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Inversion of Surface Nuclear Magnetic Resonance by Regularization with Simulated Atomic Transition Method

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Abstract

Initial water content impacts the accuracy and resolution of the inversion in surface nuclear magnetic resonance (SNMR). In order to solve this problem, a new method called as regularization combined with simulated atomic transition method (RSATA) is proposed. The inversion of SNMR is transformed into an unconstrained nonlinear global optimization problem, and it solved directly by RSATA without pre-assigning the initial water content distribution. The conjugate gradient linear iterative algorithm is adopted to look for local minimum and global extreme value when using RSATA, and has improved the inversion speed. Results show that this method is a very good solution to solve the effect of initial water content and it is also better than the existing methods on the operation efficiency and the accuracy of inversion.

Keywords**:** *regularization, simulated atomic transition algorithm (SATA), inversion, SNMR*

1. Introduction

Surface Nuclear magnetic resonance (SNMR) detection technology is one and only direct detection groundwater method [1], many scholars have developed this theory and made field tests on this technology [2-6]. The inversion of water content plays an important role in research of SNMR. While the accuracy and resolution of SNMR inversion are the key factors of inversion algorithm. In order to simplify this problem, we regard the inversion process as a mathematical model of solving functional minimum. We always calculate this minimum question by linear iteration methods, such as Steepest Descent method [7], Conjugate Gradient method [8], Newton method [9], and nonlinear iterative method [10]: Monte Carlo method [11], Simulated Annealing method (SA) [12], et al. However, the linear iterative methods depend much on the initial model although they have advantages of good stability, high computational efficiency. But it is not easy to get a reasonable initial model in complex electric conditions; while the nonlinear iterative methods based on random search can obtain the global optimal solution without depending on the initial model, but it has poor stability and slow convergence speed.

In order to solve the problem of the initial value influence and realize fast and stable inversion during the inversion, we have proposed a new method which is called as combined regularization method with simulated atomic transition method (RSATA) to solve the optimal solution of SNMR inversion. The idea of RSATA method is to model the process of atomic transition. The objective function of solving the SNMR inversion is equivalent to the energy of atomic. And the objective function tending to a smaller value is like the transition from an excited state with higher energy to that of lower energy or ground state. The probability of transition from one energy level to another can be calculated according to the Boltzman distribution. Compared with singular value decomposition (SVD), and SA for the inversion of one layer water content, the simulation results show that the RSATA is more stable and fast for efficient SNMR inversion.

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2. Forward Modeling of SNMR

Assuming that a wire antenna is laid out on the ground in a circle, the antenna is then energized by a pulse of alternating current and an alternating magnetic field can be detected using the same antenna after the pulse is terminated. Oscillating with the Larmor frequency, the SNMR signal $E(t,q)$ has an exponential envelope and depends on the pulse parameter $q = I_0\tau$:

$$E(t,q) = E_0 \exp(-t/T_2^*)\cos(w_0 t + \varphi_0) \quad (1)$$

Where T_2^* is the spin-spin relaxation time, and φ_0 is the phase of SNMR signal, w_0 is equal to the Larmor frequency of the protons $w_0 = \gamma H_0$, with H_0 being the magnitude of the geomagnetic field and γ the gyro magnetic ratio for protons. The initial amplitude $E_0(q)$ can be calculated as [4]:

$$E_0(q) = \omega_0 |M_0| \int_V \beta_{1\perp} \sin(\frac{1}{2}\gamma\beta_{1\perp} q) w(\mathbf{r}) dV(\mathbf{r}) \quad (2)$$

Assuming that stratification is horizontal and vertical distribution of resistivity is known, $\rho(\mathbf{r})$ the subsurface resistivity, $\mathbf{r} = \mathrm{r}(x, y, z)$, $\rho(\mathbf{r}) = \rho(z)$, Equation (2) can be simplified and written as:

$$E_0(q) = \int_0^L K(q, \rho(z), \alpha, z) w(z) dz \quad (3)$$

Where,

$$K(q, \rho(z), \alpha, z) = \omega_0 |M_0| \iint_{x,y} \beta_{1\perp} \sin(\frac{1}{2}\gamma\beta_{1\perp} q) dxdy \quad (4)$$

We limit integration by $x^2 + y^2 \le (2D)^2$ and $L = 2D$, where D is the antenna diameter.

3. Inversion of SNMR Data

Assume that the groundwater structure is layer distribution, and hence:

$$w(z) = \sum_j w_j \beta_j(z)$$
$$\beta_j(z) = \begin{cases} 1, z_j \le z \le z_j + \Delta z_j \\ 0, \text{其他} \end{cases} \quad (5)$$

Where $i = 1, 2, \ldots M$ is the running index of q , $j = 1, 2, \ldots N$ is the running index for the water content w, $\beta_j(z)$ is a set of basis functions. Hence, the kernel vectors are the elementary responses from the layers of water, characterized by their depth z and thickness Δz . When we use a series of different pulse, equation (2) can be discreted as:

$$E_0(q_i) = \sum_{j=1}^{\infty} K(q_i, z)\Delta z_j \beta_j(z) w_j \quad (6)$$

In a matrix notation, projected Equation (6) can be written as:

$$\mathrm{A}\cdot\mathbf{w}=\mathrm{e}_0 \tag{7}$$

Where A is a rectangle matrix of $M\times N$ with the elements $a_{i,j}=\int_{z_j}^{z_{j+1}}K(q_i,z)dz$;

$\boldsymbol{e_0}=\left(E_0(q_1),E_0(q_2),\ldots,E_0(q_M)\right)^{\mathrm{T}}$,

$E_0(q_i)$ being the set of experimental data;

$\boldsymbol{w}=(w_1,w_2,\ldots w_j,\ldots w_N)^{\mathrm{T}}$,

$w_j=w(\Delta z_j)$ being the vertical distribution of water content at specific aquifer thickness。

4. SNMR Inversion Optimization Model

4.1. SNMR Inversion based on RSATA Method

According to the characteristics of the method of SNMR, the aim of SNMR inversion is to get the water content and its depth. The underground space span of 120m is divided into 60 shares by mesh generation, and each one is an aquifer with 2m thickness. So a model with 60 equal depth layers is constructed. The water content is a column vector with sixty elements which are all between 0 and 1. The inversion of objective function is carried out according to Tikhonov regularization method. To find an approximate solution of matrix Equation (8)

$$\Phi(w)=\left\|\mathbf{d}-\mathrm{Aw}\right\|_{L_2}+\alpha^2\left\|\mathbf{W}\cdot\xi(\mathbf{w})\right\|_{L_2}=\min \tag{8}$$

Where:

A is an integral of the kernel function;

$\mathbf{d}$ being the data of experiment;

$\mathbf{W}$ being the regularizing operator.

4.2. The Introduction of TSATA Method

Inversion of simulation atomic transition was first proposed by Jiaying Wang [13]. Then a new non-linear inversion method adapted to the general geophysical inverse problem was created by Xueming Shi et al. They analyzed the correspondence between the atomic transition and geophysical inversion in Table 1 [14]. This paper will introduce this method to the inversion of SNMR, besides the regularization was combined with this method.

Table 1. The Corresponding Relation between SNMR Detection Inversion and Simulated Atomic Transition

The inversion of SNMR water content	Atomic transition
The target level of the SNMR inversion	Atomic energy level
global minimum	ground state of atom
Local minimum	excited state of atom

The steps of RSATA method are follows:

1. Give a random initial model group $\mathbf{w}=(w_1,w_2,w_3\ldots,w_{60})^{\mathbf{T}}$;
2. Use conjugate gradient linear iterative method to get target level (local extremum) and its water content through local optimization inversion. If the target level is less than the given threshold, then go to step (E);
3. Make the simulated atomic transited according to the target level. The transition probability of target level are decided by Equation (9);

$$p = \begin{cases} 1, E_i > E_j \\ \exp\left[-(E_j - E_i)/kT\right], E_i \le E_j \end{cases} \quad (9)$$

4. update the model parameter, $w^* = w^* + \delta w$, where w^* is "steady" solution, δw is random number, then go to step (B);
5. Output target level and parameter of the inversion.

5. Inversion Results and Analysis

In order to demonstrate the performance of RSATA method, we used a single layer model consisting of a 10-m-thick horizontal, homogeneous in free space at depth of 20m and three-layer model consisting of two 10-m-thick horizontal, homogeneous in free space at depth of 20m and 100m and a 8-m-thick horizontal, homogeneous in free space at depth of 60m.

In the calculation of this section we first give a water content of the model, and calculate the strength of the signal e_i at different pulse moments, then certain signal-to-noise ratio (SNR) of the Gaussian white noise is added to e_i ,so we get e ,signal-to-noise is defined by (10):

$$SNR = 20 * \log_{10} \frac{\|e_i\|_2}{\|e - e_i\|_2} \quad (10)$$

Assume that the whole section is composed of sixty 2-m-thick acquires, the geomagnetic field is 50000nT, the antenna is laid out on the ground in a circle with a diameter of 100m, and it is excited by sixty current pulses, the largest pulse is $10000 A \cdot ms$.

It can be seen from the inversion results that RSATA method is effective for single aquifer model, especially when we add the noise of 20 dB signal-to-noise ratio, the inversion result is still consistent with the model. With the complexity of the model complex, the water content of three layer aquifer model at depth of 100m was not accurate enough in Figure 3, which is less than model, let alone the water content with adding noise in Figure 4. At the same time we can see there are three more layers model in Figure 5 and Figure 6, However, from Figure 5 and Figure 6 we found that the amplitude which we calculated by inversion results in Figure 3 and Figure 4 is consistent with the amplitude which we calculated by inversion model . It is the multi-solutions problem in geophysics that we also encountered earth in SNMR.

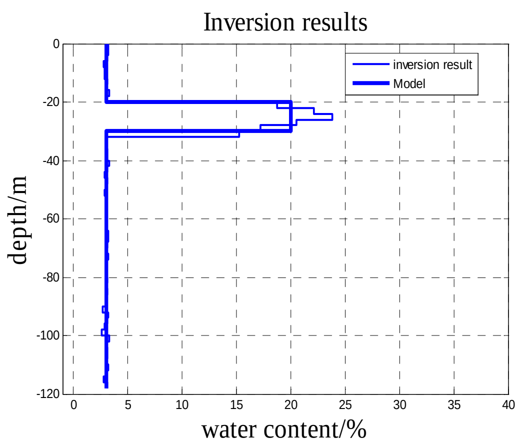

Figure 1. The Inversion Results for Single Layer without Noise

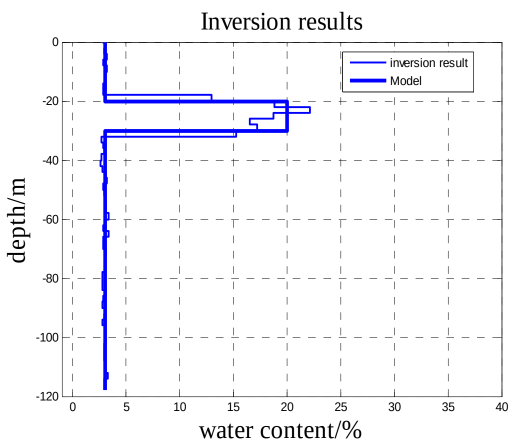

Figure 2. The Inversion Results for Single Layer with Noise of s/n=20dB

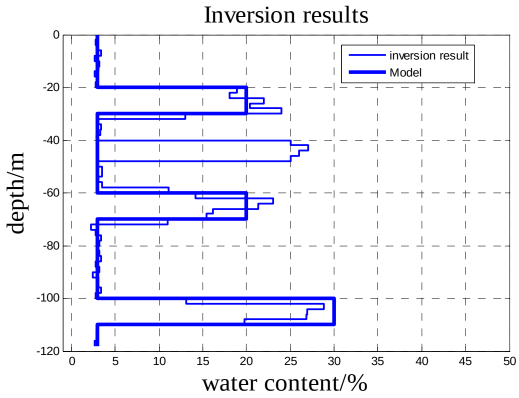

Figure 3. The Inversion Results for Three Layers without Noise

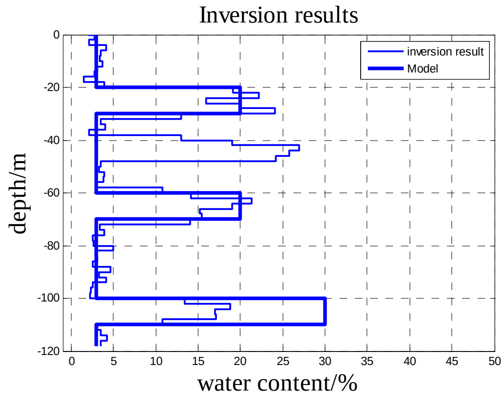

Figure 4. The Inversion Results for Three Layers with Noise of s/n=20dB

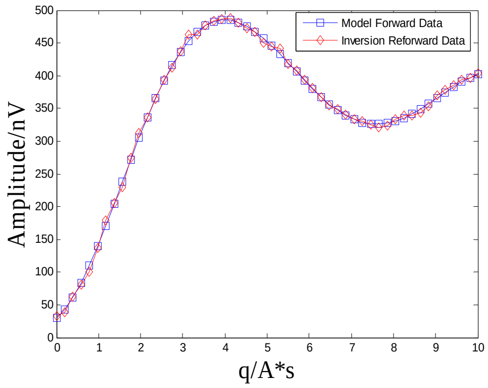

Figure 5. The SNMR Forward of 3-layer Aquifers and the Reforward of RSATA without Noise Inversion Results

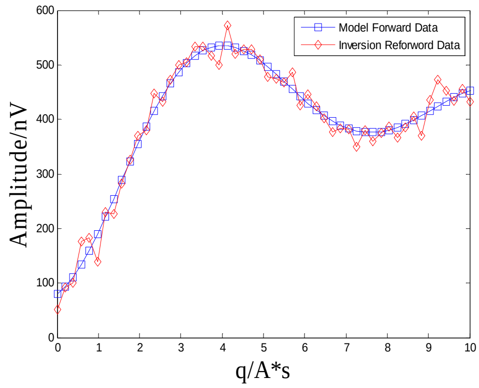

Figure 6. The SNMR Forward of 3-layer Aquifers and the Reforward of RSATA with Noise of s/n=20dB Inversion Results

Table 2. The Comparison of Different Kinds of Inversion Methods

signal-to-noise ratio	Inversion methods					
	RSATA		SVD		SA	
	accuracy /%	time/s	accuracy /%	time/s	accuracy/%	time/s
40	90.3	2.73	60.9	50.2	88.2	8.91
30	86.1	2.45	50.4	52.6	80.3	9.32
20	83.2	2.87	40.7	59.2	74.3	10.33
10	81.7	3.12	30.1	60.3	70.5	11.78

The accuracy of inversion and its rate of convergence at different noise for single layer water model by RSATA, SVD, and SA algorithm are given in Table 2. It shows that RSATA algorithm has obtained higher accuracy and bigger rate of convergence with lower SNR for observation data, while SVD needs a higher SNR at least 40dB to complete the inversion.

6. Conclusion

Regularization combined with simulation atomic transition algorithm is proposed to the inversion of SNMR in this paper. From the simulation experiments, we can see inversion results never be effected by the initial water content and this method has better performance on the inversion of single-layer and multi-layer aquifer models. Moreover, the use of the conjugate gradient linear iterative optimization algorithm to find local and globe extremum obviously increased the speed of calculation during the inversion. Compared with SVD and SA, we can see it is more fit to the inversion of low SNR signals. So more accurate underground information can be detected by this algorithm and it also provides a new way of solving other problems of low SNR.

References

[1] Lin J. Situation and progress of nuclear magnetic resonance technique for groundwater investigations. *Progress in Geophys (In Chinese)*. 2010; 25(2): 681-691.
[2] Mohnke O, Yaramanci U. Forward modeling and inversion of MRS relaxation signals using multi-exponential decomposition. *Near Surface Geophysics.* 2005; 3(3): 165-185.
[3] Gunther T, Muller-Petke M. Hydraulic Properties at the North Sea Island of Borkum Derived from Joint Inversion of Magnetic Resonance and Electrical Resistivity Soundings. *Hydrology and earth system sciences.* 2012; 16(9): 3279-3291.
[4] Dai Miao, Hu Xiang-Yun, Wu Hai-Bo. Inversion of Surface Magnetic Resonance. *Chinese Journal of Geophysics*. 2009; 52(10): 2676-2682.
[5] Thin Lai Lai Thein, Myint Myint Sein. View Synthesizing for a Large-scale Object in a Scene. *TELKOMNIKA Indonesian Journal of Theoretical and Applied Information Technology*. 2012; 10(5): 999-1004.
[6] WENG Aihua, WANG Xueqiu, LIU Guo xing, et al. Nonlinear inversion of surface nuclear magnetic resonance over electrically conductive medium. *Chinese Journal of Geophysics*. 2009; 50(3): 890-896.
[7] Yu YP, Li ZY, Gong SP, et al. The Research on 1D SNMR Inversion by Tikhonov Regularization Method. *CT Theory and Applications (In Chinese)*. 2009; 18 (2): 134-189.
[8] Li TS. Optimization principle and programming algorithm. Chang sha: National University of Defense Technology Press. 2001: 8-9.
[9] Braun M, Yaramanci U. Inversion of resistivity in magnetic resonance sounding. *J.Appl.Geophys*. 2007; 66 (2): 151-164.
[10] Legchenko AV, Baltassat JM. *Application of the surface proton magnetic resonance method for the detection of fractured granite aquifers*, Proceedings of the IV Meeting of the Environmental and Engineering Geophysical Society (European Section). Barcelona (Spain). 1998; 163-166.
[11] Guillen A, Legchenko A. Inversion of surface nuclear magnetic resonance data by an adapted Monte Carlo method applied to water resource characterization. *Journal of Applied Geophysics*. 2002; 50(2): 193-205.
[12] Legchenko A, Vouillamoz JM, Roy J. Application of the magnetic resonance sounding method to the investigation of aquifers in the presence of magnetic materials. *Geophysics.* 2010; 75(6): 91-100.
[13] Shi XM, Wang JY. Yi YY, et al. A study on the simulated atomic transition algorithm for geophysical inversion. *Chinese J. Geophys*. 2007; 50(1): 305-312.
[14] Hermagasantos Zein, Yusra Sabri, Ali Mashar. Implementation of Electricity Competition Framework with Economic Dispatch Direct Method. *TELKOMNIKA Indonesian Journal of Theoretical and Applied Information Technology.* 2012; 10(4): 625-632.