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Summary of the Doctoral thesis

Stochastické simulace a modelování v magnetotelurické metodě

Stochastic simulations and modelling in the magnetotelluric method

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Abstrakt

V této práci se zabývám vývojem stochastické obrácené úlohy pro magnetotelurickou metodu v případě 1D/2D izotropní a anizotropní úlohy a její aplikací na syntetická a reálná data. Magnetotelurická metoda je geoelektrická induktivní metoda, která využívá jako zdroj indukce v Zemi variace přírodního elektromagnetického pole, na základě jejichž zpracování a interpretace dokáže zjistit odpor horninového prostředí až do hloubek desítek kilometrů. Obrácená úloha je v magnetotelurice řešena s cílem určit skutečné rozložení elektrického odporu pod povrchem Země na základě povrchových měření. Běžné metody řešení obrácené úlohy jsou založeny na optimalizaci modelu prostředí s omezením na shodu mezi pozorovanými daty a modelovou odezvou. Naproti tomu stochastické metody jsou založené na prohledávání prostoru parametrů a vybírání modelů na základě jejich pravděpodobnosti, díky čemuž jsou vhodné pro mnohadimenzionální úlohy, které nelze charakterizovat jedním výrazným minimem. Efektivní cestou jak zmapovat velký prostor parametrů jsou simulace Monte Carlo, pomocí nichž lze efektivně třídit přijatelné modely z hlediska pravděpodobnosti. Výsledkem těchto simulací je pravděpodobnostní popis jednotlivých parametrů, nikoli jeden výsledný model.

Vzhledem k výhodám stochastické úlohy jsem vyvinul obrácenou úlohu založenou na vzorkovací metodě DREAM, která byla speciálně rozvinuta pro mnohodimenzionální problémy. Jedná se o adaptivní algoritmus Monte Carlo s Markovovými řetězci, který používá více souběžně běžících řetězců a kombinuje

několikeré vzorkování se vzorkováním z minulých stavů. Vzorkovací metodu DREAM jsem nejprve zapracoval do 1D izotropní/anizotropní a následně i do 2D izotropní/anizotropní magnetotelurické úlohy a otestoval na syntetických modelech.

V průběhu vývoje algoritmu jsem se účastnil celé řady nových terénních experimentů, během nichž jsem získal, zpracoval a interpretoval nová magnetotelurická data, na která jsem následně mohl stochastickou úlohu aplikovat. Konkrétními cíli byly tektonické jednotky západočeské seismoaktivní oblasti, východní okraj Českého masivu a okolí bradlového pásma v karpatské soustavě. U syntetických modelů podává vyvinutý algoritmus celkově dobré výsledky. U 2D reálných izotropních úloh dosahuje algoritmus horších výsledků pouze v případě velkého množství parametrů (> 500). V případě 2D anizotropních syntetických i reálných úloh dosahuje algoritmus lepších výsledků než standardní optimalizační algoritmy. Celkově vyvinutý algoritmus podává velmi dobré výsledky a přes vysoké výpočetní nároky je jeho přidanou hodnotou pravděpodobnostní zmapování prostoru řešení a odhad jeho neurčitosti.

Abstract

In the thesis I deal with the development of a stochastic inversion procedure for the magnetotelluric method in 1D/2D isotropic and anisotropic cases, and its application to both synthetic and real data. The magnetotelluric method is a geoelectric inductive technique that utilizes variations of naturally occurring electromagnetic fields as a source of the electromagnetic induction for estimating the Earth's subsurface resistivity to depths of several tens of kilometres. The purpose of the inversion procedure is to estimate a real distribution of the electrical resistivity in the Earth's subsurface from surface measurements. Common inversion procedures in magnetotellurics perform a model optimization by minimizing the misfit between the data and the model response. Stochastic methods are based on the exploration of the model parameter space, and they pick models according to their probability, which makes them effective for the solution of high-dimensional problems which do not show a single pronounced minimum of the target function. The effective ways of mapping the parameter space are sampling algorithms based on Monte Carlo simulations which allow to sort models according to their probability. Results of these methods are obtained in the form of a fully probabilistic description of the parameters, and not in the form of a single model like in the deterministic inversion procedures.

Due to the mentioned advantages of the stochastic methods, I developed a stochastic inversion procedure using a sampling method DREAM, which was specially designed for high-dimensional problems. DREAM can be

classified as an adaptive Monte Carlo Markov Chain algorithm. It runs multiple chains in parallel and combines a multi-try sampling with sampling from an archive of past states. I used at first DREAM algorithm in 1D isotropic/anisotropic case and lately for 2D isotropic/anisotropic problem and tested the technique on synthetic models.

I attended a whole series of field experiments during the development of the inversion procedure, where I measured, processed and interpreted new magnetotelluric data, which I could use later for testing the stochastic inversion. The particular targets were tectonic structures in the West Bohemia seismo-active region, the eastern termination of the Bohemian Massif and the vicinity of the Pieniny Klippen Belt in the West Carpathians. The developed algorithm gives satisfactory results in 1D case, as well as for synthetic 2D isotropic problems. The algorithm achieves worse results in 2D real isotropic examples only in case of large number of parameters (> 500). In case of 2D anisotropic problems, both synthetic and practical, the algorithm reaches better results than the classical non-probabilistic procedures. The developed stochastic algorithm gives overall satisfactory results and, despite its high computational costs, it benefits from offering full probability maps of the solution space, and thus estimates of the uncertainties of the solutions.

Contents

1. Introduction

Most of the inversion procedures applied to the magnetotelluric data perform a model optimization trying to minimize the data vs. model misfit under structural constraints. Unfortunately, these algorithms have only a limited ability to describe the ambiguity of inversion solutions and to deal with local minima, where they often get stuck. Another option is to employ stochastic methods, which are based on exploration over the space of model parameters and picking models according to their probability. The effective procedure for a parameter search are sampling algorithms based on Monte Carlo methods, which probabilistically map the solution space by many random simulations. Results of these methods are obtained as full probability descriptions of the parameters, and not in the form of a single model like is the case in deterministic inversion procedures.

2. Aims of the study

The main aim of this thesis was to develop a stochastic inversion procedure for the magnetotelluric method (MT) in 1D and 2D isotropic and anisotropic cases. The second objective was the application of this algorithm to both synthetic and real data in order to assess the effectiveness and performance of the stochastic procedure.

3. Material and methods

3.1 Magnetotelluric method

Magnetotellurics is a geoelectric inductive technique that utilizes variations of natural occurring electromagnetic fields as a source of the electromagnetic induction in the Earth. MT is commonly used to estimate the Earth's subsurface electrical resistivity from hundreds of meters to several hundred kilometers. After the time series are collected in the field and processed, an inversion procedure is typically used to determine the true resistivity in the subsurface.

3.2 DREAM algorithm

In the Bayesian approach, the model parameters, in the form of posterior probability, can be derived from prior knowledge of the model, the experimental data and the statistical model by which the observed data are theoretically modeled. This process is like a learning procedure: from a weak knowledge about the model parameters (prior probability), we can gradually, by repeated experiments, refine our understanding about the model (posterior probability conditioned on the observed data).

The Bayesian problem cannot be solved analytically in MT, so it is necessary to use a sampling algorithm for the solution. Monte Carlo simulations (Metropolis et al., 1953) can be employed to generate random samples from posterior distribution, while the resulting probability is obtained from generated samples. Because the posterior is often a high-dimensional distribution, it is necessary to use many sampling iterations to arrive at a sufficiently reliable summary statistics for the model parameters.

The Monte Carlo methods include a variety of algorithms, which use repeated random sampling in order to estimate the target distribution. Since the blind random Monte Carlo sampling is ineffective for high-dimensional problems, Monte Carlo Markov Chain methods (MCMC) were introduced (Hastings, 1970). These methods relay on a Markov chain, which randomly moves through the parameter space and visits, in turn, the individual solutions with a stable frequency. MCMC methods can also employ several chains, which search through the space simultaneously.

I choose the MT-DREAM$_{(ZS)}$ algorithm (Laloy and Vrugt, 2012) in Matlab environment to drive my stochastic inversion procedure. The underlying adaptive MCMC sampling algorithm was specially designed to explore high-dimensional distributions. It runs multiple chains in parallel and combines a multi-try sampling (Liu et al. 2000) with sampling from an archive of past states (Vrugt et al. 2008) to accelerate the convergence to a limiting distribution. For assessing the convergence, the Gelman-Rubin statistic (Gelman and Rubin 1992) is computed for the last 50% of the samples in each chain. Furthermore, the algorithm is fully parallelized and can be run on multiple processors.

3.3 Experimental data

I took part in multiple MT field campaigns during the development of the inversion algorithm. After the data collection and processing, inversion by classical procedures and geologic interpretation, I selected four data sets to test the stochastic procedure:

(1) eight MT stations from a 1 km long profile in W Bohemia near Kopanina village focused on the Mariánské-Lázně Fault
(2) seven MT stations from ca. 13 km long profile in N Slovakia near Ľubovňa town focused on the Klippen Belt structure
(3) twenty four MT stations within EMERES experiment from ca. 50 km long profile in W Bohemia focused on geodynamically active zone near Nový Kostel village

(4) four MT stations from larger geologically focused experiment in S Moravia, which exhibits anisotropic effects

3.4 Evaluation of performance

I used multiple statistical parameters to assess the effectiveness and to estimate the uncertainty of the solution. As a basic tool for the uncertainty estimation of single parameters, marginal probabilities can be used. For the whole model, credibility intervals, at α%-level, are useful parameter interval estimates (here, α =90 is used in most cases). Because classical inverse models are judged according to their RMS (root mean square) error, I applied mean deviance along the stabilized section of the Markov chain of the stochastic procedure, which can provide similar information about the data misfit.

4. Results and discussion

Overall, the developed algorithm gives satisfactory results. The DREAM code achieves very similar results compared to classic inversion procedures in case of 1D isotropic/anisotropic models, which are quite simple in terms of number of parameters (<100). A more interesting situation is in case of 2D models.

4.1 2D isotropic synthetic example

For a 2D isotropic test, I generated a synthetic model with a conductor 1x1 km of 3 Ω.m and a non-conductor 1x1.5 km of 1000 Ω.m. Both structures were embedded into a 300 Ω.m halfspace, which was covered by a 1 km thick layer of 100 Ω.m. Total number of parameters was 286 (Fig. 1).

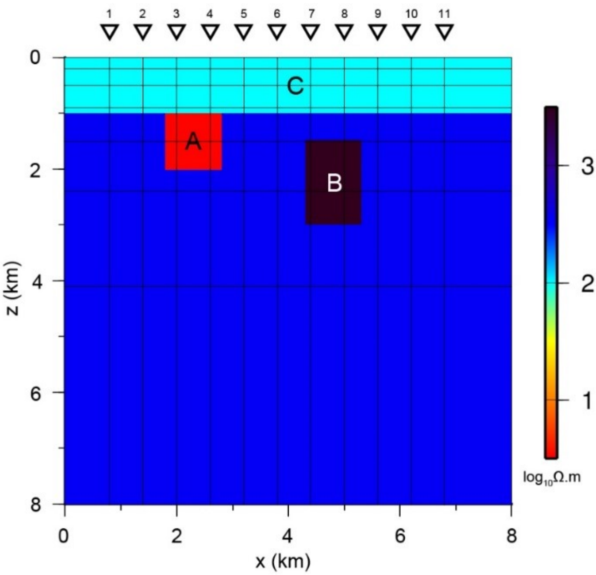

Fig. 1. Synthetic model for 2D isotropic test with conductor (A), non-conductor (B) and top most layer with lower resistivity (C).

The DREAM algorithm was employed to invert for the resistivities in the model cells. A priori, the lower and upper bounds for the resistivity were chosen $10^{-0.5}$ Ω.m and 10^{4} Ω.m, respectively, and a structural prior on minimum roughness was implemented. For the chain, 30,000 simulations were carried out. Fig. 2 shows models derived from the minimum (A) and maximum (B) bounds of the 90% credibility interval. The mean deviance over the final half of the chains, as a measure of the data vs. model fit, is reaching 0.79, which is very similar to the result of the classical inversion (RMS 0.72 by NLCG inversion by Pek et al., 2012). The difference between both models (A, B) is very small, indicating narrow parameter histograms and a relatively low uncertainty of the solution.

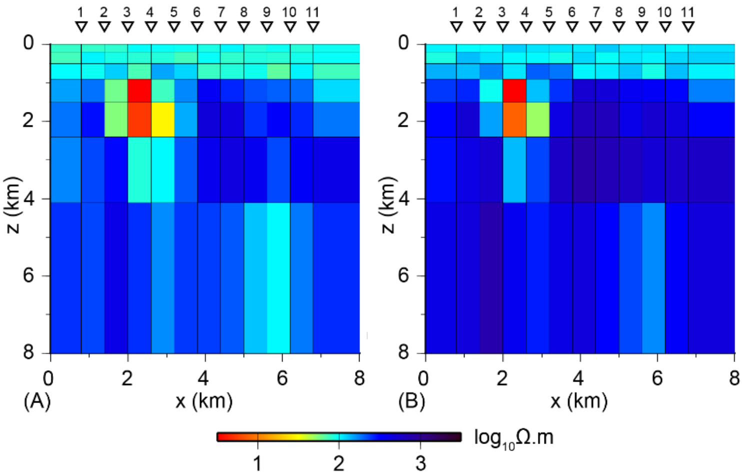

Fig. 2. Models from the minimum (A) and maximum (B) bounds of the 90% (equi-tailed) credibility interval. The conductor beneath stations 3 and 4 is resolved well, the same applies to the resistive feature under station 7.

4.2 2D isotropic experimental example

Subsequently, I tested the DREAM algorithm on multiple experimental data sets (Kopanina, Lubovna, EMERES) within a 2D isotropic model setting. Various experience has been gained: some of the DREAM inversions were, in terms of the data fit, better than the classical inversion procedure, others not.

Satisfactory results were obtained for data collected along the profile close to Ľubovňa. The DREAM algorithm was applied to invert for the model resistivities, with a priori bounds set to $10^{-0.5}$ Ω.m and 10^{4} Ω.m, and with a structural prior on minimum roughness imposed. The total number of variable model parameters was 620. The results were summarized after 100,000 simulation steps.

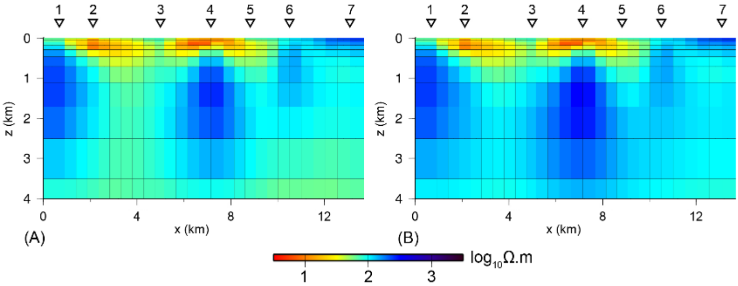

Fig. 3. Models constructed from the minimum (A) and maximum (B) bounds of the 90% credibility interval for the model resistivities.

Fig. 3. shows models constructed from the minimum (A) and maximum (B) bounds of the 90% credibility intervals for the model resistivities. The mean deviance of the data residuals is 3.9, which is better than the RMS obtained by the NLCG classical algorithm (5.45), although both algorithms sense almost the same structures. Difference between the extreme models, A and B, is very small which implicates a low uncertainty of the obtained solution.

4.3 2D anisotropic synthetic example

For a 2D anisotropic test, I used the same synthetic model as earlier in the 2D isotropic example (Fig. 1), except for a major change made in the anomalous conductor: now it exhibits uniaxial anisotropy with the principal resistivities of 3/300/3 Ω.m and 30° azimuth of anisotropy. The total number of variable parameters was thus increased to 313.

The DREAM algorithm was applied to invert for the resistivities and anisotropy azimuths in the model cells, with a priori resistivity bounds of $10^{-0.5}$ Ω.m and 10^3 Ω.m, azimuth of anisotropy from -90° to 90°, and a structural prior on minimum roughness imposed. The results were summarized after 100,000 simulations.

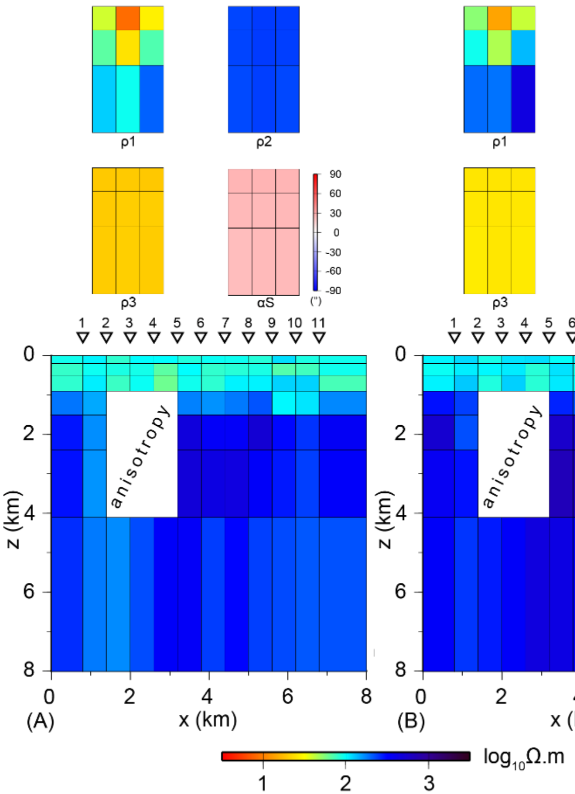

Fig. 4. Models derived from the minimum (A) and maximum (B) bounds of the 90% credibility intervals for the model resistivities.

Fig. 4 shows models constructed from the minimum (A) and maximum (B) bounds of the 90% credibility intervals for the individual model cell resistivities/azimuths. The mean deviance of the residuals is 1.02, which is very similar to the result of the classical inversion (RMS 1.04). The higher uncertainty of the parameters is observed only in the anisotropic domain of the model.

4.4 2D anisotropic experimental example

I used MT data from the profile in S Moravia to test the 2D anisotropic inverse procedure. Four stations on this profile exhibit out-of-quadrant phases and large splits between the resistivity curves, which may imply structures with strong anisotropy.

The DREAM algorithm was employed to invert for the model resistivities, with a priori resistivity limits of $10^{-0.5}$ Ω.m and 10^{4} Ω.m, azimuth of anisotropy from -90° to 90°, and prior structural constraint on minimum roughness considered. The results were summarized after 80,000 MCMC simulations. The total number of variable parameters was 590 in this case.

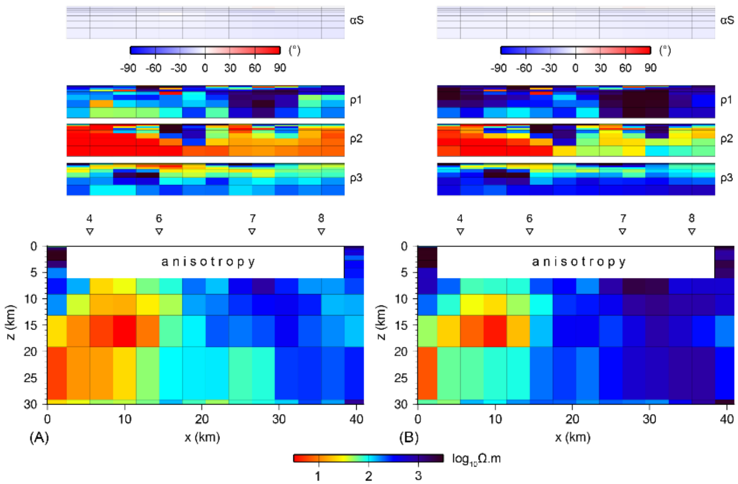

Fig. 5. Models constructed from the minimum (A) and maximum (B) bounds of the 90% credibility intervals for the resistivities in the model cells.

Fig. 5 shows models derived from the minimum (A) and maximum (B) bounds of the 90% credibility intervals for the resistivities in the model cells. The mean deviance along the chain is reaching 2.32, which is far better than the RMS obtained by the classical inversion (4.42). Difference between the min. and max. models A and B is low in isotropic parts of the model and is increasing the in anisotropic domain. Even so, the difference between the extremal models is quite low, and so is the uncertainty of the final solution.

5. Conclusions

The developed stochastic algorithm gives overall satisfactory results. The examples dealing with isotropic models are fully comparable with the classical inversion procedures, and, furthermore, they offer estimates of the uncertainty of the solution.

The real strength of the algorithm is in case of anisotropic models. While, in this case, classical inversion procedures often fail due to large number of local minima and high uncertainty of anisotropic parameters, the stochastic algorithm thoroughly searches the solution space, maps possible solutions and provides estimates of the parameters' uncertainty. The computational costs of the stochastic algorithm are high: several days compared to hours for classical inversion procedures, but the obtained solutions are substantially more complete.

The developed algorithm is well suited for small models with anisotropic structures. It can be used also for isotropic examples, but only for models containing first hundreds of parameters, because time efforts for computing larger models is too great to be useful.

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Curriculum vitae

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