electric field data continuously, whereas the ocean bottom array was installed during the April 2000 magnetic storm. Note that OB3, which was installed on the seafloor between OB2 and OB4, did not provide useful data. Colours indicate topography/bathymetry.

C.2.1 Data

Earth’s magnetic field is routinely measured at more than 150 geomagnetic observatories worldwide, of which about 120 are part of the International Real-Time Magnetic Observatory Network INTERMAGNET (Love & Chulliat, 2013). We collect minute mean definitive vector data of all available observatories at geomagnetic latitudes equatorward of $\pm 55^\circ$ for in total 6 magnetic storms. All storms occurred during the peak phase of solar cycle 23, namely in April 2000, July 2000, August 2000, March 2001, October 2003 and November 2003. For each storm, we select a time segment of 10 days, covering build-up phase, main phase and recovery phase. A summary of the data is given in Table C.1. The magnetic data are used to construct a model of the magnetospheric source, as will be described in the next subsection.

While long-term measurements of the geomagnetic field at observatories are common, the geoelectric field is usually only measured in MT field campaigns. The Japanese
observatories Kakioka (KAK), Kanoya (KNY) and Memambetsu (MMB), all part of INTERMAGNET, are an exception, as all of them have routinely measured the geoelectric field for several decades (Minamoto, 2013). We use minute mean electric field data of all three observatories to estimate distortion matrices, as outlined below.

In addition, we use minute mean electric field data from an ocean bottom MT survey, carried out from November 1999 to July 2000 in the Philippine Sea (Seama et al., 2007). The survey was based on 6 ocean bottom electro-magnetometers, deployed along a line at water depths between 3250 m and 5430 m. The stations in particular recorded the April 2000 magnetic storm and are thus of interest for our analysis. The locations of observatories and ocean bottom electro-magnetometers providing electric field data are depicted on a map in Figure C.1.

We subtract the baseline and a linear trend from both magnetic and electric data to remove main field contributions and possible instrument drift. All magnetic data are checked visually for gaps and offsets. Small gaps are interpolated, channels with low-quality data or large gaps are removed.

C.2.2 Calculation of the electric field

We expand geomagnetic and geoelectric fields by spherical harmonic basis functions as in eqs (2.17)–(2.18). The calculation of electric field time series during a magnetic storm involves the following steps:

1. Calculation of $B_m^n$ and $E_m^n$ in a 3-D conductivity model for the desired set of spherical harmonic sources and representative frequencies $\omega$. This is done using a numerical solution (Kuvshinov, 2008) based on a contracting integral equation approach (Pankratov et al., 1995). The responses are modelled at Earth’s surface on a regular $1^\circ \times 1^\circ$-mesh.

2. Spatial interpolation of $B_m^n$ to observatory locations $r_j$.

3. Interpolation of $B_m^n$ to the full set of frequencies contained in the data.

4. Fourier transformation of observed time series $B_{\text{obs}}(r_j, t)$, yielding $B_{\text{obs}}(r_j, \omega)$.

5. For each frequency $\omega$, construction of a system of linear equations (2.17) and solution of this system for coefficients $\varepsilon_m^n(\omega)$ using iteratively re-weighted least squares (e.g. Aster et al., 2005). Only the horizontal components of $B$ are used, since they are less influenced by conductivity heterogeneities than $B_r$ (as demonstrated by Olsen & Kuvshinov, 2004).

6. Interpolation of $E_m^n$ to the full set of frequencies contained in the data.

7. Calculation of $E(r, \omega)$ at any observation point by means of eq. (2.18).
8. Inverse Fourier transformation of $\mathbf{E}(r, \omega)$, yielding time series $\mathbf{E}(r, t)$.

Details of this scheme are given in Pütthe & Kuvshinov (2013c). It is noteworthy that the time-consuming solution of Maxwell’s equations in a global 3-D conductivity model (step 1) only has to be done once; the results can be recycled for every storm under investigation. Also note that the same scheme with modified steps 6–8 can be used to consistently reproduce time series of $B_r$, as done by Olsen & Kuvshinov (2004).

The 3-D conductivity model used in step 1 of the above algorithm coincides with the model shown in Figure 3.2. The laterally heterogeneous surface layer has a resolution of $1^\circ$.

**C.2.3 Estimation of distortion matrices**

Let us first, for convenience, define a local Cartesian coordinate system at each observatory, with $E_x = -E_\vartheta$ pointing north and $E_\varphi = E_\varphi$ pointing east. The radial electric field vanishes at Earth’s surface, since air is assumed to be insulating. We therefore restrict ourselves from here on to the horizontal electric field and redefine $\mathbf{E} = (E_x, E_y)^\top$.

Electric charges accumulate along conductivity contrasts. Such a charge build-up at small-scale heterogeneities, often located near the surface, generates a local quasi-static electric field, which is barely related to the electric field due to regional-scale induction (e.g. Jiracek, 1990). In the MT community, this effect is referred to as galvanic distortion. The Fourier transforms of the theoretical/modelled electric field $\mathbf{E}^{\text{mod}}(\omega)$ and the actual measured/observed field $\mathbf{E}^{\text{obs}}(\omega)$ are then related as (e.g. Groom & Bahr, 1992; Chave & Jones, 2012)

$$\mathbf{E}^{\text{obs}}(\omega) = \mathbf{G}\mathbf{E}^{\text{mod}}(\omega), \quad \mathbf{G} = \begin{pmatrix} G_{xx} & G_{xy} \\ G_{yx} & G_{yy} \end{pmatrix}. \quad (C.1)$$

$\mathbf{G}$ is the frequency-independent, real-valued distortion matrix. Due to these properties, eq. (C.1) is also valid in the time-domain, in which it reads

$$\mathbf{E}^{\text{obs}}(t) = \mathbf{G}\mathbf{E}^{\text{mod}}(t). \quad (C.2)$$

Having the observatory data and the calculated electric field obtained with the method described above, we can solve the linear system of equations (C.2) for $\mathbf{G}$. Since $\mathbf{G}$ is time-independent, the system is highly over-determined, as the relation must hold for every sample in time. We solve eq. (C.2) with iteratively re-weighted least squares (e.g. Aster et al., 2005).

We want to note that the issue of estimating the distortion matrix at a geomagnetic observatory was recently also addressed by Love & Swidinsky (2013). In contrast to us, the authors employed a local approach, i.e. they did not describe the structure of the source field. Additionally, the authors used a homogeneous half-space instead of a 3-D conductivity model. We will compare the results of both studies in Section C.3.3.
C.3 Results and discussion

We consider a large-scale magnetospheric source, which we parametrize with 15 low-degree SHE coefficients $\varepsilon_n^m(\omega)$ ($n \leq 3$, $|m| \leq 3$). Note that, in contrast to most other parts of this thesis, we do not omit terms with $|m| > 1$ to catch part of the $Sq$ variations (cf. Appendix B). We estimate time spectra of these coefficients separately for all 6 magnetic storms summarized in Table C.1. These are used to synthesize time series of the electric field at the measurement sites in Japan and the Philippine Sea shown in Figure C.1.

As widely known, geomagnetic and geoelectric fields are in magnetic quiet times dominated by the daily $Sq$ variations, which cannot fully be described by our chosen set of coefficients (e.g. Schmucker, 1999). To minimize the influence of $Sq$, we estimate distortion matrices from 3-day segments of the calculated and observed time series, which are centred around the magnetic storm of interest.

C.3.1 Ocean bottom observatories

The magnetic storm of April 2000 was the only significant event during the deployment of the ocean bottom electro-magnetometers. For the chosen 3-day window around this storm, only 4 stations (OB1, OB2, OB5 and OB6) collected trustworthy data. We present observed and predicted electric field at these sites in Figure C.2. Note that the “predicted” electric field is given by $\mathbf{E}^{mod}(t)$. Our estimates of the distortion matrix $\mathbf{G}$ are presented in Table C.2.

Since little galvanic distortion is expected for ocean bottom sites, we assumed $\mathbf{G}$ to be close to the identity matrix. Indeed, the results at most sites show diagonal elements $G_{xx}$, $G_{yy}$ close to 1 and off-diagonal elements $G_{xy}$, $G_{yx}$ close to 0. $G_{xx}$ at OB6 deviates significantly from its expected values; however, $E_x^{obs}$ at OB6 shows a number of non-physical spikes, hence this deviation might be due to data quality. At OB5, both $G_{xx}$ and $G_{yx}$ deviate clearly from the expected value, indicating that the assumption of a homogeneous layered subsurface might not hold for this station. In general, the results confirm that for oceanic sites, the amplitudes of our modellings are close to those of the actual electric field, and thus validate the concept of Püthe & Kuvshinov (2013c).

<table>
<thead>
<tr>
<th>Station</th>
<th>$G_{xx}$</th>
<th>$G_{xy}$</th>
<th>$G_{yx}$</th>
<th>$G_{yy}$</th>
<th>$R_x^2$</th>
<th>$R_y^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>OB1</td>
<td>0.90</td>
<td>0.46</td>
<td>-0.13</td>
<td>1.13</td>
<td>0.52</td>
<td>0.84</td>
</tr>
<tr>
<td>OB2</td>
<td>1.24</td>
<td>0.26</td>
<td>-0.09</td>
<td>0.78</td>
<td>0.63</td>
<td>0.78</td>
</tr>
<tr>
<td>OB5</td>
<td>1.70</td>
<td>-0.15</td>
<td>-0.59</td>
<td>1.02</td>
<td>0.64</td>
<td>0.70</td>
</tr>
<tr>
<td>OB6</td>
<td>2.04</td>
<td>-0.40</td>
<td>-0.12</td>
<td>1.34</td>
<td>0.68</td>
<td>0.91</td>
</tr>
</tbody>
</table>

Table C.2: Distortion matrices estimated for ocean bottom stations, using data of the April 2000 magnetic storm.
Figure C.2: E-field at ocean bottom observatories. Observed (blue) and predicted (red) electric field for the April 2000 magnetic storm. Left panel: $E_x$, right panel: $E_y$. Note that the time series at individual stations are shifted by 15 mV/km for clarity.

In the last two columns of Table C.2 we present coefficients of determination, which are defined analogously as in eq. (B.4). $R_x^2$ measures how well $E_{x,\text{obs}}$ correlates with the inputs $E_{x,\text{mod}}$ and $E_{y,\text{mod}}$, while $R_y^2$ measures how well $E_{y,\text{obs}}$ correlates with these inputs. Acceptable values are obtained for all stations, especially in the $E_y$-component.

C.3.2 Onshore observatories

The onshore observatories KAK, KNY and MMB provide continuous time series of the electric field. We estimate distortion matrices separately for each magnetic storm. This permits us to investigate the robustness of our estimates. Tables C.3, C.4 and C.5 contain the estimated elements of $G$ for each storm as well as mean value and standard deviation, obtained by analysis of all events. The pronounced differences between the estimates obtained at different sites are noteworthy. At KAK (Table C.3), $G_{yy}$ is large compared to all other elements, while at MMB (Table C.5), $G_{xx}$ and $G_{xy}$ are large. Maximum values for both observatories are around 3, indicating that our modelings underestimate the amplitude of the actual electric field by about this factor. At KNY (Table C.4), in contrast, the magnitudes of all elements are $<1$, indicating that our modelings overestimate the amplitude of the electric field. These very different results confirm that galvanic distortion is a very local phenomenon.

A look at the variance between individual events reveals that the estimates of $G$ are quite robust. Except for a few elements (such as $G_{yx}$ at KAK), the standard deviations have clearly smaller amplitudes than the estimates themselves. Coefficients of determination are relatively stable over different storms, but vary significantly with site and...
Results and discussion

Table C.3: Distortion matrix and statistics for observatory KAK

<table>
<thead>
<tr>
<th>Storm</th>
<th>$G_{xx}$</th>
<th>$G_{xy}$</th>
<th>$G_{yx}$</th>
<th>$G_{yy}$</th>
<th>$R^2_x$</th>
<th>$R^2_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apr-00</td>
<td>0.27</td>
<td>1.05</td>
<td>0.21</td>
<td>3.66</td>
<td>0.90</td>
<td>0.93</td>
</tr>
<tr>
<td>Jul-00</td>
<td>0.20</td>
<td>1.00</td>
<td>-0.29</td>
<td>3.11</td>
<td>0.89</td>
<td>0.92</td>
</tr>
<tr>
<td>Aug-00</td>
<td>0.12</td>
<td>0.86</td>
<td>-0.40</td>
<td>3.00</td>
<td>0.81</td>
<td>0.90</td>
</tr>
<tr>
<td>Mar-01</td>
<td>0.17</td>
<td>0.83</td>
<td>-0.16</td>
<td>3.24</td>
<td>0.76</td>
<td>0.91</td>
</tr>
<tr>
<td>Oct-03</td>
<td>-0.15</td>
<td>0.73</td>
<td>-0.91</td>
<td>2.60</td>
<td>0.76</td>
<td>0.81</td>
</tr>
<tr>
<td>Nov-03</td>
<td>0.12</td>
<td>0.92</td>
<td>-0.50</td>
<td>3.55</td>
<td>0.94</td>
<td>0.94</td>
</tr>
<tr>
<td>Mean</td>
<td>0.12</td>
<td>0.90</td>
<td>-0.34</td>
<td>3.19</td>
<td>0.84</td>
<td>0.90</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>0.15</td>
<td>0.12</td>
<td>0.37</td>
<td>0.39</td>
<td>0.08</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table C.4: Distortion matrix and statistics for observatory KNY

<table>
<thead>
<tr>
<th>Storm</th>
<th>$G_{xx}$</th>
<th>$G_{xy}$</th>
<th>$G_{yx}$</th>
<th>$G_{yy}$</th>
<th>$R^2_x$</th>
<th>$R^2_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apr-00</td>
<td>0.42</td>
<td>-0.24</td>
<td>-0.19</td>
<td>0.78</td>
<td>0.72</td>
<td>0.82</td>
</tr>
<tr>
<td>Jul-00</td>
<td>0.54</td>
<td>-0.19</td>
<td>-0.70</td>
<td>0.66</td>
<td>0.68</td>
<td>0.86</td>
</tr>
<tr>
<td>Aug-00</td>
<td>0.53</td>
<td>-0.09</td>
<td>-0.65</td>
<td>0.56</td>
<td>0.60</td>
<td>0.91</td>
</tr>
<tr>
<td>Mar-01</td>
<td>0.62</td>
<td>-0.17</td>
<td>-0.55</td>
<td>0.70</td>
<td>0.85</td>
<td>0.91</td>
</tr>
<tr>
<td>Oct-03</td>
<td>0.34</td>
<td>0.26</td>
<td>-0.57</td>
<td>0.97</td>
<td>0.71</td>
<td>0.90</td>
</tr>
<tr>
<td>Nov-03</td>
<td>0.55</td>
<td>0.24</td>
<td>-0.60</td>
<td>1.04</td>
<td>0.65</td>
<td>0.95</td>
</tr>
<tr>
<td>Mean</td>
<td>0.50</td>
<td>-0.03</td>
<td>-0.54</td>
<td>0.78</td>
<td>0.70</td>
<td>0.89</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>0.10</td>
<td>0.23</td>
<td>0.18</td>
<td>0.19</td>
<td>0.08</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table C.5: Distortion matrix and statistics for observatory MMB

<table>
<thead>
<tr>
<th>Storm</th>
<th>$G_{xx}$</th>
<th>$G_{xy}$</th>
<th>$G_{yx}$</th>
<th>$G_{yy}$</th>
<th>$R^2_x$</th>
<th>$R^2_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apr-00</td>
<td>2.60</td>
<td>3.67</td>
<td>0.43</td>
<td>1.14</td>
<td>0.62</td>
<td>0.34</td>
</tr>
<tr>
<td>Jul-00</td>
<td>2.44</td>
<td>3.84</td>
<td>0.31</td>
<td>1.19</td>
<td>0.80</td>
<td>0.70</td>
</tr>
<tr>
<td>Aug-00</td>
<td>1.80</td>
<td>1.98</td>
<td>0.03</td>
<td>0.99</td>
<td>0.51</td>
<td>0.63</td>
</tr>
<tr>
<td>Mar-01</td>
<td>2.32</td>
<td>2.46</td>
<td>0.25</td>
<td>0.92</td>
<td>0.60</td>
<td>0.59</td>
</tr>
<tr>
<td>Oct-03</td>
<td>1.24</td>
<td>2.02</td>
<td>0.08</td>
<td>0.99</td>
<td>0.41</td>
<td>0.49</td>
</tr>
<tr>
<td>Nov-03</td>
<td>2.90</td>
<td>4.00</td>
<td>0.31</td>
<td>0.89</td>
<td>0.89</td>
<td>0.77</td>
</tr>
<tr>
<td>Mean</td>
<td>2.22</td>
<td>2.99</td>
<td>0.23</td>
<td>1.02</td>
<td>0.64</td>
<td>0.59</td>
</tr>
<tr>
<td>Std. dev.</td>
<td>0.60</td>
<td>0.94</td>
<td>0.15</td>
<td>0.12</td>
<td>0.18</td>
<td>0.15</td>
</tr>
</tbody>
</table>

component. Highest $R^2$ are obtained for KAK; at MMB, they are comparably low. In this context, we want to stress again that our analysis is based on a small number of low-degree source terms. While these terms can likely reproduce variations in the large-scale magnetospheric ring current, they cannot fully describe the daily $S_q$ variations, which are always present in the data.

In Figures C.3–C.5, we compare the observed and the predicted electric field for the October 2003 magnetic storm (also known as the “Halloween storm”) at observatories
KAK, KNY and MMB. Note again that in these figures, the “predicted” electric field is given by $\mathbf{GE}^{\text{mod}}(t)$. The plotted time series reflect the different $R^2$ at different observatories. While the observed electric field at KAK and KNY is excellently reproduced, observations and predictions at MMB differ in detail. The peak amplitudes and the overall shape of the time series are, however, also well reproduced at MMB.

If comparing the results obtained for different storms, the October 2003 event stands out, both in the estimates of $\mathbf{G}$ (e.g. $G_{xx}$, $G_{yx}$ and $G_{yy}$ at KAK, $G_{xx}$ at MMB) and in the coefficients of determination (e.g. comparably small $R_y^2$ at KAK and $R_x^2$ at MMB). These
findings might indicate a violation of our assumption that the source can be described by a moderate number of low-degree spherical harmonics. This could be due to an extension of the auroral oval well beyond its usual position equatorward as far as Japan. For particularly strong magnetic storms such as the October 2003 event, the accuracy of our method might thus be limited even in mid-latitudes.

C.3.3 Galvanic and inductive effects

In this section, we investigate the importance of 3-D modelling for our analysis and, in particular, address the question if galvanic and inductive effects are correctly separated. Throughout the section, we will focus on the distortion matrix at KAK for the October 2003 storm to facilitate a comparison with the study of Love & Swidinsky (2013).

To test the importance of 3-D modelling, we repeat the above simulations in a 1-D model. For depths $>10$ km, this model is equivalent to the 3-D model, but the heterogeneous top layer is replaced by a homogeneous shell with the conductivity of the area around the specific observatory, picked from the surface conductance map. With this 1-D model, we obtain for KAK and the October 2003 storm

$$G_{1-D}^{KAK} = \begin{pmatrix} -0.19 & 0.55 \\ -1.16 & 1.89 \end{pmatrix}, \quad (C.3)$$

with $R_x^2 = 0.23$ and $R_y^2 = 0.24$. Similar results are obtained with data of the other storms; on average, $R_x^2 = 0.46$, $R_y^2 = 0.47$. These values are considerably smaller than those obtained with 3-D modelling ($R_x^2 = 0.84$, $R_y^2 = 0.90$, cf. Table C.3). The estimated
Reproducing Electric Field Observations during Magnetic Storms

distortion matrix, however, is not too different from that obtained with 3-D modelling,

\[ \mathbf{G}_{3-D}^{KAK} = \begin{pmatrix} -0.15 & 0.73 \\ -0.91 & 2.60 \end{pmatrix}. \]  

(C.4)

1-D modelling for KNY also results in a drop in \( R^2 \), but more pronounced changes in the elements of \( \mathbf{G} \), while 1-D modelling for MMB results in similar \( R^2 \) and a very different distortion matrix. For the ocean bottom observatories, we finally obtain similar \( R^2 \) and minor differences in \( \mathbf{G} \) for 1-D and 3-D modellings. This leads to the following conclusions:

1. In regions in which the conductivity structure is mostly 1-D (such as the Philippine Sea), 3-D modelling has only minor effects on the results.

2. In coastal regions (such as the locations of all three observatories in Japan), 3-D modelling is crucial to correctly predict the shape of electric field time series during a magnetic storm, indicated by strong correlations between observations and model predictions.

3. For some locations (such as MMB), modelled inductive and galvanic effects can compensate each other in their effect on the calculated electric field. 1-D modelling results in similar \( R^2 \) as 3-D modelling, but to the price of an incorrect separation of inductive and galvanic effects, indicated by a very different distortion matrix.

The distortion matrix for KAK was recently also estimated by Love & Swidinsky (2013), using data of the Halloween storm of October 2003. The authors obtained the distortion matrix

\[ \mathbf{G}_{L&S}^{KAK} = \begin{pmatrix} 0.06 & 0.21 \\ -0.42 & 1.33 \end{pmatrix}. \]  

(C.5)

Note that the distortion matrix presented in their paper is a shuffled version of the matrix above, which is due to a small difference in the definition of \( \mathbf{G} \). The distortion matrix of Love & Swidinsky has some similarity with our results for the same event, but the two matrices do not agree very well. In spite of the differences, both studies can reliably reproduce the measured time series of both \( E_x \) and \( E_y \). Love & Swidinsky (2013) state that they can reproduce 87% of the measured variations (although it is not entirely clear from the description how this value is calculated). We reach coefficients of determination of 76% for \( E_x \) and 81% for \( E_y \).

To test whether the differences in the estimated distortion matrices are caused by the differences in the conductivity models, we repeat our above simulations once again in a homogeneous half-space model with conductivity of \( 5.13 \times 10^{-4} \) S/m. This value was co-estimated (together with the distortion matrix) by Love & Swidinsky (2013). With
Figure C.6: Power spectra (upper panel) and time series (lower panel) of $\varepsilon_0^1$. Red: Estimated from observatory magnetic data, blue: predicted from solar wind parameters with the method of Temerin & Li (2002).

this model, we obtain for KAK and the October 2003 storm

$$G_{\text{homog}}^{\text{KAK}} = \begin{pmatrix} -0.04 & 0.34 \\ -0.44 & 1.24 \end{pmatrix},$$

(C.6)

with $R_x^2 = 0.47$ and $R_y^2 = 0.48$. This result is in remarkable agreement with $G_{\text{L&K}}^{\text{KAK}}$. The low coefficients of determination, however, indicate a poor agreement between measurements and modelings. Our method hence requires an accurate model of subsurface conductivity structure.

C.3.4 Towards real-time prediction

We finally want to demonstrate that our method is suitable for real-time prediction of the electric field during magnetic storms. To this purpose, we need to know the temporal evolution of the source field prior to the arrival of the storm. This requires some simplifications. As widely known, the dominant source of induction in mid-latitudes is a symmetric ring current in the magnetosphere, described spatially by the spherical harmonic $Y_1^0 = \cos \vartheta$ and temporally by the corresponding coefficient $\varepsilon_1^0$. The latter can be related to the $Dst$-index as (Olsen & Kuvshinov, 2004)

$$\varepsilon_1^0 \approx -\frac{DStd}{1 + \tilde{Q}}.$$  

(C.7)

with $\tilde{Q} = 0.27$ being a first order correction for induction effects (Langel & Estes, 1985).

A forecast of $Dst$ is possible from analysis of solar wind observations by the Advanced Composition Explorer (ACE) satellite at the L1 Lagrange point (Temerin & Li, 2002).
Depending on the solar wind speed, the $Dst$ forecasts are available approximately 1 hour in advance. Moreover, an approximate 6-day-forecast for $Dst$, which is based on direct solar observations, was recently presented by Tobiska et al. (2013). In this study, we use the $Dst$ forecast from ACE observations for the October 2003 magnetic storm and calculate $\varepsilon_0^1$ with eq. (C.7). The result is compared to $\varepsilon_1^0$ obtained with our method in the lower panel of Figure C.6. The overall shapes of observed and predicted time series are in good agreement, and the maximum amplitudes are well predicted, too. The offset in the recovery phase might be due to the use of eq. (C.7), which does not account for the time lag due to inductive effects. The most prominent difference, however, are the rapid oscillations of $\varepsilon_1^0$, which are present in the time series derived with our method, but not in that predicted from ACE observations. The $Dst$ forecast has a nominal temporal resolution of 10 minutes, but it only correctly reproduces features on time scales of hours.

This is also apparent from the power spectra, shown in the upper panel of Figure C.6. For periods shorter than a few hours, the $Dst$ forecast lacks energy.

We use the responses of our 3-D model, the estimated distortion matrix for KAK (mean values, cf. Table C.3) and the $Dst$-prediction of $\varepsilon_0^1$ to compute the electric field at KAK for the October 2003 storm. The results are shown in Figure C.7. The agreement between observations and predictions is weak. Only the very broad features of the variation of the electric field during the storm are correctly reproduced. Peak amplitudes do not match, and the characteristic fast oscillations are missing. We think that this is mostly due to the limited temporal resolution of the $Dst$ forecast. The electric field exhibits very rapid oscillations during magnetic storms, which can only be reproduced if knowing the temporal evolution of the source field on the same time scales.
C.4 Conclusions

In this study, we revisited the method of Püthe & Kuvshinov (2013c) to calculate the electric field generated in mid-latitude regions during magnetic storms. The method involves 3-D modelling of induction processes in a heterogeneous Earth and the construction of a source model described by low-degree spherical harmonics from observatory magnetic data.

We extended the work of Püthe & Kuvshinov (2013c) by investigating the fit of the modelings with electric field measurements at ocean bottom stations in the Philippine Sea and at onshore observatories in Japan. Observations and modelings are linearly related by a distortion matrix, which accounts for galvanic effects. We reliably determined such matrices with, dependent on site and component, coefficients of determination between 0.59 and 0.90. The largest matrix elements reach values around 3, indicating that the modelings underestimate the actual electric field by about this factor. However, since galvanic distortion is a very local phenomenon, it is not possible to draw conclusions from this finding on global electric field models as presented by Püthe & Kuvshinov (2013c).

The results of this study also stress the need for 3-D modelling. Correlations between observations and predictions are markedly higher if the latter are generated in a 3-D model. In addition, a correct separation of galvanic and inductive effects is only possible with a precise 3-D model. We do not claim that our model fulfils this requirement, as in the considered period range, inductive effects take place at scale lengths that are significantly smaller than its resolution. Nevertheless, the inclusion of a heterogeneous surface shell is a clear improvement to a 1-D model – and our method can easily incorporate more complex conductivity models as soon as they are available, such as that compiled by Alekseev et al. (2015) (cf. Figure 6.15). Using responses of a more complex model will not have any effect on the computational cost, because these responses are independent of the source and can therefore be computed beforehand and archived.

In a larger framework, this study can be seen as contribution to a procedure that predicts the hazard to technological systems in mid-latitude regions due to geomagnetic disturbances. By computing the electric field on Earth’s surface, our method bridges the gap between predictions of geomagnetic disturbances (e.g. Temerin & Li, 2002; Tobiska et al., 2013) and calculations of the currents induced in conductor networks (e.g. Lehtinen & Pirjola, 1985). To establish a real-time forecast system for GIC, it will be necessary to connect and automate the existing individual algorithms. In addition, as shown in this study, a more precise forecast of the temporal evolution of the source field is crucial for a correct prediction of fast fluctuating electric fields.

As already discussed by Püthe & Kuvshinov (2013c), the formalism presented above could in principle also be applied to magnetic substorms, which cause the strongest EM
signals in polar latitudes and are due to intensifications of the auroral current system. This will, however, require a precise description of the auroral source, which is extremely variable both in space and time, and connected with this, a more local approach involving a different set of basis functions.

Finally, we would like to note that the described formalism to estimate distortion matrices could also be applied in MT. If sufficiently long time series, containing magnetic storms, are collected, the method outlined above can be used to correct for the static shift.
List of Figures

1.1 Concept of EM induction (courtesy of Jin Sun). According to Maxwell’s equations, a primary time-varying current generates a primary (external) time-varying magnetic field. The latter induces an electric field in the conducting Earth, which in turn drives a secondary current, generating a secondary (internal) magnetic field. Measurements taken on or above Earth’s surface contain contributions of both primary and secondary fields.

1.2 Map of geomagnetic observatories delivering magnetic data as this thesis is written. Colours indicate topography/bathymetry.

2.1 A system transforms an input signal into an output signal. Without knowledge of the physics, the only visible part of the system is its transfer function. By adding an appropriate physical model, it is possible to gain insight into the system’s properties from its transfer functions.

2.2 C-responses estimated from magnetic data from observatory IRT. a) Conventional approach, b) multi-frequency approach (with a suitable regularization parameter).

3.1 Variability of observed C-responses, estimated at 77 mid-latitude observatories with the Z/H-method from 16 years of observatory data (1997–2012). The solid lines indicate the theoretical prediction, corresponding to the 1-D conductivity profile derived from satellite data by Kuvshinov & Olsen (2006). The top panel shows squared coherencies.

3.2 3-D conductivity model. Left: Surface conductance (in S), representing the uppermost 10 km. White dots indicate the locations of geomagnetic observatories for which C-responses were estimated (cf. Figure 3.1) and of which data were used to determine the SHE of the magnetospheric source. Right: 1-D conductivity profile beneath the surface shell.

3.3 Time series of the external coefficients $q^m_n$, $s^m_n$ (in nT) that describe the source in our model study. Ticks indicate January 1 of the respective years. Note that the real coefficients $q^m_n(t)$, $s^m_n(t)$ shown in this figure are related to the complex coefficients $\varepsilon^m_n(t)$ in the following way: $\varepsilon^m_n = (q^m_n - is^m_n)/2$ if $m > 0$, $\varepsilon^m_n = (q^{|m|}_n + is^{|m|}_n)/2$ if $m < 0$, and $\varepsilon^0_n = q^0_n$. Also note the different scales of the individual plots.

3.4 Power spectral density of the external coefficients $\varepsilon^m_n$, which were derived from 16 years of observatory data. Here, the power spectral density is defined as $P(\varepsilon^m_n(\omega)) = |\varepsilon^m_n(\omega)|^2$. 
3.5 Variability of observed (a) and modelled (b)–(d) $C$-responses for the locations of 77 observatories at geomagnetic latitudes between $\pm 10^\circ$ and $\pm 55^\circ$. (b) Variability due to the ocean effect. (c) Variability due to a complex source. (d) Variability due to ocean and source effect. The black lines in all plots denote, as a reference, the globally uniform $C$-response corresponding to the 1-D model that has been excited by $\varepsilon_1^0$. 40

3.6 Maps of modelled $C$-responses (in km) for periods of 2.0 days, 13.6 days and 91.3 days, respectively. Top: real part, bottom: imaginary part of $C$. (a) 1-D model, excited by $\varepsilon_1^0$. (b) 3-D model, excited by $\varepsilon_1^0$ (showing the ocean effect). (c) 1-D model, excited by the full set of $\varepsilon_n^m$ (showing the source effect). (d) 3-D model, excited by the full set of $\varepsilon_n^m$ (showing ocean and source effects). The solid black lines indicate geomagnetic latitudes of $\pm 10^\circ$ and $\pm 55^\circ$, respectively. Observed responses at observatory locations are added as coloured dots to panel (d). 41

3.7 Transfer functions estimated for the observatory Hermanus (HER, South Africa) at a geomagnetic latitude of 34°S. The bottom left panel shows $C$-responses. The bottom right panel shows squared coherencies for $C$ and multiple squared coherencies for the alternative transfer functions $T_n^m$, $U_n^m$ and $V_n^m$. The further panels show the transfer functions $T_n^m$ ($n \leq 3$, $|m| \leq 1$). For all responses, the real part is presented in blue, the imaginary part in red. The 90% confidence interval is indicated for each estimate. Modelled transfer functions, corresponding to the conductivity model shown in Figure 3.2, are marked by solid lines. 43

3.8 Transfer functions $U_n^m$ estimated for the observatory Hermanus (HER, South Africa). See also caption of Figure 3.7. 44

3.9 Transfer functions $V_n^m$ estimated for the observatory Hermanus (HER, South Africa). See also caption of Figure 3.7. 45

3.10 Squared coherencies for $C$ (black) and multiple squared coherencies for $T_n^m$ (magenta), $U_n^m$ (orange) and $V_n^m$ (green) at different geomagnetic observatories. Geomagnetic latitude is indicated. 46

3.11 Network of geomagnetic observatories (white dots) and abandoned submarine telecommunication cables in the North Pacific region. Reprinted from Utada et al. (2003). Voltage data from the cable TPC-1 are used in this study. 48

3.12 Transfer functions $\Xi$ (bottom left panel) and $K_n^m$, estimated for the cable TPC-1 (North Pacific). The bottom right panel shows squared coherencies. See also caption of Figure 3.7. 49

4.1 Expected development of the Swarm constellation. With time, Swarm C separates in local time from Swarm A and B, reaching an angular distance of approximately 90° after 4 years. Image: ESA. 51

4.2 Target conductivity model in S/m. Note that the conductivity of the top layer has been obtained by scaling the surface conductance map (Figure 3.2) to a thickness of 10 km. 53

5.1 Processing scheme for the iterative 1-D inversion. Inputs and output are marked by grey and red boxes, respectively. Note that by the term “3-D model”, we denote the 1-D model plus a laterally heterogeneous surface shell. 56
5.2 Demonstration of the convergence of $C^{\text{obs}}(\omega)$ and $C^{3-D}(\omega)$ within five iterations of the inversion scheme. Note that the series with positive values represent Re $C$, those with negative values Im $C$. ........................................ 58

5.3 Recovered conductivity model (blue) in comparison to the uniform initial model (green) and the laterally averaged target conductivity model (red; compare with Figure 4.2). ........................................ 59

5.4 Availability of observatory and satellite data for the CHAMP phase (a) and the Swarm phase (b). The small amount of observatory data during the Swarm phase is due to the fact that many observatories had not yet published their measurements when this study was started. .............. 60

5.5 a) Estimated (uncorrected) $C$-responses in this study in comparison to those obtained by Kuvshinov & Olsen (2006). b) $C$-responses corrected for induction in the oceans; solid lines indicate $C$-response predictions corresponding to the recovered conductivity models (Figure 5.8). Top panels show squared coherencies. .................................................. 62

5.6 L-curve relating misfit term $\phi_d$ and regularization term $\phi_m$. The results shown in Figure 5.8 correspond to point 3, at which both $\phi_d$ and $\phi_m$ are minimized. .................................................. 65

5.7 The inverse Hessian (absolute values, in logarithmic units) at the point of convergence $m_0$. See main text for details. .................................................. 66

5.8 1-D conductivity models recovered by Kuvshinov & Olsen (2006) (solid black line) and in this study (1-D inversion without correction: solid blue line, 1-D inversion with correction: solid red line, quasi-1-D inversion: solid yellow line). Narrow red lines indicate uncertainties of the recovered (corrected) model, estimated from analysis of the inverse Hessian. In grey, we show 400 near-independent models obtained from Monte Carlo sampling. 67

5.9 Results of the grid-based sampling: Posterior pdf $\Sigma(m)$ for an 8-layer model and different regularization parameters $\lambda$. Each plot shows the stacked pdfs of $9^8$ different models. .................................................. 70

5.10 1-D conductivity profiles estimated in this study (blue line) and computed using laboratory-based conductivity data for various mantle water contents and temperatures. Ol and wads refer to major upper mantle and transition-zone minerals olivine and wadsleyite, respectively. $T_{\text{ad}}$ is the temperature at the location where the mantle adiabat intersects the conductive geotherm at 150 km depth. For the computations related to variations in water content (black lines) we assumed a mantle adiabat of 1300°C with an intersection depth of 100 km, whereas for the mantle adiabats (grey lines) we fixed water content to 0.001 wt% (ol) and 0.01 wt% (wads). $\sigma_0=1$ S/m. .................................................. 74

6.1 Effect of the different parametrizations in a test 3-D inversion. a) Target model, b)-d) block parametrization (b) no merging, c) merging of $2 \times 2$ cells, d) merging of $3 \times 3$ cells), e)-f) spherical harmonic parametrization (e) $L = 10$, f) $L = 20$). More information in the text. .................................................. 90

6.2 Recovery of a 1-layer chequerboard target model (a) from ideal, noise-free synthetic data, using different parametrizations of the model domain and different optimization schemes. Middle row (b-d): block parametrization, bottom row (e-g): spherical harmonic parametrization. First column (b & e): QN, second column (c & f): LMQN, third column (d & g): NLCG. Colours denote electrical conductivity in logarithmic units. .................................................. 92
6.3 Illustration of the Wolfe conditions in an inexact line search. Only trial step lengths $\alpha^*$ in intervals 1 and 2 are accepted. In the widely shaded intervals, the curvature condition is not fulfilled. In the densely shaded interval, the sufficient decrease condition is not fulfilled.  

6.4 Left: Reference chequerboard conductivity structure of the anomalous layer used in the resolution studies. Conductivity is described as $\log_{10}(\sigma/\sigma_b)$, where $\sigma_b$ is the background conductivity of the respective layer. Right: 1-D background conductivity structure $\sigma_b$ in the top 1600 km.

6.5 Results of the resolution study. Each column corresponds to an individual inversion, which aims at recovering the conductivity structure of an anomalous layer buried in the depth range indicated at the top of the respective column. The depth of the resolved layers is indicated on the right. Conductivity is plotted as $\log_{10}(\sigma/\sigma_b)$, where $\sigma_b$ is the background conductivity of the respective layer (cf. Figure 6.4).

6.6 Synthetic regular grids of observatories (a) and cables (b) for resolution studies.

6.7 Results of test inversions of various ground- and sea-based transfer functions. a) $T_m^m$, b) $U_m^m$, c) $V_m^m$, d) $K_m^m$.

6.8 Selected elements of the $Q$-matrix, estimated from noise-free test data using the conventional approach (cf. Section 2.5.1). Rows correspond to $k = 1$, $l = -1 / k = 3$, $l = -2 / k = 5$, $l = 5$. Columns correspond to $n = 1$, $m = -1 / n = 1$, $m = 0 / n = 3$, $m = 0 / n = 3$, $m = 1$. Black dots show the real part of the estimated responses, red dots the imaginary part. Solid lines correspond to theoretical predictions from the target model shown in Figure 4.2.

6.9 Selected elements of the $Q$-matrix, estimated from the SCARF test data set using the conventional approach. See also the caption of Figure 6.8.

6.10 Selected elements of the $Q$-matrix, estimated from the SCARF test data set using the multi-frequency approach. See also the caption of Figure 6.8.

6.11 a) Conductivity model recovered from ideal $Q$-responses, i.e. theoretical predictions from the target model. b) Conductivity model recovered from $Q$-responses that were estimated by multivariate analysis from the SCARF test data set. c) Conductivity model recovered from $Q$-responses describing induction by the $\varepsilon_0^1$ source term, prior selection. Units are S/m.

6.12 Sketch of the $Q$-matrix used in this study. Black colour marks the diagonal elements – note that not all of them are actually in the diagonal of the matrix due to the “missing” source terms for $|m| > 1$. Red colour marks the elements used for different inversions. Due to the chosen ordering of the coefficients, the second column of the $Q$-matrix corresponds to induction by $\varepsilon_0^1$. a) corresponds to the results presented in Figure 6.13a, b) corresponds to the results presented in Figure 6.13b, and c) corresponds to the results presented in Figure 6.13c. Note that the diagonal element of the second column is used in all three inversions.

6.13 Conductivity model recovered by inverting $Q$-responses describing induction by the $\varepsilon_0^1$ source term, posterior selection. a) all elements, b) elements from $Q$-matrix rows with diagonal element, c) elements from $Q$-matrix rows without diagonal element. Units are S/m.

6.14 Coefficient of determination $R^2$, measuring the proportion of the data that are described by nine low-degree spherical harmonics.
6.15 3-D conductivity model compiled by Alekseev et al. (2015). Colours indicate electrical conductivity in units of S/m.  
6.16 $Q$-matrix recovered from 10 years of satellite and observatory data. Blue and red dots denote the real and the imaginary part, respectively, of the individual responses. Confidence limits for a confidence level of 90% are indicated. Solid lines correspond to predictions from the conductivity model shown in Figure 6.15. 
6.17 $Q$-matrix recovered from 10 years of satellite and observatory data, continued. The last column presents multiple squared coherencies for the respective row of the $Q$-matrix (i.e. for the respective induced coefficient $\eta_l^k$). 
B.1 Synthesized spectra of the radial component $B_r$ (left: real part, right: imaginary part) for a period of $T = 24$ h and cases 1–4 (see text). Estimated spectra at observatory locations are plotted as coloured dots. 
B.2 Synthesized spectra of the latitudinal component $B_\vartheta$ (left: real part, right: imaginary part) for a period of $T = 24$ h and cases 1–4 (see text). Estimated spectra at observatory locations are plotted as coloured dots. 
B.3 Evolution of the current function $\Psi$ in time. The dip equator is marked in black. 
B.4 Variability of the dominant coefficients $\varepsilon_m^n$ over a year for a period of $T = 24$ h. Left: Coefficients in the complex plane, right: absolute values of the coefficients in comparison to the $F_{10.7}$ index. 
B.5 Variability of the dominant coefficients $\varepsilon_m^n$ over a year for a period of $T = 12$ h. Left: Coefficients in the complex plane, right: absolute values of the coefficients in comparison to the $F_{10.7}$ index. 
C.1 E-field measurement sites. The three Japanese observatories provide electric field data continuously, whereas the ocean bottom array was installed during the April 2000 magnetic storm. Note that OB3, which was installed on the seafloor between OB2 and OB4, did not provide useful data. Colours indicate topography/bathymetry. 
C.2 E-field at ocean bottom observatories. Observed (blue) and predicted (red) electric field for the April 2000 magnetic storm. Left panel: $E_x$, right panel: $E_y$. Note that the time series at individual stations are shifted by 15 mV/km for clarity. 
C.3 E-field at KAK. Observed (blue) and predicted (red) electric field for the October 2003 (Halloween) magnetic storm. Top panel: $E_x$, bottom panel: $E_y$. 
C.4 E-field at KNY. Observed (blue) and predicted (red) electric field for the October 2003 magnetic storm. 
C.5 E-field at MMB. Observed (blue) and predicted (red) electric field for the October 2003 magnetic storm. 
C.6 Power spectra (upper panel) and time series (lower panel) of $\varepsilon_0^1$. Red: Estimated from observatory magnetic data, blue: predicted from solar wind parameters with the method of Temerin & Li (2002). 
C.7 E-field at KAK – revisited. Observed electric field (blue) and electric field predicted from $Dst$ forecast (red) for the October 2003 magnetic storm.
List of Tables

1.1 Past and recent missions of satellites measuring the magnetic field. *Expected lifetime. ................................................................. 14

5.1 Observed and corrected C-responses with uncertainties (in km) and squared coherencies as functions of period (in seconds). ......................... 63
5.2 Conductivity models obtained in the deterministic 1-D inversion. Depth (to the top of the respective layer) in km, and conductivity in S/m. Model $\sigma_1$ is obtained with the iterative correction scheme (red curve in Figure 5.8), model $\sigma_2$ is obtained with the direct quasi-1-D inversion (yellow curve in Figure 5.8). ......................................................... 68

6.1 Performance of the different optimization schemes in block parametrization on a regular $5^\circ \times 5^\circ$ grid ($N_m = 2592$). From left to right: number of iterations to reach convergence, average number of forward calls per iteration, average time to compute the searching direction $p$. Note that the total time (last column) includes all processing steps and in particular the solution of the forward problem. ......................................................... 93

6.2 Performance of the different optimization schemes in spherical harmonic parametrization with a cut-off degree 7 ($N_m = 64$). See caption of Table 6.1 for more details. ......................................................... 93

B.1 Mean coefficients of determination $R^2$, measuring the correlations between measurements and predictions from a truncated Fourier synthesis of the first $p_{\text{max}}$ time harmonics. ................................................................. 122

B.2 Coefficients $\varepsilon_{m}^{n}$ ($\Re$ and $\Im$ denote the real and the imaginary part, respectively) and their uncertainties $\delta\varepsilon_{m}^{n}$ for 4 time harmonics ($p = 1..4$) and cases 1–4, estimated from observatory magnetic data on the equinoctial day 2010/03/22. ................................................................. 125

B.3 Coefficients of determination $R^2$, measuring the correlations between estimated and synthesized magnetic field time spectra for 6 time harmonics. 127

B.4 Coefficients of determination $R^2$ for case 2, with data weighted according to the observatory distribution. ................................................................. 130

B.5 Coefficients of determination $R^2$ for a period of $T = 24$ h and quiet days of different seasons, obtained with the method of case 2. ................................................................. 131

C.1 Overview of the magnetic data used in this study. The second column contains the peak Dst values for each storm. The last column contains the number of observatories from which data were used to construct the source field model. ................................................................. 135
List of Tables

C.2 Distortion matrices estimated for ocean bottom stations, using data of the April 2000 magnetic storm. .......................................................... 139
C.3 Distortion matrix and statistics for observatory KAK .......................... 141
C.4 Distortion matrix and statistics for observatory KNY .......................... 141
C.5 Distortion matrix and statistics for observatory MMB ....................... 141
Bibliography


Bibliography


Kuvshinov, A. 2008. 3-D Global induction in the oceans and solid Earth: Recent progress in modeling magnetic and electric fields from sources of magnetospheric, ionospheric and oceanic origin. Surv Geophys, 29, 139–186.


Bibliography


Acknowledgements

I am deeply grateful to Alexey Kuvshinov for his exceptional support over the last three years. Alexey is a veritable fountain of ideas, whose curiosity and scientific creativity are inspiring. From the very beginning, Alexey showed great faith in me and welcomed me as a researcher on an equal level. When I needed his advice, he always had time for a discussion. I truly enjoyed working with Alexey, and I really appreciate him as a supervisor who also spends part of his free time with his students. The holidays in Australia, the road trip in Japan, and the several excursions to the Rhine river were events that I will always remember.

Many thanks to the rest of my committee – Andrew Jackson, Jakub Velímský, and Nils Olsen. Global EM induction only has a small community within the larger area of geomagnetic research. I am happy to have found a committee of designated experts, who are willing to give feedback to my research.

In particular, I am extremely thankful to Nils for inviting me to join his research group at DTU and work with him for four months as part of my PhD. I was received very cordially by the entire group and I immediately felt welcome. Thanks to their hospitality, the time in Denmark was definitely one of the highlights of my life in recent years. I especially want to thank Stavros Kotsiaros for accepting an intruder in his office and acquainting me with the Copenhagen night life.

The three years of my PhD will remain as a very positive memory, thanks to the great environment I found at the Department of Earth Sciences. In particular, I want to mention the “induction crew”, consisting of Jenneke Bakker, Friedemann Samrock, and Stephan Koch, with whom I had many inspiring conversations, and with whom I also shared unforgettable experiences at various conferences around the world. I also want to emphasize the good times I had with my office mates, who never forgot teasing me when I arrived late at work. In the context of this thesis, special thanks go to Laura Ermert, Nienke Blom, Friedemann Samrock, and Charitra Jain for proofreading some important sections and polishing my style of writing. I am also very grateful to Moritz Müller for helping me with organizing the defence party. Finally, I want to thank you, dear reader, for centring your attention on this thesis. I sincerely hope you enjoyed reading it. Let’s raise our glasses!
Christoph Püthe

Personal information

Date of birth 1986/09/18
Place of birth Stuttgart, Germany
Citizenship German
Marital status single
Address Langstrasse 81, CH-8004 Zürich
E-mail christoph.puethe@erdw.ethz.ch

Education

2012–2015 PhD student in geophysics at the Department of Earth Sciences, ETH Zürich (CH), including a four-month research stay at DTU Space, Technical University of Denmark, in Autumn 2014.

2010–2012 MSc student in geophysics at the Department of Earth Sciences, ETH Zürich (CH). Graduation in 2012 as Master of Science ETH.

2007–2010 BSc student in geophysics at the Department of Earth Sciences, ETH Zürich (CH). Graduation in 2010 as Bachelor of Science ETH.


Work experience

2011–2012 Research assistant at the Department of Earth Sciences, ETH Zürich (CH).
2009–2011 Teaching assistant at the Department of Mathematics, ETH Zürich (CH).
2006–2007 Military service, Deutsche Bundeswehr (D).
Publications


Miscellaneous

Language skills
- German (native)
- English (C2)
- French (B2)
- Spanish (B1)
- Russian (A2)

Computer skills
- Programming languages: Fortran, Matlab, C
- Operating systems: Windows, Linux
- Others: LATEX, Office