



# On the adequacy of identified Cole–Cole models <sup>☆</sup>

Jianping Xiang<sup>a</sup>, Daizhan Cheng<sup>b</sup>, F.S. Schlindwein<sup>c,\*</sup>, N.B. Jones<sup>c</sup>

<sup>a</sup>Department of Geology, Central South University of Technology, Changsha 410083, People's Republic of China

<sup>b</sup>Institute of Systems Science, Chinese Academy of Sciences, Beijing 100080, People's Republic of China

<sup>c</sup>Department of Engineering, University of Leicester, Leicester LE1 7RH, UK

Received 3 November 2000; received in revised form 20 October 2002; accepted 1 November 2002

## Abstract

The Cole–Cole model has been widely used to interpret electrical geophysical data. Normally an iterative computer program is used to invert the frequency domain complex impedance data and simple error estimation is obtained from the squared difference of the measured (field) and calculated values over the full frequency range. Recently a new direct inversion algorithm was proposed for the ‘optimal’ estimation of the Cole–Cole parameters, which differs from existing inversion algorithms in that the estimated parameters are direct solutions of a set of equations without the need for an initial guess for initialisation. This paper first briefly investigates the advantages and disadvantages of the new algorithm compared to the standard Levenberg–Marquardt “ridge regression” algorithm. Then, and more importantly, we address the adequacy of the models resulting from both the “ridge regression” and the new algorithm, using two different statistical tests and we give objective statistical criteria for acceptance or rejection of the estimated models. The first is the standard  $\chi^2$  technique. The second is a parameter-accuracy based test that uses a joint multi-normal distribution. Numerical results that illustrate the performance of both testing methods are given. The main goals of this paper are (i) to provide the source code for the new “direct inversion” algorithm in Matlab and (ii) to introduce and demonstrate two methods to determine the reliability of a set of data before data processing, i.e., to consider the adequacy of the resulting Cole–Cole model.

© 2003 Elsevier Science Ltd. All rights reserved.

**Keywords:** Inversion algorithm; Induced polarization; Statistical methods; Ridge regression; Multi-normal distribution; Matlab

## 1. Introduction

The Cole–Cole model was first introduced for describing electrochemical reactions (Cole and Cole, 1941). Since then it has been widely used as a method to interpret electrical geophysical data: The spectral induced polarization (SIP) has been widely used in geological surveys. Interpretation is often based on the Cole–Cole model (Pelton et al., 1978; Luo and Zhang, 1998; He, 1996; Milson, 1996; He et al., 1995). The model can be described as (Major and Silic, 1981).

$$Z(\omega) = Z_0 \left\{ 1 - m \left[ 1 - \frac{1}{1 + (j\omega\tau)^c} \right] \right\}, \quad (1)$$

where  $Z(\omega)$  is the complex impedance at angular frequency  $\omega$  (in ohms),  $Z_0$  is the value of  $Z(\omega)$  at  $\omega = 0$  (ohms),  $m$  is the limited polarizability (also called chargeability),  $\tau$  is the time constant (s) and  $c$  is the frequency dependence factor.

The chargeability lies in the range  $0 \leq m \leq 1$ , and the requirement for the complex impedance to be a function whose amplitude monotonically decreases with increasing frequency restricts  $c$  to the range  $0 \leq c \leq 1$  (Major and Silic, 1981). To determine the Cole–Cole model four parameters,  $Z_0$ ,  $m$ ,  $\tau$ ,  $c$  must be estimated (Luo and Zhang, 1998). The existing methods for the estimation of these parameters are based on nonlinear iterative inversion (Luo and Zhang, 1998, Jaggar and Fell 1988), which

<sup>☆</sup>Code on server at <http://www.imag.org/CGEditor/index.htm>

\*Corresponding author.

E-mail addresses: dcheng@iss03.iss.ac.cn (D. Cheng), fss1@leicester.ac.uk (F.S. Schlindwein).

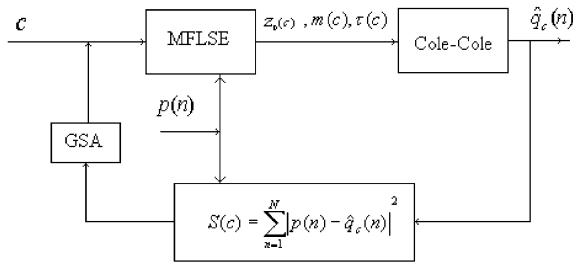


Fig. 1. Flow chart of direct inversion algorithm.

are based on the standard Levenberg–Marquardt ‘ridge regression’ algorithm.

Recently, Xiang et al., (2001) proposed a new algorithm, called the “direct inversion”, to identify the parameters in the Cole–Cole model. The algorithm consists of two essential parts: the first is the multi-fold least-squares estimation (MFLSE), which uses the assumed parameter  $c$  and the field data to estimate the other parameters,  $Z_0(c)$ ,  $m(c)$ ,  $\tau(c)$ . Part 2 is the Golden Section Algorithm (GSA), which is used to search the optimal value of  $c$  that minimizes the square error given by

$$S(c) = \sum_{n=1}^N [p(n) - \hat{q}_c(n)]^2.$$

The algorithm can be described with the help of the flow chart shown in Fig. 1. The new algorithm is robust when up to 0.1% noise is added to the original data. This is adequate for practical use.

In this paper, we start by applying both methods to previously published field data. Then the adequacy of the models obtained by both the old (Jaggar and Fell’s ridge regression) and the new (Xiang’s) algorithm is investigated by two different kinds of statistical testing. Finally, a further improvement for Xiang’s algorithm is presented. The Matlab source code for the Improved

coefficients of the Cole–Cole model of Eq. (1). In this section we briefly describe the algorithm.

Assume the field data of size  $N + 1$  given by  $\omega_i$ ,  $Z_i = Z(\omega_i)$ ,  $i = 1, \dots, N + 1$ . First, for a given  $0 \leq c \leq 1$ , we can calculate the best estimations of the parameters  $Z_0(c)$ ,  $m(c)$ ,  $\tau(c)$  by the following (Xiang et al., 2001).

1. Estimate  $\tau(c)$ :

$$\begin{aligned} A_k &= \frac{\cos(c\pi/2)\omega_k^c\omega_{k+1}^c}{\omega_k^c - \omega_{k+1}^c}, \\ C_k &= \frac{\sin(c\pi/2)\omega_k^c\omega_{k+1}^c}{\omega_k^c - \omega_{k+1}^c}, \\ D_k &= \frac{\omega_{k+1}^c}{\omega_k^c - \omega_{k+1}^c} \end{aligned} \tag{2}$$

and

$$B_k = R_k - D_k, \quad k = 1, \dots, N, \tag{3}$$

$$\tau^c := X = \frac{\sum_{k=1}^N (A_k B_k + I_k C_k)}{\sum_{k=1}^N (A_k^2 + C_k^2)}, \tag{4}$$

where  $R_k$  and  $I_k$  are the real and imaginary part of  $Z_k$ , respectively, i.e.,  $Z_k = R_k + jI_k$ ,  $k = 1, \dots, N$ .

2. Estimate  $Z_0(c)$ :

Calculate parameters  $\mu_k, \lambda_k, \phi_k, \varphi_k$ :

$$\frac{1}{Z_{k+1} - Z_k} = \mu_k + j\lambda_k, \quad \frac{Z_{k+1}}{Z_{k+1} - Z_k} = \phi_k + j\varphi_k. \tag{5}$$

Get intermediate variables:

$$P = \frac{\sum_{k=1}^N \frac{\omega_k^c \omega_{k+1}^c}{(\omega_k^c - \omega_{k+1}^c)} [\cos(c\pi/2)\mu_k + \sin(c\pi/2)\lambda_k]}{\sum_{k=1}^N \left( \frac{\omega_k^c \omega_{k+1}^c}{\omega_k^c - \omega_{k+1}^c} \right)^2}, \tag{6}$$

$$H = \frac{\sum_{k=1}^N \frac{\omega_k^c \omega_{k+1}^c}{(\omega_k^c - \omega_{k+1}^c)} \left[ \cos(c\pi/2)\phi_k + \sin(c\pi/2)\varphi_k + \cos(c\pi/2) \left( \frac{\omega_{k+1}^c}{\omega_k^c - \omega_{k+1}^c} \right) \right]}{\sum_{k=1}^N \left( \frac{\omega_k^c \omega_{k+1}^c}{\omega_k^c - \omega_{k+1}^c} \right)^2}, \tag{7}$$

new Xiang’s ‘direct inversion’ algorithm is publically available on the IAMG server.

## 2. Algorithm for identification of the Cole–Cole model

In a previous publication (Xiang et al., 2001) we derived in detail all the equations for the “direct inversion” technique to estimate the value of the

$$M(c) = \begin{pmatrix} A_k P - \mu_k \\ C_k P - \lambda_k \end{pmatrix} \quad k = 1, \dots, N, \tag{8}$$

$$L(c) = \begin{pmatrix} A_k H - \phi_k - D_k \\ C_k H - \varphi_k \end{pmatrix} \quad k = 1, \dots, N. \tag{9}$$

Finally, we have the multi-fold least-squares estimation as

$$Z_0(c) = [M^T(c)M(c)]^{-1}M^T(c)L(c). \tag{10}$$

3. Estimate  $m(c)$ :

$$m(c) = \frac{\sum_{k=1}^{N+1} \left| \frac{(j\omega_k\tau)^c}{1 + (j\omega_k\tau)^c} \left( \frac{Z_0 - Z_k}{Z_0} \right) \right|}{\sum_{k=1}^{N+1} \left| \frac{(j\omega_k\tau)^c}{1 + (j\omega_k\tau)^c} \right|^2}. \tag{11}$$

Using this set of parameters and the Cole–Cole model, a set of estimated data, which depends on the choice of  $c$ , is obtained as  $\hat{Z}_c(\omega_k)$ .

Secondly, the GSA (or any alternative minimization method) can be used to find the optimal value for  $c$  by minimizing the total square error

$$S(c) = \sum_{k=1}^{N+1} (Z_k - \hat{Z}_c(\omega_k))^2. \tag{12}$$

### 3. Brief comparison with ridge regression

The following 19-valued set of field data listed in Table 1 is from Jaggar and Fell (1988) and was used in our tests. We suspect that the last value on the phase ( $-7.930e+0$ ) and perhaps the penultimate for the amplitude are either typos on the original publication or outliers due to noise, but we left both untouched. Actually the fact that these values might be incorrect corresponds to additional noise introduced in the field data set. This makes some estimations of the Cole–Cole model invalid when using all data points ( $N = 19$ ) since the modelling techniques will attempt to fit the outliers as well as the ‘good’ data. This was one of the reasons that made us develop the techniques described in this paper for testing the adequateness of the estimated parameters (and therefore the resulting model), and associate to it a ‘level of confidence’.

Using the field data provided in Table 1, we can compare the results obtained by the new algorithm with those obtained by Jaggar and Fell (1988) using ridge-regression. The parameters estimated by using first  $N$  data values are given in Table 2 (Xiang et al., 2001).

The last row of Table 2 is the estimation obtained as suggested by Jaggar and Fell (1988). Note that the initial guess for Jaggar and Fell’s approach using  $N = 19$  is,  $c = 0.700$ ,  $Z_0 = 21.90$ ,  $\tau = 1.100e - 03$ ,  $m = 0.13$ .

To compare the accuracy of the resulting estimations, we used the square errors, as defined in Eq. (12), listed in Table 3.

In Table 3 there are three models for Xiang’s inversion ( $N = 13$ ,  $N = 16$ ,  $N = 17$ ) that provide a

Table 1  
Field data from Jaggar and Fell (1988)

Frequency (1/s)	Amplitude ( $\Omega$ m)	Phase (mrad)
1.000e−2	2.200e+1	0.000e+0
2.154e−2	2.199e+1	0.000e+0
4.642e−2	2.197e+1	0.000e+0
1.000e−1	2.198e+1	0.000e+0
2.150e−1	2.197e+1	0.000e+0
4.640e−1	2.196e+1	−1.52e+0
1.000e+0	2.195e+1	−3.36e+0
2.154e+0	2.191e+1	−6.11e+0
4.642e+0	2.184e+1	−1.049e+1
1.000e+1	2.172e+1	−1.637e+1
2.154e+1	2.154e+1	−2.483e+1
4.642e+1	2.124e+1	−3.248e+1
1.000e+2	2.083e+1	−4.014e+1
2.154e+2	2.036e+1	−3.856e+1
4.642e+2	1.996e+1	−3.319e+1
1.000e+3	1.961e+1	−2.953e+1
2.154e+3	1.940e+1	−1.746e+1
4.642e+3	1.927e+1	−1.980e+0
1.000e+4	1.884e+1	−7.930e+0

Table 2  
Estimated parameters via Xiang’s ‘‘direct inversion’’ of field data

Data size $N$	Estimated $c$	Estimated $Z_0$	Estimated $\tau$	Estimated $m$
12	0.6896	21.9901	0.0013	0.1235
13	0.6702	21.994	0.0010	0.1343
14	0.6812	21.992	0.0013	0.1223
15	0.6824	21.9902	0.0012	0.1226
16	0.6502	21.9907	9.4159e−004	0.1341
17	0.6502	21.9907	8.1710e−004	0.1373
19	0.691	21.90	1.165e−3	0.128

Table 3  
The comparison of model errors using first  $N$ -values of field data

Model	Overall error
Jaggar–Fell $N = 19$	0.3164
Xiang inversion $N = 12$	0.3250
Xiang inversion $N = 13$	0.1684
Xiang inversion $N = 14$	0.3732
Xiang inversion $N = 15$	0.3595
Xiang inversion $N = 16$	0.1682
Xiang inversion $N = 17$	0.1930

better estimation than the Jaggar–Fell model over all the 19 data values.

The advantage of the new ‘‘Xiang inversion’’ algorithm over the Jaggar–Fell’s ‘‘ridge regression’’ technique is the following.

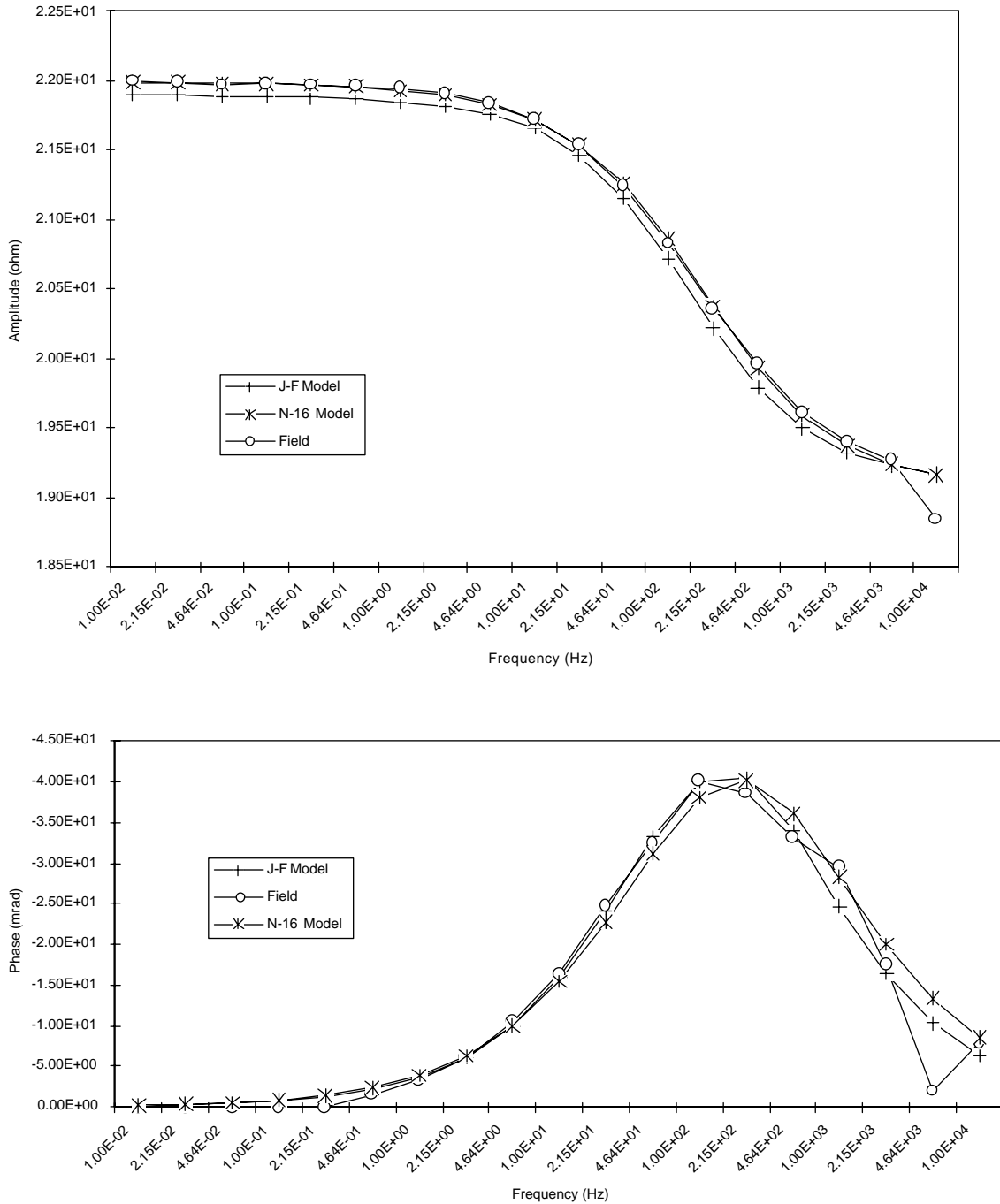


Fig. 2. Comparison of amplitude (top) and phase (bottom) of field data and results obtained by using Jaggar–Fell and Xiang’s methods. Note that points  $N = 18$  and  $19$  are outliers. Field data are directly from the listing published by Jaggar and Fell (1988). Note that phase is expressed in milliradians.

In the ridge regression, an initial estimation is found via forward modelling. This is then inverted iteratively for convergence. If convergence has not occurred the calculated parameters become the new initial estimates, and the iteration continues. The convergence and the

results depend heavily on this initial guess. The new algorithm does not need such initial guess. The inverted parameters are direct solutions to a set of equations.

From the previous tables and Fig. 2, one can clearly see that the last two data values ( $N = 18$  and  $19$ ) are

Table 4  
Estimated parameters with outlier-data values (Xiang’s inversion)

Data size $N$	Estimated $c$	Estimated $Z_0$	Estimated $\tau$	Estimated $m$	Error $s$
18	0.5725	21.9921	4.5647e-004	0.1555	0.5518
19	0.4392	21.9952	7.2398e-005	0.2282	2.5321

outliers. If the data set does contain some outlier points the Xiang algorithm might find (wrong) estimated values as listed in Table 4 for the situation where the last 2 points were included.

It seems that these two sets of parameters are not acceptable. This is a disadvantage of the new algorithm: it seems to be less robust to outliers than the classical regression technique. But neither the new nor the classical ‘ridge regression’ method produces a “confidence” level. A critical question that begs asking is “when is the estimation of the model parameters—and therefore, the model itself—obtained with the available (maybe noisy, maybe including outliers) data acceptable”? The major purpose of this paper is to consider the adequacy of the resulting Cole–Cole model.

#### 4. Adequacy of the estimated Cole–Cole model

In this section we use some standard statistics (Dobson, 1990) to test the adequacy of the Cole–Cole model. First, we assume the measurement error is approximately normal with zero mean and variance  $\sigma^2$

$$E = |Z_k - \hat{Z}_k| \sim N(0, \sigma^2). \tag{13}$$

We use the square error  $S$  as the statistic to minimise. Let us assume  $\sigma = 0.1$  (as the a priori information).

Then we can use a  $\chi^2$  distribution to test the adequacy of the model. That is,

$$\frac{S}{\sigma^2} \sim \chi^2(N). \tag{14}$$

Let the confidence level  $L$  be 0.9, 0.95, and 0.99, respectively. Then the critical values for rejecting the model from chi-square tables are listed in Table 5.

Using Tables 2 and 3, if we consider the first  $N$  data values for the modelling, but all available 19 values for the error calculation, we can conclude the following:

- With confidence level 0.90, we should reject the Jaggar–Fell model, and Xiang models with  $N = 12$ ,  $N = 14$ ,  $N = 18$ , and  $N = 19$ .
- With confidence level 0.95, we reject the Jaggar–Fell Model, and Xiang models with  $N = 12$ ,  $N = 14$ ,  $N = 18$ , and  $N = 19$ .
- With confidence level 0.99, we reject the Xiang models  $N = 14$ ,  $N = 18$ , and  $N = 19$ .

Table 5  
Critical values for rejecting Cole–Cole model

Model	$L = 0.90$	$L = 0.95$	$L = 0.99$
Xiang $N = 12$	0.18549	0.21026	0.26217
Xiang $N = 13$	0.19812	0.22362	0.27688
Xiang $N = 14$	0.21064	0.23685	0.29141
Xiang $N = 15$	0.22309	0.24996	0.30578
Xiang $N = 16$	0.23542	0.26296	0.32000
Xiang $N = 17$	0.24769	0.27587	0.33409
Xiang $N = 18$	0.25989	0.28869	0.34805
Xiang $N = 19$	0.27204	0.30144	0.36191

Using  $\chi^2$  testing for the Cole–Cole model, one critical point is to determine the variance  $\sigma$ . In this example we assumed  $\sigma = 0.1$ . With hindsight and checking the models and the field data it seems reasonable, but this choice was arbitrary and we have no evidence that this particular value would generally be adequate. Moreover, the purpose for the inversion is to identify the parameters for the Cole–Cole model. But the above statistical method ignored the roles played by the different parameters in the statistic. We therefore propose an alternative method to test the confidence of the estimated parameters. The technique is based on the estimation errors and considers the model we are trying to estimate.

#### 5. Adequacy investigation based on parameter errors

Let  $Z_0, m, \tau, c$  be the estimated parameters for a Cole–Cole model. We want to investigate the estimation errors. The problem becomes a standard inverse problem (Meju, 1994, Press et al., 1992, Tarantola, 1987, Menke, 1984). Assume the following: (A1)  $Z_0, m, \tau, c$  are the true parameters of the real model. Then we propose the statistic as  $\sqrt{S}$ . For a given confidence level  $L$  we seek a critical value  $E = E(L)$ , such that

$$P(\sqrt{S} > E) < 1 - L. \tag{15}$$

As long as the condition expressed by Eq. (15) holds, we reject (A1). That is, we should reject the resulting estimated Cole–Cole model.

Suppose the measured data are noisy. We may then treat the estimated parameters  $\hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}$  as random

variables and that they have normal distributions. The distributions are determined by a confidence level and the required accuracy. Say the required accuracy of  $Z_0$  is  $\mu_Z$ . Then the distribution of  $\hat{Z}_0 \sim N(Z_0, \sigma_Z^2)$  is determined by

$$P\left(\frac{|\hat{Z}_0 - Z_0|}{Z_0} \geq \mu_Z\right) \leq 1 - L_r. \tag{16}$$

If  $L_r = 0.90, 0.95,$  and  $0.99,$  then, from the table of the Normal distribution, we know that  $\mu_Z Z_0 / \sigma_Z = 1.64, 1.95$  and  $2.575,$  respectively. Then the distribution of  $Z_0$  is completely determined by  $L$  and  $\mu_Z$ . Similarly, the distributions of the other three parameters can be determined.

Since the parameter errors should be small enough, we can use a linear approximation

$$Z(\omega) - \hat{Z}(\omega) = \frac{\partial Z}{\partial Z_0} \Big|_0 (Z - \hat{Z}_0) + \frac{\partial Z}{\partial m} \Big|_0 (m - \hat{m}) + \frac{\partial Z}{\partial \tau} \Big|_0 (\tau - \hat{\tau}) + \frac{\partial Z}{\partial c} \Big|_0 (c - \hat{c}),$$

where

$$\frac{\partial Z}{\partial Z_0} = 1 - m \left(1 - \frac{1}{1 + (j\omega\tau)^c}\right),$$

$$\frac{\partial Z}{\partial m} = -Z_0 \left(1 - \frac{1}{1 + (j\omega\tau)^c}\right),$$

$$\frac{\partial Z}{\partial \tau} = -Z_0 m \frac{c(j\omega)^c}{[1 + (j\omega\tau)^c]^2 \tau^{1-c}}.$$

$$\frac{\partial Z}{\partial c} = -Z_0 m (\omega\tau)^c \frac{e^{\pi(-\sin(\pi c/2) + j \cos(\pi c/2))/2} + (\cos(\pi c/2) + j \sin(\pi c/2)) \ln(\omega\tau)}{[1 + (j\omega\tau)^c]^2}.$$

Now we construct a  $2(N + 1) \times 4$ -matrix  $F$  as

$$F_{2k-1,1} = \text{Re} \left[ \frac{\partial Z}{\partial Z_0}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right],$$

$$F_{2k-1,2} = \text{Re} \left[ \frac{\partial Z}{\partial m}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right],$$

$$F_{2k-1,3} = \text{Re} \left[ \frac{\partial Z}{\partial \tau}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right],$$

$$F_{2k-1,4} = \text{Re} \left[ \frac{\partial Z}{\partial c}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right],$$

$$F_{2k,1} = \text{Im} \left[ \frac{\partial Z}{\partial Z_0}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right],$$

$$F_{2k,2} = \text{Im} \left[ \frac{\partial Z}{\partial m}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right],$$

$$F_{2k,3} = \text{Im} \left[ \frac{\partial Z}{\partial \tau}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right],$$

$$F_{2k,4} = \text{Im} \left[ \frac{\partial Z}{\partial c}(\omega_k, \hat{Z}_0, \hat{m}, \hat{\tau}, \hat{c}) \right].$$

Let  $Y$  be the measurement error with separated real and imaginary parts, then it is easy to see that  $Y$  satisfies the following linear equations:

$$Y = F \begin{pmatrix} Z_0 - \hat{Z}_0 \\ m - \hat{m} \\ \tau - \hat{\tau} \\ c - \hat{c} \end{pmatrix}. \tag{17}$$

Then  $Y$  is a vector of random variables with a  $2 \times (N+1)$ -dimensional normal distribution. Moreover, the mean of  $Y$  is zero and the covariance matrix is (Tarantola, 1987, p. 210, Eq. 4.51)

$$\text{Cov}(Y) = F \text{Cov}(\sigma_{z_0}^2, \sigma_m^2, \sigma_\tau^2, \sigma_c^2) F^T.$$

We choose  $\sqrt{S}$  as a statistic. Note that  $\sqrt{S} = \sqrt{Y^T Y}$ .

It is difficult to test this high-dimensional normal distribution. But we may consider the worst direction, i.e., the one with largest variance. On this direction the edge distribution is  $N(0, \rho)$ , where  $\rho$  is the spectrum radius of  $\text{Cov}(Y)$ . It is obvious that if on this direction we can find a  $E$  such that

$$P(\sqrt{S} > E) < \frac{1-L}{2}. \tag{18}$$

Then the condition expressed by Eq. (15) holds everywhere. Of course, it is a conservative estimation. But it provides a confidence criterion to reject improper models.

Assume  $L = 0.90, 0.95,$  and  $0.99.$  Then, respectively,

$$E = 1.64\sqrt{\rho}, 1.95\sqrt{\rho}, 2.575\sqrt{\rho}.$$

Consider the above field data, now we have to determine  $\sqrt{\rho}$ . Again we need a priori information. We assume

$$Y \sim N(0, 0001FF^T). \tag{19}$$

Then with  $L_r = 0.99.$  We then have the results in Table 6.

So, under confidence levels 0.90 and 0.95, Xiang  $N = 18$  and  $N = 19$  models are rejected; under confidence level 0.99, Xiang  $N = 19$  Model is rejected.

Next, we assume the parameter errors are all 0.005 with  $L_r = 0.99.$  Then we have the results for the confidence test in Table 7.

Table 6  
Adequacy test with parameter error of 1%

Model and number points	$\sqrt{S}$	$E(L = 0.9)$	$E(L = 0.95)$	$E(L = 0.99)$
Jaggar–Fell $N = 19$	0.5625	0.5842	0.6982	0.9173
Xiang $N = 12$	0.0542	0.4820	0.5760	0.7567
Xiang $N = 13$	0.0602	0.4999	0.5974	0.7849
Xiang $N = 14$	0.0822	0.5164	0.6171	0.8107
Xiang $N = 15$	0.0874	0.5318	0.6355	0.8350
Xiang $N = 16$	0.1241	0.5464	0.6530	0.8579
Xiang $N = 17$	0.2191	0.5607	0.6697	0.8798
Xiang $N = 18$	0.7197	0.5742(Reject)	0.6862(Reject)	0.9015
Xiang $N = 19$	1.5912	0.5874(Reject)	0.7020(Reject)	0.9223(Reject)

Table 7  
Adequacy test with parameter error of 0.5%

Model	$\sqrt{S}$	$E(L = 0.9)$	$E(L = 0.95)$	$E(L = 0.99)$
Jaggar–Fell $N = 19$	0.5625	0.2921(Reject)	0.3491(Reject)	0.4586(Reject)
Xiang $N = 12$	0.0542	0.2410	0.2880	0.3784
Xiang $N = 13$	0.0602	0.2499	0.2987	0.3924
Xiang $N = 14$	0.0822	0.2582	0.3086	0.4054
Xiang $N = 15$	0.0874	0.2659	0.3178	0.4175
Xiang $N = 16$	0.1241	0.2732	0.3265	0.4289
Xiang $N = 17$	0.2191	0.2802	0.3348	0.4399
Xiang $N = 18$	0.7197	0.2871(Reject)	0.3431(Reject)	0.4508(Reject)
Xiang $N = 19$	1.5912	0.2937(Reject)	0.3510(Reject)	0.4611(Reject)

Now, under confidence level 0.90, 0.95, and 0.99, Jaggar–Fell Model, Xiang  $N = 18$  and 19 models are rejected.

**Remark.** The a priori information Eq. (19) is fundamental in the test. This assumption formally contains the more general case. But the motivation is from the following fact: Assume the parameter errors are all 0.01 and they are independent. As pointed by an anonymous reviewer, the independence of the parameters can not be assumed. Using the posterior covariance operator in data space (Tarantola, 1987, p. 210, Eq. (4.51)), the posterior covariance is not diagonal. An improvement is as follows: Using Tarantola’s equation (4.51) to calculate the posterior covariance matrix.

$$Cov_p(P) = Cov_p \begin{pmatrix} Z_0 - \hat{Z}_0 \\ m - \hat{m} \\ \tau - \hat{\tau} \\ c - \hat{c} \end{pmatrix}$$

to modify the a priori information Eq. (19), it yields  $Y \sim N(0, F Cov_p(P) F^T)$ .

Taking this as a priori information with some modification (based on more experimental knowledge), we can essentially avoid the assumption of uniform,

uncorrelated model-parameter error. But as the testing process remains unchanged.

### 6. Some improvements on Xiang’s approach

In later investigation, a shortcoming of new (Xiang’s) algorithm was exposed. Recall the overall quadratic error Eq. (12). The local minimum may not be unique. The numerical experience shows that there may be 1–3 or even more local minima. So the GSA may not be applicable to the whole interval  $c \in (0, 1)$ . A modification to resolve this is to divide the whole interval into several sub-intervals, say 10, and then using the GSA in each sub-interval. Finally, the overall minimum is obtained by comparing the minima on each sub-interval. In fact, the computation load is still light. The source code presented here incorporates such an improvement.

The main advantage of the new direct inversion algorithm proposed in Xiang et al., (2001) is that it does not need the initial estimation of the parameters. That does not mean that it always gives better results than ridge regression. In fact, if the initial value is good enough, ridge regression should reach better results. But for the Cole–Cole model, the ridge regression algorithm is too sensitive to the initial guess. In Jaggar and Fell’s (1988) approach, the initial guess is very close to the

optimal value. This suggests to us that the ridge regression algorithm may be used to further refine the results obtained by Xiang's new approach. Avoiding complex formulas, we sketch our improved algorithm as follows:

*Step 1:* Calculate the gradient of the overall error with respect to parameters as

$$G_0 = \text{grad}(S(z_0, m, \tau, c))|_{(z_0^0, m^0, \tau^0, c^0)}.$$

*Step 2:* Find a suitable small  $\delta > 0$  (such as Armijo step length, etc., which are standard in nonlinear programming), and then set new parameters

$$(z_0^1, m^1, \tau^1, c^1) = (z_0^0, m^0, \tau^0, c^0) - \delta G_0.$$

*Step 3:* Use the new parameters to get theoretical values of  $Z(\omega_i)$ , then go back to Step 1. Stop when the overall error is no longer reduced.

Detailed formulas are included in the source code. Using this method gave the best result in our previous work (refer to Table 3), i.e. for Xiang inversion  $N = 16$ . We can get an even better result:  $c = 0.645717$ ,  $Z_0 = 21.990231$ ,  $\tau = 9.359236e - 04$ ,  $m = 0.134683$ .

The overall error is  $S = 0.165957$ . Compare it with Table 3, one sees that the result has been improved (if only a little).

## 7. Conclusion

The new inversion algorithm introduced in Xiang et al. (2001) for identifying a Cole–Cole model was investigated. Based on the published field data and results provided by Jaggar and Fell (1988), a comparison between the new Xiang's inversion algorithm and the standard 'ridge regression' technique was completed. Two statistical methods are proposed to test the adequacy of the resulting Cole–Cole models. One is the standard  $\chi^2$  test. The other one uses a parameter-error based statistic with the assumption that the measured data have a joint multi-normal distribution. Numerical results show that both methods provide a reasonable criterion for testing the adequacy of the resulting Cole–Cole models, with the second technique having the advantages that no arbitrary decision has to be taken for the statistics of the measured data.

Finally, two improvements have been introduced: (1) using Golden Section on sub-intervals to avoid convergence to a local minimum, (2) using gradient algorithm to further improve the (Xiang's) direct inverse algorithm.

The following problems remain for further study: (1) More experimental data are needed for further study, particularly, for a priori information. (2) How to use the posterior information to improve the results.

## Acknowledgements

The authors would like to thank the financial support of the Royal Society of UK for funding J.X. We greatly appreciate the excellent critical proof reading, suggestions and constructive criticism by Dr. Max Meju. The authors also acknowledge Dr. Michael J Phillips for the excellent comments on the paper. The authors are also in debt to the anonymous referees for many constructive comments. Particularly, the connection of this work with the inverse problem theory.

## References

- Cole, K.S., Cole, R.H., 1941. Dispersion and absorption in dielectrics. I. alternating current field. *Journal of Chemical Physics* 1, 341–351.
- Dobson, A.J., 1990. *An Introduction to Generalized Linear Models*, 2nd Edition. Chapman & Hall, London, 192pp.
- He, J., 1996. Frequency domain electrical methods for searching resources of non-ferrous metals in China. *International Journal of the Society of Materials Engineering for Resources* 4 (1), 72.
- He, J., Li, D., Tang, J., 1995. Equivalent circuit of nonlinear effect of spectral IP. *Transactions of Nonferrous Metals Society of China* 5, 1–7.
- Jaggar, S.R., Fell, P.A., 1988. Forward and inverse Cole–Cole modelling in the analysis of frequency domain electrical impedance data. *Exploration Geophysics* 19, 463–470.
- Luo, Y., Zhang, G., 1998. Theory and application of spectral induced polarization. *Geophysical Monograph Series No. 8*, Society of Exploration Geophysicists, Tulsa, Oklahoma, 171pp.
- Major, J., Silic, J., 1981. Restrictions on the use of Cole–Cole dispersion models in complex resistivity interpretation. *Geophysics* 46, 916–931.
- Meju, M., 1994. *Geophysical Data Analysis: Understanding Inverse Problem Theory and Practice*. Society of Exploration Geophysicists, Tulsa, Oklahoma, 296pp.
- Menke, W., 1984. *Geophysical Data Analysis, Discrete Inverse Theory*. Academic Press, Orlando, FL, 260pp.
- Milson, J., 1996. *Field Geophysics*. Geological Society of London Handbook Series, Wiley, New York, NY, 198pp.
- Pelton, W.H., Ward, S.H., Hallof, P.G., Sill, W.R., Nelson, P.H., 1978. Mineral discrimination and removal of inductive coupling with multifrequency IP. *Geophysics* 43, 588–609.
- Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T., 1992. *Numerical Recipes in C*, 2nd Edition. Cambridge University Press, New York, 994pp.
- Tarantola, A., 1987. *Inverse Problem Theory, Methods for Data Fitting and Model Parameter Estimation*. Elsevier, Amsterdam, The Netherlands, 613pp.
- Xiang, J., Jones, N.B., Cheng, D., Schlindwein, F.S., 2001. Direct inversion of the apparent complex resistivity spectrum. *Geophysics* 66 (5), 1399–1404.