Non-linear Inversion for Surface Nuclear Magnetic Resonance Data in Layered Electrically Conductive Media

Hairu Zhang[1], Guofu Wang[2], Faquan Zhang[2]

1. *State Key Laboratory of Acoustics, Institute of Acoustics, Chinese Academy of Sciences, Beijing 100190, China;*

2. *School of Information and Communication Engineering, Guilin University of Electronic Technology, Guilin 541004, China*

ABSTRACT

The inversion for surface nuclear magnetic resonance (SNMR) data in layered electrically conductive media can be concluded as the problem to solving a matrix equation $An=E$, where A is a kernel function matrix, E is a initial amplitude sequence of the measured data and n is the unknown water content distributions sequence. The precision of A mainly depends on the estimation to the spacial resistivity distributions. Because of the intrinsic error existing in both A and E and the big condition number of A, a regularization - total least square (R-TLS) model of the SNMR inversion is firstly proposed in this paper. Then the model is transformed into a constrained nonlinear optimization problem, and the solution to the optimization problem is obtained by using an proposed improved particle swarm optimization (IPSO) algorithm. Although $An=E$ is generally an ill-conditioned and highly underdetermined equation, the proposed algorithm still works effectively. The whole proposed approach is examined by using synthetic data and practical field data, which well demonstrates the capability of the approach. The results of the synthetic data example demonstrate that proposed approach can well derived the construction information of the hypothesis model under poor relative error of the resistivity distributions ($ERROR_{layer}$ = 17.7%) and poor SNR (SNR = 5dB) at the root mean square 5.11%, while all existing approaches are useless at all in this example. And the inversion results by the proposed approach for the practical field example, when SNMR has been used in combination with Vertical Electrical Sounding (VES), can well meet with the construction information from an in-site borehole under poor SNR (SNR = 6.9dB) at the root mean square 2.92%.

KEYWORDS: Surface nuclear magnetic resonance; Total least square; Regularization; Non-linear optimization; Particle swarm optimization; Vertical electrical sounding

INTRODUCTION

Simple in operation, rich in information and unique in solution, the surface nuclear magnetic resonance (SNMR) is a geophysical technique specifically developed for hydrogeological investigations. Along with its unintermittent growth and its exploration, this technique has been applied successfully to the detection of groundwater, archaeological work, test of shallow groundwater quality, etc [1]-[3]. SNMR energizes the hydrogen nuclei in the groundwater by transmitting an electromagnetic pulse at the Larmor frequency followed by a certain dead time, when the pulse is terminated. The resonance signal emitted by the hydrogen nucleus is then received. Receptions of the SNMR data are carried out by varying the pulse moment. The structure of underground aquifer can be derived from the inversion of the SNMR data [4].

In recent years, the SNMR technology has been paid much attention to by many experts and scholars and certain achievements have been made. With the development of research work, the one-dimensional forward and inversion theory has been ripening, and it provides theoretical foundation for further study to two-dimensional and three-dimensional forward and inversion [5]-[6]. The inversion algorithms of SNMR data are all based on the forward equation $An = E$, where A is a kernel function matrix, E is a initial amplitude sequence of the measured data and n is the unknown water content distributions sequence. The precision of A mainly depends on the estimation to the spacial resistivity distributions. However, the array A is estimated from the prior information about the resistivity distributions which is obtained by the other geophysical methods or the drilling data around the site. An improved simulated annealing algorithm (ISA) was proposed to improve the stability of the existing inversion algorithms and speed up the convergence [7]. The QT inversion that considers the entire data set and inverts the data set directly for water-content distribution was designed to improve the accuracy [8]. The full decay inversion of SNMR data was proposed to improve the accuracy by the gated integration technique [9], which is similar to the QT inversion in the solution methods. However, the existing inversion algorithms are all based on the assumption that the prior information about the resistivity distributions is objective and reliable. Because of the initial data errors, the accuracy of the result will decrease. We find that the existing inversion algorithms are all useless when the estimation of the resistivity distributions is poor, especially when the resistance is less than 50Ω•m. In solving the equation containing errors in both A and E, the total least square model outperforms the least square model, which is used to improve the accuracy in this paper. Besides, $An = E$ is a ill-conditioned equation for the big condition numbers of A. The regularization has high-performance in solving the ill-conditioned equation [10]. Therefore, the R-TLS model of the SNMR inversion is proposed in this paper to improve the stability and accuracy of the inversion result, which is transformed into a constrained nonlinear optimization problem. Then the IPSO algorithm is described to solve the constrained nonlinear optimization problem, which still works effectively under $An = E$ being a highly underdetermined equation.

NON-LINEAR INVERSION OF SNMR DATA IN LAYERED MEDIA

The spatial distribution of the excited magnetic field in layered media

In horizontally stratified Earth models, the radial and vertical components of the magnetic field for the i th geological layer are then given by[11]

$$H_{ir}\left(r,z\right)=\frac{I_0 a}{2}\int_0^{\infty}\left[a_i e^{-u_i z}-b_i e^{u_i z}\right]u_i J_1\left(\lambda r\right)J_1\left(\lambda a\right)d\lambda\,, \quad (1)$$

$$H_{iz}\left(r,z\right)=\frac{I_0 a}{2}\int_0^{\infty}\left[a_i e^{-u_i z}+b_i e^{u_i z}\right]\lambda J_0\left(\lambda r\right)J_1\left(\lambda a\right)d\lambda\,, \quad (2)$$

where I_0 is the pulse moment amplitude, $u_i=\sqrt{\lambda^2+i\varpi u_0/\rho_i}$, ϖ is the Larmor frequency, u_0 is the permeability of vacuum, ρ_i is the resistivity of the i th geological layer, $J_0\left(\bullet\right)$ and $J_1\left(\bullet\right)$ are respectively the zero and one order Bessel function of the first kind, both a_i and b_i are geotechnical parameters.

Forward modeling of SNMR data

In horizontally stratified Earth models, the discrete model of SNMR data can be written as [6]

$$E_0\left(q_i\right)=\sum_{j=1}^{\infty}K\left(q_i,z_j\right)n_j\Delta z_j\,, \quad (3)$$

where q_i is the i th pulse moment, n_j and Δz_j are respectively the water content and thickness of the j th geological layer. The kernel function in the columnar coordinates is given by

$$K\left(q_i,z_j\right)=\varpi M_0\sum_{m=1}^{M}\sum_{n=1}^{N}b_{1\perp mnj}\sin\theta_{imnj}r_m\Delta r_m\Delta\Phi_n\,, \quad (4)$$

where M_0 is magnetic moment of unit volume, $b_{1\perp}=u_0 H_{1\perp}/I_0$, $H_{1\perp}$ is the vertical component of excitation field to the local geomagnetic field, θ_{imnj} is the excitation angle of the location

$\left(r_m,\Phi_n,z_j\right)$, Δr_m and $\Delta\Phi_n$ are respectively the radial and vertical length of the differential element $\left(r_m,\Phi_n\right)$, M and N are respectively the radial and vertical number of the differential element.

For a series of pulse moments q_i and a limited detecting depth, the Eq.(3) can be expressed as

$$An = E\,, \tag{5}$$

where $E=\left(E\left(q_1\right),E\left(q_2\right),...,E\left(q_{I_N}\right)\right)^T$, I_N is the number of pulse moments, $A_{ij}=K\left(q_i,z_j\right)\Delta z_j$, $n=\left(n_1,n_2,...,n_{M_N}\right)^T$, M_N is the number of aquifers.

Inversion modeling of SNMR data by a constraint R-TLS method

In the SNMR inversion, the precision of the kernel function array A mainly depends on the estimation to the resistivity distributions, which is obtained by the other geophysical methods. Because of the disturbances from various noises, there are many errors, including systematic errors and gross errors, in the obtained data. Hence, the R-TLS model of SNMR inversion is proposed to improve the stability and accuracy of the inversion result as follows.

$$\begin{array}{l}\min\left\|\left(A,E\right)-\left(A^*,E^*\right)\right\|_F\\ \begin{cases}A^*n=E^*\\ \left\|Ln\right\|_2\le\delta\\ 0\le n_i\le 1, i=1,2,...,M_N\end{cases}\end{array}, \tag{6}$$

where A^* and A are respectively the measured and real kernel function array, E^* and E are respectively the measured and real initial amplitude array, $\left\|\bullet\right\|_F$ is F-norm operator, δ is a positive constant, the array L controls the degree of the smoothness constraint n, which is usually the first or second derivative. The Eq.(6) can be translated into the constraint Lagrange equation which is given by

$$\begin{cases}L\left(A^*,n,\mu\right)=\left\|\left(A,E\right)-\left(A^*,A^*n\right)\right\|_F^2+\mu\left(\left\|Ln\right\|_2^2-\delta^2\right)\\ 0\le n_i\le 1, i=1,2,...,M_N\end{cases}, \tag{7}$$

where μ is the Lagrange multiplier. When δ converges to zero, the Eq.(7) can be expressed as

$$\begin{cases}\min\left\{\dfrac{\left\|An-E\right\|_2^2}{1+\left\|n\right\|_2^2}+\xi\left\|Ln\right\|_2^2\right\}\\ 0\le n_i\le 1, i=1,2,...,M_N\end{cases} \tag{8}$$

where ξ is regularized factors the R-TLS model constraint object function.

IPSO algorithm applied to solve water resource characterization

Particle Swarm Optimization (PSO) is a popular and bionic algorithm which takes advantage of simple algorithm, facile realization, fast convergence rate, etc. It is widely used in non-linear optimization, neural network training, complex system control, etc[12]. In the following, the IPSO algorithm is described for solving the Eq.(8).

Step 1: Population initialization. The number of particles M_N in solution space is equal to the number of aquifers. $n_0 = \left(n_{01}, n_{02}, ..., n_{0M_N}\right)^T$ is an initialization particle swarm vector, which range from 0 to 1. $v_0 = \left(v_{01}, v_{02}, ..., v_{0M_N}\right)^T$ is an initialization speed vector, which v_{0i} ranges from -1 to 1. The maximum number of iteration is defined as $N_{\max}$. The number of iterations Num is initialized as zero. The threshold $Threshold\_Val$ of the limited inversion accuracy is initialized as 10^{-8}.

Step 2: Each particle has its objective function value which is decided by a fitness function:

$$\begin{cases} v_h^* = w\Delta v_i + c_1 r_1\left(p_{best} - n_h\right) + c_2 r_2\left(g_{best} - n_h\right) \\ v_h = \begin{cases} v_h^*, \left|v_h^*\right| > v_{threshold} \\ v_{threshold}, \left|v_h^*\right| \le v_{threshold} \end{cases} \\ n_{h+1}^* = n_h + v_h \\ n_{h+1} = \begin{cases} 0, n_{h+1}^* < 0 \\ n_{h+1}^*, 0 \le n_{h+1}^* \le 1 \\ 1, n_{h+1}^* > 1 \end{cases} \end{cases} \tag{9}$$

where i is the i th particle, w is weights for limiting shift step length, Δv_i is the direction vector, c_1 and c_2 are the limited factors, which are respectively initialized as 0.0005 and 0.001, r_1 and r_2 are random numbers, which range from 0 to 1. p_{beat} is the position with the best fitness found in the i th particle. g_{beat} is the position with the best fitness found so far for the i th particle. The threshold $v_{threshold}$ of the limited speed is initialized as 0.005, which can avoid getting in the local best solution when solving the precise solutions.

The direction vector Δv is defined as

$$\Delta v=\begin{pmatrix} \Delta v_{11} & \Delta v_{12} & \cdots & \Delta v_{1M_N} \\ \Delta v_{21} & \Delta v_{22} & \cdots & \Delta v_{2M_N} \\ \vdots & \vdots & \ddots & \vdots \\ \Delta v_{M_N 1} & \Delta v_{M_N 2} & \cdots & \Delta v_{M_N M_N} \end{pmatrix},$$

where $\Delta v_{ij} \in \{x \mid -1,0,1\}$. Δv is a randomly generated matrix each particle, which is written as $\Delta v=\left(\Delta v_1,\Delta v_2,\ldots,\Delta v_{M_N}\right)$, where $\Delta v_i=\left(\Delta v_{1i},\Delta v_{2i},\ldots,\Delta v_{M_N i}\right)^T$.

In the course of iterative optimization of IPSO algorithms, variable searching step is used to improve the accuracy of the calculation and speed up the convergence.

$$w=\left(1-Num/N_{\max}\right)\Delta w,$$

where Δw is constant step with the value of 0.05.

Step 3: The score F_{score} of each particle is calculated by substituting each n_{h+1} into the Eq.(8), which is introduced to evaluate the results of the each particle. Then, p_{beat} and g_{beat} are updated.

Step 4: Judgment of terminal condition. If $Num > N_{\max}$ or $F_{score} \le Threshold$, the iterates stops and the result of inversion is g_{beat}, otherwise it returns to execute **Step 2**.

APPLICATIONS

Tests with synthetic data

To verify the performance of the new algorithm, the synthetic model parameters are setted at first. Then the real initial amplitude array E and kernel function array A are obtained by Eq.(4) and Eq.(5). The measured initial amplitude array E^* is produced by adding noise to E. The measured kernel function array A^* is obtained by substituting the estimated layered model containing relative errors into Eq.(4). Finally, the new algorithm (IPSO) is used to solve the Eq.(4). Besides, a comparison experiment is made to compare with existing algorithms, including the current best algorithm (ISA algorithm [7]), to verify the advantages of the IPSO algorithm. Table 1 shows the comparison results for some existing inversion algorithms in some working conditions.

Table 1: Performance comparisons about the existing inversion algorithms

Inversion algorithms	Subsurface resistance		SNR	Kernel function $A_{M\times N}$
	Resistance	Existential error		
SVD[7]	High resistance	Neglect	>20dB	$M \geq N$
Monte Carlo method[13]	Unrestricted	Neglect	>5dB	Unrestricted
Simulated Annealing algorithm[6]	Unrestricted	Neglect	>5dB	Unrestricted
QT[8]	Unrestricted	Neglect	>2dB	Unrestricted
ISA[7]	Unrestricted	Neglect	>2dB	Unrestricted

Here, signal to noise ratio (SNR) is defined as

$$\mathrm{SNR} = 20\log_{10}\frac{\|d\|_2}{\|d-d^*\|_2}, \tag{10}$$

where d^* and d are respectively the measured data and the real data. The relative errors $ERROR_{layer}$ of the estimated layered model is defined as

$$ERROR_{layer} = \frac{1}{M_N}\sum_{i=1}^{M_N}\frac{|\rho_i-\rho_i^*|}{\rho_i}\times 100\%, \tag{11}$$

where ρ_i^* and ρ_i are respectively resistivities of the estimated and real layered model. The root mean square (RMS) of the inversion results is used to evaluate the inversion algorithm's performance, which is defined as

$$\mathrm{RMS} = \sqrt{\frac{1}{M_N}\sum_{i=1}^{M_N}\left(n_i-n_i^*\right)^2}\times 100\%, \tag{12}$$

where n_i and n_i^* are respectively water content in each layer of the real and inversion result model.

Both the IPSO and ISA inversion algorithms have been tested with synthetic data. Inversions for a layered hydrogeological scenarios is presented, calculated for a square loop antenna with 75m long sides in a geomagnetic field of 44,630nT at an inclination of 24°and a maximum pulse moment of 6.5As. The vertical calculation grid is set to 1m with a maximum depth of 70m. The multi-layer geo-electrical structure model in Fig.1a describes the real model of two layer resistivity with between 0 and 15m depth having $10^4\,\Omega\cdot\mathrm{m}$ as well as below 15m having $10\,\Omega\cdot\mathrm{m}$ and the estimated model of two layer resistivity with between 0 and 14m depth having 9,700 $\Omega\cdot\mathrm{m}$ as well as below 14m having $12\,\Omega\cdot\mathrm{m}$ ($ERROR_{layer}$=17.7%). The measured data shown in Fig.1b is the real data with SNR=5dB random noise. The water content model in Fig.1c describes the scenario of a single aquifer with a sharp upper boundary at 25m as well as a sharp lower boundary at 40m and 30 vol.% of mobile water. The inversion grid employed consists of 70 equidistant layers with a thickness $\Delta z = 1\mathrm{m}$.

The results of ISA inversion and IPSO inversion for SNMR amplitudes are shown in Fig.1b and Fig.1c. It can be observed that the results of IPSO inversion agree well with the information of the hypothesis model at the root mean square 5.11%, while ISA inversion is useless at the root mean square 10.13%. Hence, it is difficult to ascertain the hydrogeological structure and groundwater by the existing methods under poor $ERROR_{layer}$ and SNR. However, the IPSO inversion method has many advantages over those available, which is in accordance with the actual results.

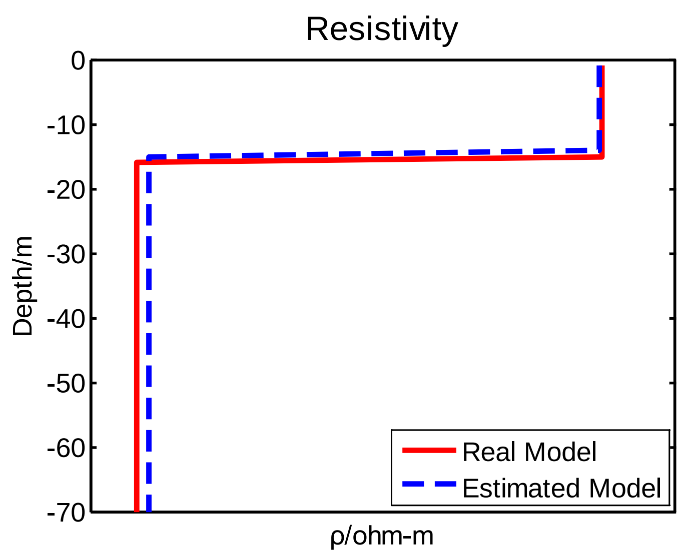

Figure 1a: The resistivity models using SNMR inversion

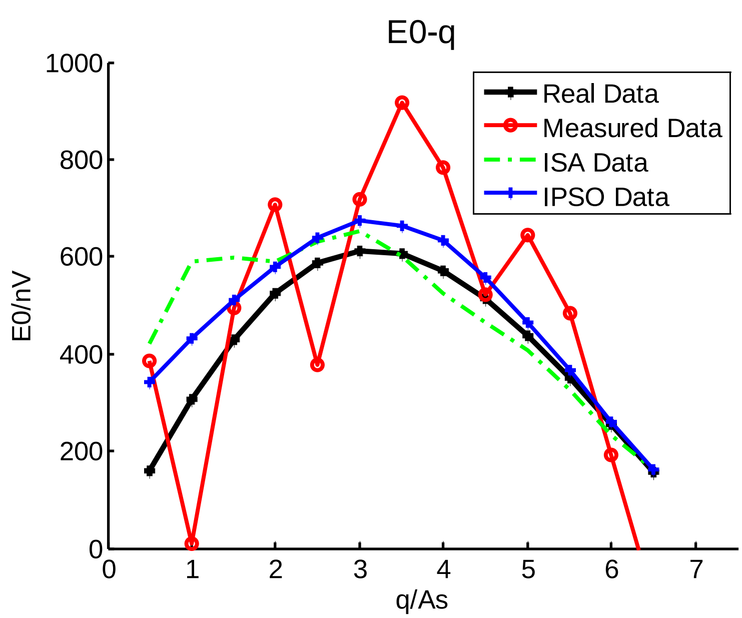

Figure 1b: SNMR data and model fit for ISA inversion and IPSO inversion

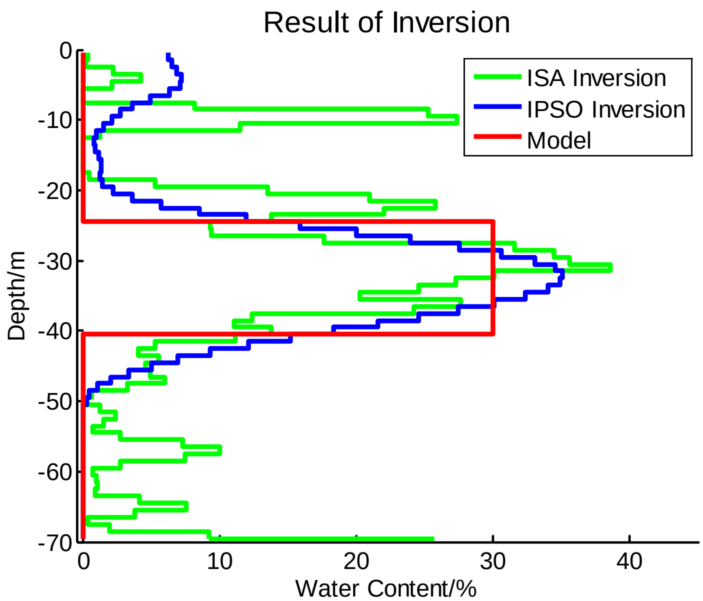

Figure 1c: Results of ISA inversion and IPSO inversion for SNMR amplitudes

Field test case

Inversions have been carried out for the data obtained from a SNMR sounding (Fig. 2a) at Site1 in Area 1 in the Vientiane basin, Laos [3]. SNMR has been used in combination with VES and borehole in field test. The measurements were conducted using a square antenna loop with a diameter of 100m and a maximum pulse moment of 5As. The local geomagnetic field intensity was 43,770nT with an inclination of 24°. The inversion grid employed consists of 70 equidistant layers with a thickness $\Delta z = 1\text{m}$. The measured data shown in Fig.2a contains SNR=6.9dB ambient noise. From a VES, the electrical resistivity in Fig.2b has been found to be about 550$\Omega\cdot\text{m}$ between 0 and 4m depth, about 5,000$\Omega\cdot\text{m}$ between 4 and 11m depth and about 20$\Omega\cdot\text{m}$ below 11m. At this site, borehole measurements confirmed a two-layer case with alluvial deposits between 0 and 38m and sandstone of Cretaceous and Jurassic age between 38 and 70m. The water content model in Fig.2c describes a three-layer case with the first aquifer between 3 and 16m having about 4% mobile water, the second aquifer between 16 and 32m having about 14% mobile water and the third aquifer between 32 and 70m having about 1% mobile water.

The SNMR data are respectively interpreted using IPSO inversion and the inversion software Samovar v6.2 [3]. The results of inversion are shown in Fig.2a and Fig.2c. The blue line in Fig.2a corresponds to a best fit inversion made with the amplitude data. The blue curve (RMS=2.92%) and the green curve (RMS=3.65%) in Fig.2c agree well the information from an in-site borehole. Hence, the IPSO inversion method has many advantages such as low dependence to initial model, stable result and strung anti-noise ability.

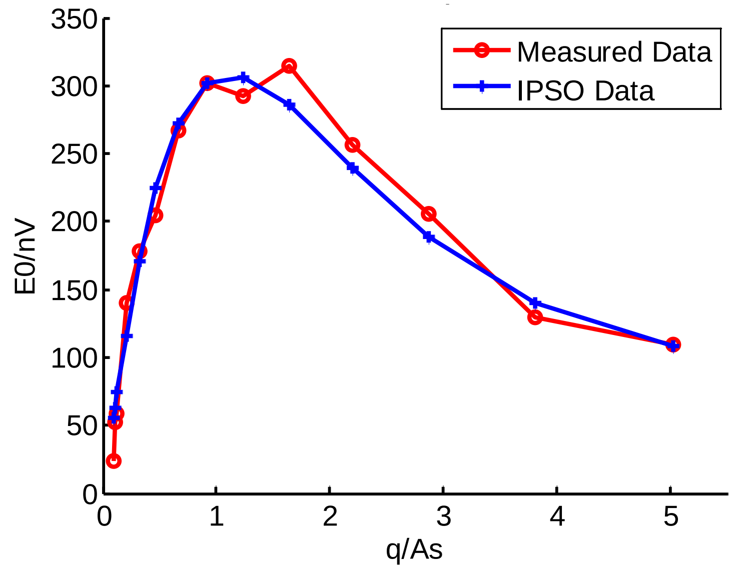

Figure 2a: SNMR data and model fit for IPSO inversion

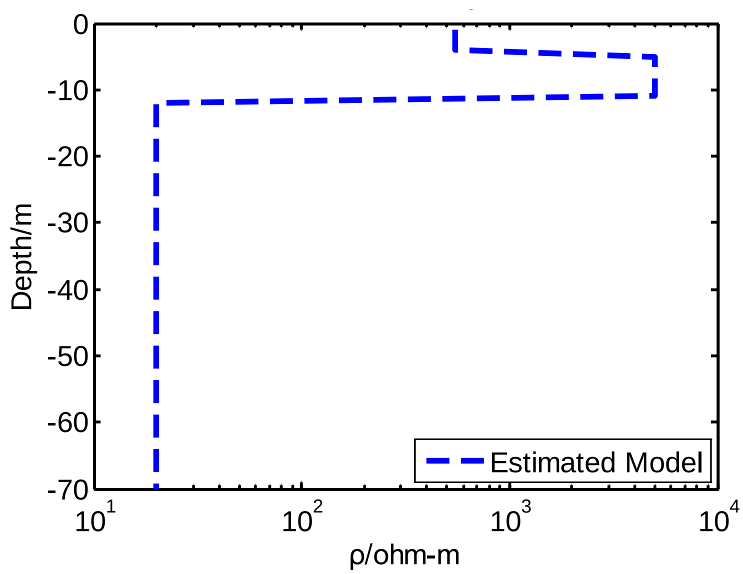

Figure 2b: The resistivity model using SNMR inversion

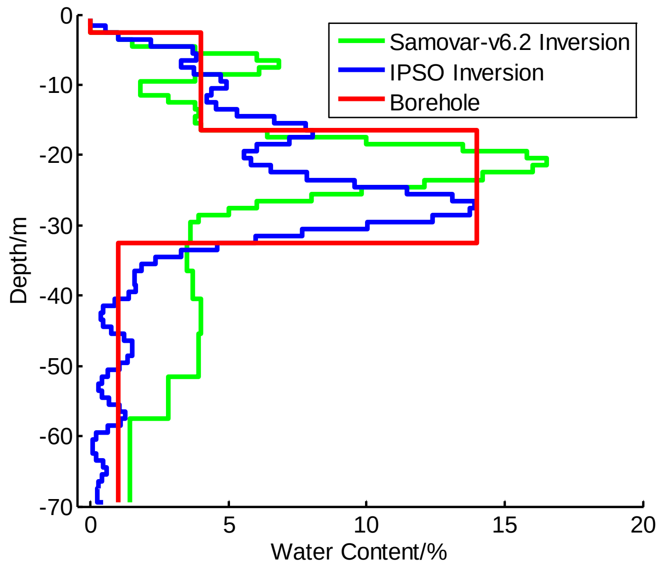

Figure 2c: Results of Samovar v6.2 inversion and IPSO inversion for SNMR amplitudes

CONCLUSIONS

For horizontally layered conductivity and water content distributions the existing inversion algorithms are all based on the assumption that the prior information about the resistivity distributions is objective and reliable, which certainly results in low inversion precision. These algorithms are useless if the estimation to the resistivity distributions is poor, especially when the resistance is less than 50Ω•m. Besides, the kernel function matrix A has generally big condition numbers. Hence, the R-TLS model is proposed to improve the stability and accuracy of the SNMR inversion result, which is transformed into a constrained nonlinear optimization problem. To obtain the inversion results, the IPSO algorithm is designed, which applies to solving underdetermined equation and removes the max number of aquifers limitation. The results of the synthetic data example show that the new algorithm agree well the construction information of the hypothesis model under poor conditions ($ERROR_{layer}$=17.7%, SNR=5dB) at the root mean square 5.11%, while ISA inversion is useless at the root mean square 10.13%. The IPSO inversion method has many advantages such as low dependence to initial model, stable result, and strung anti-noise ability. The results of the field example show that both the new algorithm (RMS=2.92%) and the inversion software Samovar v6.2 (RMS=3.65%) agree well the construction information from an in-site borehole, and the former algorithm has slightly higher precision the posterior one.

ACKNOWLEDGMENTS

This work was funded by the National Natural Science Foundation of China (Nos. 11434012, 61362020 and 61371186) and the Joint NSFC-ISF Research Program, jointly funded by the National Natural Science Foundation of China and the Israel Science Foundation (No. 41561144006).

REFERENCES

[1] Nadiah Hanim Shafie, Umar Hamzah, and Abdul Rahim Samsudin: "2D Gravity Inversion Technique in the Study of Cheshire Basin," *Electronic Journal of Geotechnical Engineering*, 2014 (19.S) pp 4381-4394. Available at ejge.com.

[2] Hairu ZHANG, Shan OUYANG, Guofu WANG, et al. "Active Contour Model to the Inversion of Surface Nuclear Magnetic Resonance Data," *Journal of Computational Information Systems*, Vol. 11, No.2, pp. 719-726, 2015.

[3] Hairu Zhang, Shan Ouyang, Jingjing Li, et al. "A High-Performance Waveform Inversion Method of GPR Data for Stratified Media Reconstruction," *Electronic Journal of Geotechnical Engineering*, 2015 (20.S) pp 11803-11814. Available at ejge.com.

[4]Yaramanci U., Legchenko A., Roy J.. "Magnetic Resonance Sounding," *Journal of Applied Geophysics*, Vol. 66, No. 3, pp. 71-72, 2008.

[5] Legchenko A., Descloitres M., Vincent C., et al. "Three-dimensional magnetic resonance imaging for groundwater," *New Journal of Physics*, Vol. 13, No. 025022, pp. 1-17, 2011.

[6] Mohnke, O., Yaramanci, U.. "Smooth and block inversion of surface NMR amplitudes and decay times using simulated annealing," *Journal of Applied Geophysics*., Vol. 50, No. 1–2, pp. 163–177, 2002.

[7] DAI Miao, HU Xiangyun, WU Haibo, et al. "Inversion of surface nuclear magnetic resonance for groundwater exploration," *Chinese Journal of Geophysics*, Vol. 52, No. 5, pp. 1166-1173, 2009.

[8] Mueller-Petke M., Yaramanci U.. "QT inversion - comprehensive use of the complete surface NMR data set," *Geophysics*, Vol. 75, pp. 199–209, 2010.

[9] Ahmad A. B ehroozmand, Esben Auken, Gianluca Fiandaca, et al. "Efficient full decay inversion of MRS data with a stretched-exponential approximation of the T_2^* distribution," *Geophysical Journal International*, Vol. 190, pp. 900–912, 2012.

[10] Shou Guofa, Xia Ling, Jiang Mingfeng, et al. "Truncated Total Least Squares: A New Regularization Method for the Solution of ECG Inverse Problems," *IEEE Transactions on Biomedical Engineering*, Vol. 55, No. 4, pp. 1327-1335, 2008.

[11] Patra H. P., Mallick K.. "Geosounding principles 2--Time-retying Geolectric Soundings," *Netherland: Elesiver Scientific publishing*, 1980.

[12] Hsien-Hsin Chou, Ling-Yuan Hsu, Hwai-Tsu Hu. "Turbulent-PSO-Based Fuzzy Image Filter With No-Reference Measures for High-Density Impulse Noise," *IEEE Transactions on Cybernetics*, Vol. 43, No. 1, pp. 296-307, 2013.

[13] A. Guillen, A. Legchenko. "Inversion of surface nuclear magnetic resonance data by an adapted Monte Carlo method applied to water resource characterization, " *Journal of Applied Geophysics*, Vol. 50, pp. 193-205, 2002.

Editor's note.

This paper may be referred to, in other articles, as:

Hairu Zhang, Guofu Wang, and Faquan Zhang: "Non-linear Inversion for Surface Nuclear Magnetic Resonance Data in Layered Electrically Conductive Media" *Electronic Journal of Geotechnical Engineering*, 2016 (21.14), pp 4445-4457. Available at ejge.com.