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Joint use of singular value decomposition and Monte-Carlo simulation for estimating uncertainty in surface NMR inversion

Anatoly Legchenko [a,*], Jean-Christophe Comte [b], Ulrich Ofterdinger [c], Jean-Michel Vouillamoz [a], Fabrice Messan Amen Lawson [d], John Walsh [e]

[a] Univ. Grenoble Alps, Institute of Research for Development, IGE, Grenoble, France
[b] University of Aberdeen, School of Geosciences, UK
[c] Queen's University Belfast, Northern Ireland, UK
[d] University of Abomey Calavi, Cotonou, Bénin
[e] School of Earth Sciences, College of Engineering, Mathematical & Physical Sciences, Dublin, Ireland

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ABSTRACT

We propose a simple and robust approach for investigating uncertainty in the results of inversion in geophysics. We apply this approach to inversion of Surface Nuclear Magnetic Resonance (SNMR) data, which is also known as Magnetic Resonance Sounding (MRS). Solution of this inverse problem is known to be non-unique. We inverse MRS data using the well-known Tikhonov regularization method, which provides an optimal solution as a trade-off between the stability and accuracy. Then, we perturb this model by random values and compute the fitting error for the perturbed models. The magnitude of these perturbations is limited by the uncertainty estimated with the singular value decomposition (SVD) and taking into account experimental errors. We use 10^6 perturbed models and show that the large majority of these models, which have all the water content within the variations given by the SVD estimate, do not fit data with an acceptable accuracy. Thus, we may limit the solution space by only the equivalent inverse models that fit data with the accuracy close to that of the initial inverse model. For representing inversion results, we use three equivalent solutions instead of the only one: the "best" solution given by the regularization or other inversion technic and the extreme variations of this solution corresponding to the equivalent models with the minimum and the maximum volume of water. For demonstrating our approach, we use synthetic data sets and experimental data acquired in the framework of investigation of a hard rock aquifer in the Ireland (County Donegal).

1. Introduction

NMR phenomenon can be observed in nuclei possessing both magnetic moment and angular momentum (hydrogen H^1, for example). It consists of selective absorption and transmission of electromagnetic energy by atomic nuclei. Surface NMR method (SNMR), also known as Magnetic Resonance Sounding (MRS) is an application of the NMR phenomenon to groundwater investigation (Semenov, 1987; Schirov et al., 1991; Legchenko and Valla, 2002; Legchenko, 2013; Behroozmand et al., 2015). The resonance behavior of proton magnetic moments ensures that the method is sensitive only to groundwater. Thus, the method is selective. The capacity of a non-invasive detection of groundwater is the competitive advantage of MRS compared to other geophysical tools. For performing MRS measurements, we use a wire loop on the ground. MRS is a large-scale method and the investigated volume depends on the size of the loop. Usually, the same loop acts as a coincident transmitting/receiving antenna. However, separated transmitting and receiving loops can be also used (Legchenko and Pierrat, 2014). The system is tuned to the Larmor frequency (the resonance frequency for hydrogen nuclei of water) known from measurements of the earth's magnetic field. Additionally to detection of groundwater, MRS allows locating water-saturated geological formations. One sounding consists of generating a pulse of oscillating electrical current in the transmitting loop and measuring the amplitude of MRS signal after the pulse is terminated. These measurements are performed with different values of the current in the loop. The shape of the sounding curve allows resolving aquifers using inversion procedure.

Inversion of MRS data is ill-posed. One of the most popular methods of MRS inversion is the Tikhonov regularization (Tikhonov and Arsenin, 1977). It allows obtaining the Tikhonov solution based on the assumption of the smoothness of the inverse model and selecting the parameter of regularization taking into account experimental errors. The Tikhonov solution is unique, but different equivalent solutions may be also obtained using other inversion procedures. For example, assumptions on the solution shape other than the smoothness constrain can be used for

* Corresponding author.
E-mail addresses: anatoli.legtchenko@ird.fr (A. Legchenko), jc.comte@abdn.ac.uk (J.-C. Comte), U.Ofterdinger@qub.ac.uk (U. Ofterdinger), Jean-Michel.Vouillamoz@ird.fr (J.-M. Vouillamoz), messan.lawson@ird.fr (F.M.A. Lawson), ei.dcu@hslaw.nhoj (J. Walsh).

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performing blocky inversion (Mohnke and Yaramanci, 2002). Uncertainty in the inverse model can be estimated using different methods. The singular value decomposition (SVD) allows estimating resolution of the MRS inverse problem assuming that the problem is linear (Weichman et al., 2002; Müller-Petke and Yaramanci, 2008). Guillen and Legchenko (2002a) reported application of the linear programming algorithm to investigation of the solution space. Weng (2010) reported application of the Occam's inversion using a non-linear formulation of the MRS inverse problem. Inversion for the electrical resistivity (Braun and Yaramanci, 2008) as well as inversion using MRS data measured in varying geomagnetic field (Legchenko et al., 2016) also require application of non-linear algorithms. For both, linear and non-linear MRS inverse problems the Monte Carlo inversion has been reported successful (Guillen and Legchenko, 2002b; Chevalier et al., 2014). Parsekian and Grombacher (2015) applied the bootstrap statistics for accelerating uncertainty estimate suitable for linear as well as non-linear inverse problems. One can see that many different approaches can be used but regardless of the inversion scheme, knowledge of the uncertainty in the selected solution is a matter of practical importance.

We developed a simple and robust approach for investigating uncertainty in each particular inverse model by applying random perturbations to this model. We present the case of application of this approach to the inverse models obtained with the Tikhonov regularization method, but random perturbations can be also applied when using any other inversion algorithm. We carried out field tests aiming to evaluate MRS efficiency and to optimize the methodology of MRS application to investigation of hard-rock aquifers. Any hard-rock aquifer is an important, but difficult target for geophysics and hydrogeology because of their high heterogeneity and generally low water content. In this paper, we use MRS data measured in Ireland, but our results can be easily extended to other parts of the world.

In Ireland, highly heterogeneous weathered/fractured hard rock aquifers underlay over 60% of the island (Comte et al., 2012). These aquifers have generally low permeability and porosity and are typical for post-glaciated temperate regions covering large areas in the Northern hemisphere (Comte et al., 2012; Cassidy et al., 2014). The recent glaciations have eroded the shallow part of the bedrock and overlaid this formation by highly heterogeneous glacial and fluvioglacial materials of variable thicknesses. Geological heterogeneity controls the groundwater recharge and aquifer properties (Misstear et al., 2008; Comte et al., 2012; Cai and Ofterdinger, 2016). Under these conditions, sparse borehole information may be often incomplete and the MRS method has the potential to provide a valuable contribution to investigation of groundwater resources.

2. Background

For performing MRS measurements, we use the coincident loop configuration. The loop is energized by pulses of alternating current $i(t) = I_0 \cos(\omega_0 t)$ and acts as the transmitter. The pulse moment $q = I_0 \tau$ is a product of the current amplitude I_0 and pulse duration τ. After the pulse is cut off, the loop is switched to the receiver. In non-magnetic rocks, one pulse is sufficient for measuring the free induction decay signal e_0 as a function of the pulse moment q. Assuming the horizontal stratification, the amplitude of MRS signal can be computed as

$$e_0(q) = \frac{\omega_0}{I_0} \int_V B_\perp M_\perp w(z) dV, \tag{1}$$

where $B_\perp$ is the transversal component of the loop magnetic field, $M_\perp$ is the transversal component of the nuclear magnetization and $w(z)$ is the water content distribution versus depth (Legchenko and Valla, 2002). Under near resonance conditions

$$M_\perp = M_0 \sin(\gamma B_\perp \tau / 2). \tag{2}$$

The water content in the subsurface $w(z)$ is solution of the integral Eq. (1). For resolving this equation, we approximate it by a system of algebraic equations

$$\mathbf{Aw} = \mathbf{e_0}, \tag{3}$$

where $\mathbf{A} = [a_{i,j}]$ is a rectangular matrix of $I \times J$, $\mathbf{e_0} = (e_{01}, e_{02}, \dots, e_{0i}, \dots, e_{0I})^T$ is the set of experimental data and $\mathbf{w} = (w_1, w_2, \dots, w_j, \dots, w_J)^T$ is the water content.

Discretization of the Eq. (1) consists of defining the number and values of the pulse moment and the depth z_j and the thickness Δz_j of layers in the inverse model that compose columns in the matrix $\mathbf{A}$ with respect to

$$\Delta z_j = z_{j+1} - z_j, \quad z_{\max} = \sum_{j=1}^{J} \Delta z_j, \tag{4}$$

where $\Delta z_1 \le \Delta z_2 \le .. \le \Delta z_j \le .. \le \Delta z_J$ and $z_{\max}$ is the maximum depth of water saturated formation that may contribute to measured MRS signal. In general, the number of pulses should be minimized for accelerating fieldwork but should not be less than the number of layers in the Eq. (4) for not degrading resolution (Legchenko and Shushakov, 1998; Dalgaard et al., 2016). We recommend selecting pulses so that each pulse moment q_i corresponds to the maximum of the MRS signal from one model layer Δz_j. In practice, this rule is usually not respected because pulses are set by the hardware following approximately the logarithmic distribution of the pulse moments. For selecting the thickness of each layer (Δz_j), we compute the correlation matrix $\mathbf{R}$ composed of the Pearson correlation coefficients between columns of the matrix $\mathbf{A}$

$$\mathbf{R} = \mathbf{DA^TAD} \tag{5}$$

where $\mathbf{D}$ is a diagonal matrix with the elements

$$d_{j,j} = \frac{1}{\sqrt{\sum_{i=1}^{I} a_{i,j}^2}}. \tag{6}$$

The discretization rule consists of selecting Δz_j and the correlation coefficient (r) between the neighboring layers so that $r = r_{j,j+1} = r_{j+1,j+2} = \dots = r_{J-1,J}$. Thus, varying r we may obtain different distributions with respect to Eq. (4). Straightforward application of this rule may provide very thin shallow layers. In practice, extensive horizontal thin layers are a rare case and we limit the minimal thickness by setting $\Delta z_j \ge 0.5$ m.

The singular value decomposition (SVD) allows investigating resolution of the MRS inverse problem. For that, we present the matrix $\mathbf{A}$ as a product of three orthogonal matrixes: $\mathbf{U}$, $\mathbf{V}$, and $\mathbf{S}$ (Aster et al., 2005)

$$\mathbf{A} = \mathbf{USV^T}, \tag{7}$$

where $\mathbf{U}$ is an $I \times I$ matrix representing the data space, $\mathbf{V}$ is an $J \times J$ matrix representing the model space and $\mathbf{S}$ is an $I \times J$ diagonal matrix with non-negative diagonal elements (singular values). The model resolution matrix $\mathbf{R}_m$ describing how well the recovered model is able to represent the original model is

$$\mathbf{R}_m = \mathbf{VFV^T}, \tag{8}$$

where $\mathbf{F}$ is an $J \times J$ diagonal matrix representing the effect of regularization (the filter factor). Without regularization $\mathbf{F} = \mathbf{I}$ with $\mathbf{I}$ being the identity matrix. The model will be perfectly recovered by the inversion if $\mathbf{R}_m = \mathbf{I}$.

The discretization is an iterative procedure. It consists of: 1) selecting the number and distribution of pulse moments (often I is provided by the hardware during fieldwork and cannot be increased); 2) selecting