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Uncertainty estimates for surface nuclear magnetic resonance water content and relaxation time profiles from bootstrap statistics

A.D. Parsekian [a,*], D. Grombacher [b]

[a] Department of Geology & Geophysics, University of Wyoming, Laramie, WY, United States
[b] Department of Geophysics, Stanford University, Stanford, CA, United States

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ABSTRACT

A method for estimating uncertainty in surface nuclear magnetic resonance (NMR) water content and relaxation times utilizing bootstrapping statistics is presented. Bootstrapping is particularly well suited for assigning uncertainty to the surface NMR data set due to the primary factor that degrades surface NMR data quality: ambient electromagnetic noise. We use synthetic forward modeled data with various noise levels applied (the "known uncertainty"), and then demonstrate that a bootstrap resampling of the observed synthetic data can produce an uncertainty estimate that closely represents the "known uncertainty". Finally, we present two field data sets collected under different magnitude ambient noise levels as examples illustrating the result of this approach under realistic noise conditions. This approach for estimating uncertainty is computationally intensive, but straightforward to implement and produces useful uncertainty estimates on both water content and relaxation time results for smooth surface NMR sounding models.

1. Introduction

Hydrogeophysical measurements have emerged as valuable tools for imaging the subsurface in hydrogeological investigations, estimating hydrologic parameter values and observing hydrologic processes. Evaluation of uncertainty in hydrogeophysical results has been recognized as important when producing data that may be used in a broader hydrogeologic context (Ferré et al., 2009), particularly when these data are used for parameterizing models, and when comparing the hydrogeophysical data to direct "traditional" hydrogeologic measurements. Surface nuclear magnetic resonance (NMR) is a valuable geophysical measurement due to the direct, unambiguous sensitivity to subsurface water content. Recent studies have leveraged this technology for a range of groundwater applications including, for example, aquifer characterization (e.g. Davis et al., 2013), glacial hydrogeology (Lehmann-Horn et al., 2011a), and parameterizing hydrological models (Baroncini-Turricchia et al., 2014).

One of the most common limitations to surface NMR data acquisition is ambient electromagnetic noise that may make signal analysis more challenging and contribute to inaccuracies (Trushkin et al., 1994). Many common sources of ambient electromagnetic noise are related to anthropogenic infrastructure near a measurements site including power lines, cars, trains or radio transmitters. Natural electromagnetic noise sources, such as lightning, are also frequently encountered. Although noise cancelation techniques involving reference loops (i.e. loops deployed specifically for the purpose of monitoring ambient electromagnetic noise for later digital subtraction) are often able to significantly reduce noise levels in the measured surface NMR data (Walsh, 2008), low signal to noise ratios (SNR) remain a common challenge. The uncertainty of a surface NMR measurement is dependent on the measurement quality, i.e. the SNR (Müller-Petke et al., 2011) and the result of low SNR is increased uncertainty in the estimated aquifer properties. Other factors may contribute to uncertainty in surface NMR measurements such as geometrically imperfect loop shapes that are modeled using simple loop geometries (Lehmann-Horn et al., 2011b), poorly known background magnetic field (B_0) at a measurement site (Walbrecker et al., 2011) or instrument bias, however here we focus only on uncertainty attributed to signal quality (i.e. ambient electromagnetic noise) because we assume it is the most dominant and frequently encountered factor. We aim to demonstrate an approach for estimating uncertainty that addresses the question: Under a given noise condition, how precisely can I estimate water content and relaxation time?

Currently, several common surface NMR inversion routines available to the geophysics community are deterministic (Muller-Petke and Yaramanci, 2010; Walsh, 2008; Behroozmand et al., 2012), meaning that the same result will be obtained each time the computation is executed. Often inversion routines that have a large, fixed number of layers, referred to as smooth inversions, are preferred for determining water content and T_2^* depth profiles because of the assumption that geologic properties change gradually through space. Uncertainty in smooth inversions has been evaluated previously using statistical parameters of the ensemble of stacked measurements and the diagonal elements of

* Corresponding author.
E-mail address: aparseki@uwyo.edu (A.D. Parsekian).

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the covariance matrix (e.g. Müller-Petke et al., 2011), or by testing how parameters may be varied within the magnitude of the noise (Günther and Müller-Petke, 2012), however these approaches are not exclusively driven by the observed data. Alternatively, stochastic inversion schemes may be used to assess uncertainty, however they require a priori information about the subsurface (e.g. how many layers are present in the subsurface) (Guillen and Legchenko, 2002; Mohnke and Yaramanci, 2002) and typically produce blocky models with few layers. Smooth inversions may be preferable in situations where a priori knowledge of the number of layers in the subsurface is unavailable and also may result in gradual transitions in water content that are consistent with conceptual expectations of hydrostratigraphy. As surface NMR results become more readily utilized in the hydrogeology community there is a demand for methods to seamlessly assign uncertainty to the resulting data sets. Although existing approaches for assigning uncertainty are effective, given the importance of this topic to the utility of surface NMR measurements we believe that there is value in a stochastic assessment of uncertainty that results in statistical distributions of NMR parameters. Furthermore, to our knowledge, the existing approaches for assigning uncertainty have not been validated against synthetic data with noise at a known amplitude.

For this study we test a non-parametric bootstrap resampling to assess uncertainty in surface NMR parameters. This approach was chosen due to the ease of adding the bootstrap algorithm to existing open source inversion routines (i.e. MRSMatlab, Müller-Petke and Yaramanci, 2010), because the resulting uncertainty is driven directly by the data, and because no prior information is needed beyond the signal itself. The objective of this study is to demonstrate the effectiveness of bootstrap resampling for surface NMR using comparisons between synthetic data with known noise and synthetic data with bootstrap analysis applied. We also aim to illustrate the result of bootstrap uncertainty assignment on field data sets.

2. Background: surface NMR and bootstrapping

A comprehensive presentation of the underlying physics related to surface NMR has been covered in several excellent reviews (Weichman et al., 2000; Legchenko and Valla, 2002; Hertrich, 2008), and therefore we briefly present only the most important points here. In the presence of a background magnetic field (B_0), the magnetic moments of hydrogen atoms in water molecules tend to preferentially align along the direction of B_0 (Earth's magnetic field is used for surface NMR), resulting in the formation of a net magnetization. The surface NMR experiment involves the perturbation and measurement of this magnetization in order to gain insight into subsurface properties such as water content, pore-sizes, and permeability. To perturb the magnetization, an electromagnetic field is generated by pulsing an oscillatory current in a wire loop at the Earth's surface. If the oscillation frequency is selected to be equal to the Larmor frequency ω_0 ($|\omega_0| = |\gamma B_0|$, where γ is the gryomagnetic ratio of the hydrogen atom), the magnetization is perturbed out of alignment with B_0. After the excitation pulse is switched off, the component of the magnetization transverse to B_0 precesses at ω_0, while the magnetization relaxes back to equilibrium, resulting in a measureable NMR signal.

To investigate subsurface properties at different depths a parameter called the pulse moment, q, determined by the product of the amplitude of the oscillatory current and the pulse duration, is varied; large q values are used to probe the greatest depths while small q values are sensitive to shallow depths. This allows surface NMR to produce depth profiles of the volumetric water content (VWC) and T_2^* relaxation time, a parameter that controls the time-dependence of the signal and that may be used in some situations to provide insight into pore-scale properties (e.g. Grunewald and Knight, 2011). In this paper we aim to quantify uncertainty in the VWC and T_2^* profiles. To avoid confusion, throughout the text we report all VWC values in terms of volumetric units [$m^3\ m^{-3}$] while uncertainty is uniformly presented as a percentage [%].

The general surface NMR forward model described by Weichman et al. (2000):

$$V(q,t) = -\int_{vol} \omega_0 M_0 e^{2i\xi(r,\omega)} \sin\left(\gamma q B_\perp^+(r)\right) B_\perp^-(r) e^{-t/T_{2*}(r)} w(r) d^3 r \qquad (1)$$

where $V(q,t)$ is the measured voltage of the NMR signal in the surface loop at a time t following a pulse moment q. The M_0 term represents the amplitude of the equilibrium magnetization. The exponential term containing ξ describes the signal phase related to the subsurface conductivity. The sine term describes the component of the magnetization that has been rotated into a plane transverse to the B_0 direction. The $B_\perp^+(r)$ and $B_\perp^-(r)$ represent the co- and counter-rotating components of the applied magnetic field, and contribute to the perturbation of the magnetization and determine the receive sensitivity, respectively. The exponential containing T_2^* describes the decaying envelope of the NMR signal, while $w(\mathbf{r})$ represents the spatial distribution of the water content in the subsurface. In practice, a simplified version of Eq. (1) is most commonly used where the forward model is reduced from 3D to 1D by laterally integrating Eq. (1). The only spatial variable remaining in the forward model is the depth, z. This simplification contains the implicit assumption that the subsurface is laterally homogeneous (referred to as a layercake Earth). In this case, the forward model takes the form of M\char252ller-Petke and Yaramanci (2010)

$$V(q,t) = \int_{depth} K(q,z) w(z) e^{-t/T_{2*}(z)} dz \qquad (2)$$

where the $K(q,z)$ term is the kernel function that describes all the terms in Eq. (1) except the exponential containing T_2^* and $w(z)$. Eq. (2) represents the forward model used in this study. The pulse moments, which are generally set by the hardware to logarithmically span from a low pulse moment (~0.1 A s) to the highest pulse moment (~10 A s) to allow an efficient time-saving use of the finite bus voltage, control each measurement spatial sampling of the subsurface. As such, the pulse moments used in a study influence the ability to resolve the $w(z)$, and $T_2^*(z)$ profiles. The subsurface model is described as a series of depth layers, initially thin layers close to the surface and thicker layers at greater depths where the surface NMR measurement is less sensitive. In each depth layer, a single water content and a single T_2^* value is present. This simplification describes a mono-exponential decay within a single depth layer. However, multi-exponential signals are still well-described by this model given that multiple depth layers, and thus multiple independent T_2^* values contribute to the total signal. The goal of the standard surface NMR experiment is to estimate $w(z)$ and $T_2^*(z)$. To estimate the depth profiles in this paper we utilize the QT inversion described by M\char252ller-Petke and Yaramanci (2010) that optimizes for both the water content and T_2^* profiles at once. The inversion involves iterating the $w(z)$ and $T_2^*(z)$ profiles until the data misfit is below the predetermined threshold (typically until $\chi^2 \approx 1$). This is an deterministic process resulting in a best-fitting pair of $w(z)$ and $T_2^*(z)$ profiles that describe the data. This inversion scheme improves the stability of the inversion and resolution of the result by accounting for the information shared between neighboring points in the data space. The challenge that we aim to address is to characterize the uncertainty in the estimated water content and relaxation time depth profiles.

Bootstrapping has been used for uncertainty assessment of geophysical measurements such as seismic (e.g. Sacchi, 1998), magnetics (Constable and Tauxe, 1990) and logging NMR (Parsekian et al., 2015). Our non-parametric bootstrap (e.g. Efron, 1979) strategy randomly resamples the entire surface NMR data set at a predetermined fraction of the original data and inverts this subsample. This statistical approach is well understood to be effective at estimating parameter variance when the distribution of the statistic of interest is unknown (e.g.