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Research paper

Bayesian inference of spectral induced polarization parameters for laboratory complex resistivity measurements of rocks and soils

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ABSTRACT

Spectral induced polarization (SIP) measurements are now widely used to infer mineralogical or hydrogeological properties from the low-frequency electrical properties of the subsurface in both mineral exploration and environmental sciences. We present an open-source program that performs fast multi-model inversion of laboratory complex resistivity measurements using Markov-chain Monte Carlo simulation. Using this stochastic method, SIP parameters and their uncertainties may be obtained from the Cole-Cole and Dias models, or from the Debye and Warburg decomposition approaches. The program is tested on synthetic and laboratory data to show that the posterior distribution of a multiple Cole-Cole model is multimodal in particular cases. The Warburg and Debye decomposition approaches yield unique solutions in all cases. It is shown that an adaptive Metropolis algorithm performs faster and is less dependent on the initial parameter values than the Metropolis-Hastings step method when inverting SIP data through the decomposition schemes. There are no advantages in using an adaptive step method for well-defined Cole-Cole inversion. Finally, the influence of measurement noise on the recovered relaxation time distribution is explored. We provide the geophysics community with a open-source platform that can serve as a base for further developments in stochastic SIP data inversion and that may be used to perform parameter analysis with various SIP models.

1. Introduction

In recent years, there has been an increase in interest towards spectral induced polarization (SIP) to solve various problems in mineral exploration, hydrogeology, and environmental sciences. SIP data consists of complex resistivity measurements (phase shift and amplitude) in the frequency domain, typically between 1 mHz and 100 kHz. Mathematical models that describe SIP phenomena are often used to describe field or laboratory complex resistivity measurements. These models usually involve parameters known as chargeability and characteristic relaxation time. Empirical models such as the Pelton Cole-Cole resistivity model (Pelton et al., 1978) and the Debye decomposition approach (Nordsiek and Weller, 2008) were proposed to parameterize the SIP response. Other models are derived from equivalent circuits (see Dias (2000)). Chargeability and relaxation time are also involved in mechanistic models that describe the polarization effect observed when rocks are subjected to alternating electrical fields. The models of Wong (1979), Revil et al. (2015) and Misra et al. (2016a, 2016b) describe the polarization of metallic grains disseminated in a rock's pore space. Mechanistic models have also been proposed to explain the polarization of rocks in the absence of metallic minerals (Vinegar and Waxman, 1984; Revil and Florsch, 2010; Revil et al., 2012). SIP models can be validated using synthetic samples with well-known physical properties (e.g. Leroy et al.,2008; Gurin et al., 2015).

Experimental evidence shows that there is a strong relationship between the magnitude of electrical polarization and the surface-area to pore volume ratio (S_{por}), as first described by Börner and Schön (1991). Additional data then strengthened this relationship (Slater et al., 2006; Kruschwitz et al., 2010) and it was shown by Weller et al. (2010b) that values of chargeability can be used to infer S_{por}. A direct relationship between the Cole-Cole time constant and pore size has also been established (Kruschwitz et al., 2010; Niu and Revil, 2016). In the presence of metallic grains and without considering oxidation processes, it is the metallic grain size distribution that dictates the shape of the SIP responses of unconsolidated sands (Wong, 1979; Gurin et al., 2013, 2015). The approximations used in mechanistic models are not always representative

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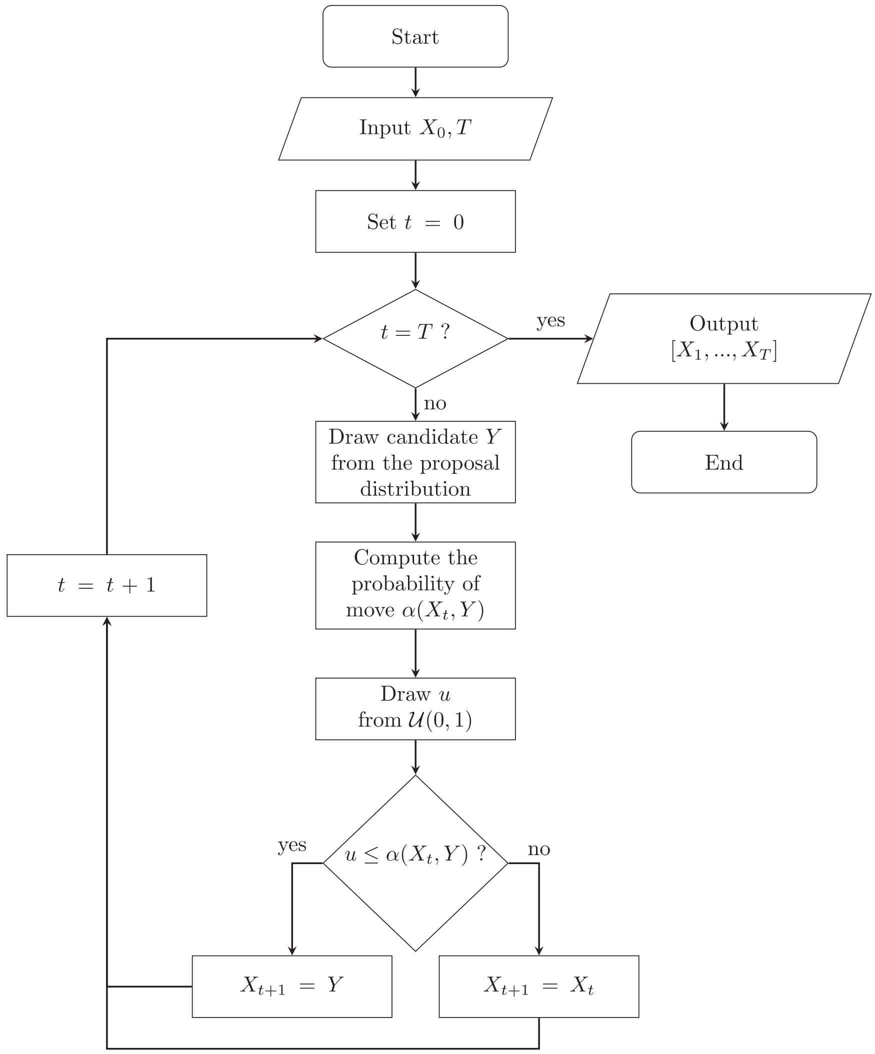

Fig. 1. Flowchart of the Metropolis-Hastings algorithm.

of real geological material. Extensive experimental data sets are needed to see if these models hold for more complex media such as the deformed and altered rocks that are often host to ore deposits. Studies that aim to characterize the SIP responses of rock samples from such deposits require fast and robust batch inversion codes.

In the SIP literature, three different approaches are often used to interpret SIP data. In the first, no curve fitting is required and only the basic features (peak value, frequency of the peak) of the imaginary part of conductivity are considered (e.g. Börner and Schön, 1991; Kruschwitz et al., 2010). The second approach consists of fitting the SIP data with a generalized Cole-Cole model or any of its variants. In this approach the optimization problem is overdetermined and fitting can be done using the nonlinear least squares formulation of Tarantola and Valette (1982). Lastly, interpretation of the SIP data can be done by performing a deconvolution of the complex resistivity spectra into a linear superposition of relaxations models. A Debye (Nordsiek and Weller, 2008) or Warburg (Revil et al., 2014) transfer function is typically used in the deconvolution scheme. In this approach, the problem is underdetermined and requires optimized regularization (Florsch et al., 2012, 2014).

Techniques based on the least-squares optimization have inconveniences. First, the inversion result is very dependent on the initial parameter estimation (e.g. Nordsiek and Weller (2008) and Weigand and Kemna (2016) for Debye decomposition). Batch inversion over large collections of laboratory measurements can prove to be a frustrating and time-consuming process for this reason. Second, they do not allow a straightforward estimation of the uncertainty around the recovered parameters. These two problems can be avoided by using a more global optimization approach such as a Markov-chain Monte Carlo (MCMC) simulation. With MCMC algorithms, the influence of the starting values diminishes as the simulation progresses. They also allow the propagation of measurement uncertainties during the inversion process. SIP parameter uncertainty is often neglected while attempts are made to establish relationships between SIP responses and rock properties (e.g. Zisser et al., 2010; Placencia-Gomez et al., 2013).

We developed BISIP, an open-source Python program to perform fast **B**ayesian **I**nversion of **S**pectral **I**nduced **P**olarization data using either Debye or Warburg decomposition, the Cole-Cole model, or any other empirical model based on simple circuits. An adaptive MCMC algorithm is implemented in BISIP. This approach offers significant advantages in terms of computation time when inverting SIP data with the decomposition approach, by comparison with the non-adaptive routine proposed by Keery et al. (2012). In this paper, parameter analysis of double Cole-Cole and Warburg decomposition inversions of synthetic data contaminated with varying levels of noise and of real SIP data measured on mineralized rocks from the Canadian Malartic gold deposit.

2. Bayesian inference using MCMC

From a Bayesian point of view, all model parameters and data are random quantities. If X denotes a vector of random variables (e.g. a data set) and θ represents a vector of model parameters, then the probability distribution of the parameters given the random variables is