GEMTIP inversion of complex resistivity data using a hybrid method based on a genetic algorithm with simulated annealing and regularized conjugate gradient method

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Summary

This paper demonstrates that an ellipsoidal model of the generalized effective-medium theory of induced polarization (GEMTIP) can be used to effectively invert complex resistivity (CR) data into petrophysical parameters of rocks, including matrix resistivity, volume fraction, etc. The inversion of the CR data has proven to be very challenging due to the nonuniqueness and instability of this problem. This paper introduces a new hybrid method based on a genetic algorithm with simulated annealing and regularized conjugate gradient minimization (SAAGA-RCG). This fast and effective approach combines the advantages of both the SAAGA and RCG methods and converges into the global minimum. The case study presents the results of inversion of the observed CR data and their comparison with a QEMSCAN analysis for representative mineral rock samples.

Introduction

The induced polarization (IP) effect has been used in mineral exploration (e.g., Pelton et al., 1978; Nelson, 1997) and in oil and gas prospecting for a long time (e.g., Zonge and Wynn, 1975; Pelton et al., 1978; Vanhala, 1997). Zhdanov (2008) introduced the generalized effective-medium theory of induced polarization (GEMTIP) using a rigorously formulated complex resistivity (CR) model to describe the relationships between the resistivity of the multiphase heterogeneous rocks and their petrophysical and structural properties.

The GEMTIP model can be used to study the petrophysical properties of rocks by inverting the CR data for the GEMTIP parameters. The inversion of CR data is a very challenging task because of the nonuniqueness and instability of this inverse problem. In this paper, we introduce a hybrid approach to inversion of the CR data for GEMTIP model parameters by combining the genetic algorithm with simulated annealing -- SAAGA -- at the initial phase of the iterative inversion with the regularized conjugate gradient (RCG) method at the final stage for rapid convergence to the global minimum. We demonstrate that the novel hybrid inversion algorithm is faster and more effective than the original SAAGA method, and it converges rapidly into the global minimum. We present a case study of inverting the observed CR data and a comparison of the results of the inversion with the OEMSCAN analysis of representative mineral rock samples.

GEMTIP model of a three-phase medium with ellipsoidal inclusions

The pertrophysical properties of the rock samples were analyzed using the GEMTIP model, developed by Zhdanov (2008). This theory makes it possible to present the effective resistivity as the function of geometrical and IP parameters of the rock - volume fraction of grains (f), average grain size (\overline{a}) , ellipticity of the grains (e), matrix resistivity (ρ_0), time constant (τ) , and decay coefficient (C). In the case of a three-phase medium with ellipsoidal inclusions, the GEMTIP model can be described by the following formula:

$$\rho_e = \rho_0 \{1 + \frac{1}{\sum_{l=1}^{2} \sum_{\alpha=x,y,z} \frac{f_l}{3\gamma_{l\alpha}} \left[1 - \frac{1}{1 + (i\omega\tau_l)^{C_l} \frac{\gamma_{l\alpha}}{2\overline{\alpha_l}\lambda_{l\alpha}}} \right] \}^{-1}, (1)$$

where \bar{a}_l is an average value of the equatorial $(a_{lx} \text{ and } a_{ly})$ and polar (a_{lz}) radii of the ellipsoidal grains. The coefficients $\gamma_{l\alpha}$ and $\lambda_{l\alpha}$ are the structural parameters defined by geometrical characteristics of the ellipsoidal inclusions (Zhdanov et al., 2009).

The GEMTIP equation (1) can be used to obtain the nonlinear relationships between the CR data and the GEMTIP parameters, which in compact form can be written as the following operator equation:

$$\mathbf{d} = \mathbf{G}_{IP}(\mathbf{m}).$$

(2)

In the last formula we denote by \mathbf{m} the vector of the unknown model parameters,

 $\mathbf{m} = [\rho_0, e_1, \tau_1, C_1, f_1, e_2, \tau_2, C_2, f_2], \quad (3)$ and vector **d** of the observed data is formed by the values of the CR resistivity at different frequencies, $\rho_{ei} = \rho_e(\omega_i)$ One has to solve the inverse problem (2) in order to find the GEMTIP parameters from the CR data.

Adaptive genetic algorithm with simulated annealing (SAAGA)

This section summarizes the adaptive genetic algorithm with simulated annealing (SAAGA). The SAAGA method is an iterative solver, which generates the best solution from the solution set (population) on each iteration using the genetic and annealing operations. The detailed steps of the SAAGA method are as follows:

1. Misfit functional

The GEMTIP inversion is based on minimization of the following misfit functional:

$$\varphi(\mathbf{m}) = \|\mathbf{d} - \mathbf{G}_{IP}(\mathbf{m})\|^2 = \min, \quad (4)$$

where a standard least-square norm is used; \mathbf{m} is the vector of unknown GEMTIP parameters (3), and \mathbf{d} is the vector of observed CR data.

2. Search subspace and search interval

The search subspace is selected from the model parameter space by determining the lower and upper bounds of the scalar components m_i of model \mathbf{m} , m_i^- and m_i^+ , respectively. The search intervals, $[m_i^-, m_i^+]$, for every scalar component, m_i , are divided into 2^{N_i} segments, where numbers N_i determine the total number of free parameters in the search subspace. In this paper, we use $N_i=10$, i=1,2,3,4, which means that the search space of each GEMTIP parameter is divided into 2^{10} segments.

3. Selection of initial population and individuals

A possible solution (called an individual) is randomly generated from the search subspaces for each GEMTIP parameter. Following the conventional technique of the GA algorithm, each scalar parameter, m_i , is encoded into the binary number. Then all the binary numbers for different scalar components of the vector **m** are connected into a string to form a binary representation of each individual.

Finally the above steps are repeated Q times, obtaining Q individuals, $\mathbf{m}^{(k)}$, k=1,2,...,Q, to form the initial population.

4. Fitness function

The fitness function is defined by the following expression:

$$f(k) = 1 / \sum_{l=1}^{Q} e^{\frac{\varphi(k) - \varphi(l)}{2\sigma}},$$
 (5)

where k=1,2,...,Q, $\varphi(k) = \varphi(\mathbf{m}^{(k)})$ is the misfit functional for the individual $\mathbf{m}^{(k)}$; and σ is the standard deviation of $\varphi(k)$ over the entire initial population.

5. Selection

The "roulette rule" is used to determine which individual should be selected. The chances are higher for the individuals which have larger fitness values. In the first step of this process, the fitness function is normalized as follows:

$$\tilde{f}(k) = \frac{f(k)}{\sum_{k=1}^{Q} f(k)}.$$
(6)

In the second step, the "roulette" space for each individual is defined by the following function:

$$s(k) = \sum_{j=1}^{\kappa} \tilde{f}(j).$$
⁽⁷⁾

In the third step, a randomly generated number a ($0 \le a \le 1$) is used to determine the reproduction chance for each individual. If $s(k) \le a < s(k)$, then the k^{th} individual will be selected. This step is repeated Q times to form a new generation with the same population size.

6. Crossover and mutation

In the framework of the GA method a new population is produced from the initial population by crossover and mutation operations (Whitley, 1994). It is well known that moderately large values of crossover probability, P_c $(0.5 < P_c < 1)$, and small values of mutations probability, P_m (0.001 < $P_m < 0.05$), are essential for the successful work of the GA methods. We also apply the adaptive genetic algorithm by adjusting the probabilities of crossover and mutation in each iteration (Srinivas and Patnaik, 1994).

7. Annealing operation

It is known that the convergence of the GA algorithm could be very slow. To overcome this difficulty, we have introduced the adaptive genetic algorithm combined with the simulated annealing (SA) method (Kirkpatrick et al., 1983), which can be described by the following steps:

a) Generate a new model set, $\mathbf{m}^{(n+1)} = \mathbf{m}^{(n)} + \Delta \mathbf{m}$, where $\mathbf{m}^{(n)}$ is the solution produced by the GA; and $\Delta \mathbf{m}$ is the perturbation (step) of this solution. A random search is applied to the current model $\mathbf{m}^{(n)}$ to produce the model, $\mathbf{m}^{(n+1)}$.

b) Calculate the fitness difference (Δt) between the new model and the current model:

$$\Delta t = f(\mathbf{m}^{(n+1)}) - f(\mathbf{m}^{(n)}), \qquad (8)$$

where *f* is the fitness function.

c) If $\Delta t > 0$, then we accept the new model $\mathbf{m}^{(n+1)}$; otherwise we accept this new model if:

$$a < e^{\Delta t/T_e},\tag{9}$$

where *a* is a random number generated from [0,1]; and T_e is the parameter of the SA method called *initial temperature*. d) In a simulated annealing method, one usually considers two additional parameters called *cooling velocity*: number of iterations, N_S , before the step, $\Delta \mathbf{m}$, is adjusted; and number of iterations, N_T , before the temperature, T_e , is reduced. After the SA iterations reach the second cooling velocity, N_T , the temperature, T_e , is reduced according to the following formula:

$$T_e = \lambda_T T_e, \tag{10}$$

where λ_T is the temperature reduction factor. We use $N_T=2$ and $\lambda_T=0.85$.

Regularized SAAGA method

The original formulation of the SAAGA method presented above was based on the direct minimization of the misfit functional (4) between the observed and predicted data. However, the GEMTIP inverse problem is ill-posed and minimization of the misfit between the observed and predicted data may result in an unstable solution (Zhdanov, 2002). In order to overcome the ill-posedness of the inversion, we apply the SAAGA method for minimization

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of the Tikhonov parametric functional with the minimum norm stabilizer,

$$P^{\alpha}(\mathbf{m}) = \|\mathbf{d} - \mathbf{G}_{IP}(\mathbf{m})\|^2 + \alpha \|\mathbf{W}_m \mathbf{m} - \mathbf{W}_m \mathbf{m}_{apr}\|^2,$$
(11)

where α is a regularization parameter, \mathbf{W}_m is the weighting matrix of the model parameters, and \mathbf{m}_{apr} is some a priori model selected based on all available rock physics data for the rock sample under consideration (Zhdanov, 2002).

A simple probabilistic interpretation of this approach is that, by using the Tikhonov parametric functional in the framework of the SAAGA method, we increase significantly the chances of selection for those individuals, whose GEMTIP parameters are close to the a priori model. Another important characteristic of the developed method is that the initial population has a normal distribution with the mean values close to the a priori values of the GEMTIP model parameters.

We apply the regularized adaptive genetic algorithm with simulated annealing (SAAGA) on the first phase of the solution of the GEMTIP inverse problem in order to overcome the presence of the local minima of the misfits functional. However, it is well known that the convergence of the GA and SA methods can be very slow. In order to speed up the convergence, we apply the regularized conjugate gradient method in the second phase of the iterative inversion to make the solution converge into a global minimum.

The stopping criterion for the first phase of the inversion is based on the condition that the difference of the misfits between the last several iterations is smaller than a given threshold value, *e*. Once the best individual from the population is "mature" enough to satisfy stopping criterion above, we apply the regularized conjugate gradient method to determine the global minimum.

Regularized conjugate gradient (RCG) method

The regularized conjugate gradient (RCG) method is an iterative process of finding the minimum of the parametric functional (11), by updating the model parameters on each iteration using conjugate gradient direction, \tilde{I}^{α} , according to the following formula:

$$\mathbf{m}_{n+1} = \mathbf{m}_n + \delta \mathbf{m} = \mathbf{m}_n - \widetilde{k_n^{\alpha}} \mathbf{l}^{\widetilde{\alpha}}(\mathbf{m}_n).$$
(12)

The conjugate gradient directions are given by the expression:

$$\mathbf{l}^{\alpha}(\mathbf{m}_{n+1}) = \mathbf{l}^{\alpha}(\mathbf{m}_n) + \beta_n^{\alpha} \mathbf{l}^{\alpha}(\mathbf{m}_{n-1}), \qquad (13)$$

In the initial step we use the direction of the regularized steepest ascent:

$$\mathbf{\tilde{l}}^{\alpha}(\mathbf{m}_0) = \mathbf{l}^{\alpha}(\mathbf{m}_0), \qquad (14)$$

The step length k_n^{α} is calculated based on the linear line search of the minimum of the corresponding parametric functional:

$$P^{\alpha}(\mathbf{m}_{n+1}) = P^{\alpha}[\mathbf{m}_n - \hat{k}_n^{\alpha} \mathbf{\tilde{l}}^{\alpha}(\mathbf{m}_n)] = \Phi(\hat{k}_n^{\alpha}) = \min.$$
(15)

Thus, the step length \tilde{k}_n^{α} can be determined based on the following expression:

$$\widehat{k_n^{\alpha}} = \frac{(\mathbf{l}_n^{\alpha}, \mathbf{l}_n^{\alpha})}{\left\|\mathbf{F}_n \widetilde{\mathbf{l}}_n^{\widetilde{\alpha}}\right\|^2 + \alpha \left\|\mathbf{W}_m \widetilde{\mathbf{l}}_n^{\widetilde{\alpha}}\right\|^2},\tag{16}$$

The coefficients β_n^{α} are computed as follows: $\beta_n^{\alpha} = \|\mathbf{l}^{\alpha}(\mathbf{m}_n)\|^2 / \|\mathbf{l}^{\alpha}(\mathbf{m}_{n-1})\|^2.$ (17)

The numerical scheme of the RCG method can be found in Zhdanov (2002)

Synthetic model study

The synthetic data set was obtained from the forward modeling considering a model formed by a homogeneous host rock filled with two types of grains with two grain sizes. It comprises a rock matrix with a resistivity of 200 Ohm-m and two inclusions with grain ellipticity of 1.0 and 4.0, respectively. The known values of the time constant, relaxation parameter, and the volume fraction of these two inclusions are 0.01, 0.9, 15% and 0.9, 0.9, 10%, respectively. The stopping criterion is set as the misfit of the imaginary effective resistivity is less than 0.5%.



The inversion stopped at the total iteration number of 228 (computation time = 220 s) with 0.48% misfit. Figure 1 presents both the synthetic and predicted resistivity curves for the three-phase ellipsoidal GEMTIP model plotted against frequency. Figure 2 shows the misfit plot of the imaginary resistivity versus the iteration number. The recovered GEMTIP parameters are very close to the true values, and the fitting of the synthetic data by the predicted data is good. Thus, the synthetic model study demonstrates

that the hybrid SAAGA algorithm with RCG method provides a robust solution of the inverse problem.



Case study

This section analyzes the experimental data obtained from a rock sample provided by the CEMI at the University of Utah. The complex resistivity data were measured over a frequency range from 10^{-2} to 10^{3} Hz. Also, the sample has been analyzed by the QEMSCAN system at the Department of Geology and Geophysics at the University of Utah to determine a variety of quantitative parameters of rock samples including the mineral distribution, volume fraction of different mineral grains, etc.

The rock sample was collected from a Cu-Au porphyry deposit. Figure 3, panel (a) shows a representative section of this sample produced by the QEMSCAN system. This sample contains 0.18% bornite, 0.13% chalcopyrite, and 6.64% pyrite. The two main grains in this sample are chalcopyrite and pyrite, which are shown by orange and yellow colors, respectively, in the section. It is known that bornite does not usually produce any IP effect; thus, the major sources of the IP response are the grains of pyrite and chalcopyrite with a total volume fraction of 6.77%.



The hybrid SAAGA algorithm with the RCG method was applied to recover the GEMTIP parameters for this sample. Figure 4 presents the plots of the observed and predicted imaginary parts of the CR data produced by the hybrid approach. Table 1 summarizes the inversion results for the final misfit of 3.5%. Note that, the difference between the recovered by GEMTIP inversion volume fractions and the results of the QEMSCAN analysis is below 2%.



Figure 4: Plots of the observed and predicted imaginary parts of the CR spectrum obtained using the hybrid regularized SAAGA algorithm with the RCG method.

$\rho_0(\Omega \cdot m)$		470.96	
Grain 1: Pyrite		Grain 2: Chalcopyrite	
e_1	3.72	<i>e</i> ₂	1.83
$\tau_1(s)$	5.46	$\tau_2(s)$	0.03
C_1	0.41	<i>C</i> ₂	0.64
$f_1(\%)$	4.58	$f_2(\%)$	1.80

Table 1: GEMTIP inversion results for the rock sample obtained using the hybrid regularized SAAGA algorithm with RCG method.

Conclusion

The three-phase ellipsoidal generalized effective-medium theory of induced polarization (GEMTIP) can be used to interpret the IP effect for multiphase rocks by inverting the complex resistivity (CR) data into the rock's induced polarization parameters. In this paper we have developed a novel hybrid approach which combines the SAAGA algorithm with the regularized conjugate gradient (RCG) method and is based on the minimization of the Tikhonov parametric functional, and the normal distribution for the initial population. The model and case studies indicate that this novel approach combines the advantages of both the SAAGA method and the RCG method, and the inversion converges rapidly into the global minimum.

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