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Resistivity Inversion with Householder's Transformation

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Abstract: A Householder's transformation is applied to the resistivity inversion problem. The conventional resistivity inversion method is sometimes numerically unstable in interpreting a resistivity sounding data because it usually solves the normal equation derived from an observation equation. The resistivity inversion method using Householder's transformation solves the observation equation directly, so that it is numerically more stable than the conventional method. A theoretical, ill-conditioned Schlumberger sounding data was chosen to test the inversion scheme with Householder's transformation.

INTRODUCTION

Many recent papers have demonstrated the technique of determining the plane-layered earth by fitting model to field data. The technique called "resistivity inversion" or "automatic interpretation" uses a nonlinear least-squares method (Inman et al., 1973; Inman, 1975; Rijo et al., 1977; Pelton et al., 1978; Sasaki, 1981; Kim, 1981). Principal advantages of the resistivity inversion over the conventional curve matching are that the inversion method requires minimal interaction between interpretor and data, and gives statistics in estimating the accuracy of solutions.

The least-squares method has been widely used in geophysical problems. The conventional least-squares method, however, is sometimes numerically unstable in processing a large amount of data, because it usually solves the normal equation derived from an observation equation. The least-squares method which directly solves the observation equation is known to be more stable than the conventional method (e.g., Saito, 1983).

In this paper, a Householder's orthogonal transformation is applied to the inversion of resistivity sounding data. The Householder's transformation is used to solve the observation equation without converting it into the normal equation. In this paper, the usefulness of the resistivity inversion using Householder's transformation will be demonstrated by interpreting a theoretical Schlumberger sounding data. The theoretical data is generated by a four-layer earth model, and it contains approximately two percent random noise. All numerical results shown in this paper are computed in single precision arithmetic.

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NONLINEAR LEAST-SQUARES METHOD

In this section, only a brief summary of the least-squares inversion method is presented. More detailed discussions regarding geoelectrical applications have been given by Glenn et al. (1973) and Inman (1975). A description of the statistical estimates in geoelectrical soundings can be found in Glenn and Ward (1976).

Linear least-squares

An observation equation for least-squares problem is expressed by

$$\boldsymbol{Y}=\boldsymbol{A}\boldsymbol{X}+\boldsymbol{R}, \qquad (1)$$

where $\boldsymbol{Y}(y_i,\ i=1,\dots,n)$ is the vector of observed data, $\boldsymbol{A}(a_{ij},\ i=1,\dots,n$ and $j=1,\dots,m)$ the $n\times m$ matrix of coefficients or weights, $\boldsymbol{X}(x_j,\ j=1,\dots,m)$ the vector of parameters to be determined and $\boldsymbol{R}(r_i,\ i=1,\ldots,n)$ the vector of residuals. The least-squares problem should be overdetermined, i.e., $n>m$. The condition of least-squares is to minimize

$$\boldsymbol{R}^T\boldsymbol{R}=(\boldsymbol{Y}-\boldsymbol{A}\boldsymbol{X})^T(\boldsymbol{Y}-\boldsymbol{A}\boldsymbol{X}), \quad (2)$$

where the superscript T denotes transpose. Minimizing of (2) generates the following normal equation

$$(\boldsymbol{A}^T\boldsymbol{A})\boldsymbol{X}=\boldsymbol{A}^T\boldsymbol{Y}. \quad (3)$$

Since (3) is m simultaneous equations, a least-squares solution can be obtained, for example, by the Gaussian eliminate method. If the problem is exactly linear, only one determination of $\boldsymbol{X}$ will be necessary. All electrical sounding problems, however, are nonlinear and several iterations are required to obtain a satisfactory solution from a given initial guess.

Weighted least-squares

Thus far, it is assumed that the observed data contains an uniform error. This may be a rather poor assumption when one considers several data sets simultaneously. In such a case, the weighted least-squares method should be used, and (2) is rewritten by

$$\boldsymbol{R}^T\boldsymbol{W}^T\boldsymbol{W}\boldsymbol{R}=\min, \quad (4)$$

where $\boldsymbol{W}(w_i,\ i=1,\ldots,n)$ is the weight vector. The fraction of the standard deviation σ_i of each data is usually used as the weight, i.e.,

$$w_i=1/\sigma_i. \quad (5)$$

In this way, very noisy data do not contribute the same degree of influence over the inversion as relatively noise-free data.

In practice, it is convenient to transform variables as follows:

$$y_i'=y_i/\sigma_i,$$

and

$$a_{ij}'=a_{ij}/\sigma_i. \quad (6)$$

The variable transformation produces

$$\boldsymbol{Y}'=\boldsymbol{A}'\boldsymbol{X}+\boldsymbol{R}', \quad (7)$$

where $\boldsymbol{R}'$ is the new residual vector. Thus the weighted least-squares is reduced to a simple least-squares with the variable transformation.

Damped least-squares

Although (3) is exceedingly fast when it converges, it is unfortunately highly unstable and usually diverges unless the data error is small and the initial guess is very accurate. In order to ensure convergence from poor initial guesses, the normal equation (3) should be modified as

$$(\boldsymbol{A}^T\boldsymbol{A}+v^2\boldsymbol{I})\boldsymbol{X}=\boldsymbol{A}^T\boldsymbol{Y}, \quad (8)$$

where $\boldsymbol{I}$ is the identity matrix and v^2 the some positive quantity (Marquardt, 1963). This technique is known as Marquardt's method or damped least-squares method. If v^2 is very large, (8) approaches the gradient method, which is slow but always converges. At the other extreme, if v^2 is very small (8) approaches (3) of Gauss-Newton step, which is very fast but may diverge. Routines which carefully select an appropriate value for v^2 at each iteration in the inversion process are called ridge regression algorithm (Marquardt, 1963). Note that, even in the damped least-squares, all parameter statistics to be mentioned below must be calculated with $v^2=0$.

Parameter statistics

Once the inversion process produces a model which yields the best fits to the observed data, one can obtain an estimate of data variance from the reduced chi-square,

$$\chi^2=\boldsymbol{R}^T\boldsymbol{R}/(n-m), \quad (9)$$

where n is the number of data points, m the number of parameters and $(n-m)$ the degree of freedoms. From the estimate of data variance, the parameter covariance matrix $\boldsymbol{C}_v(c^v{}_{ij},\ i=1,\ldots,m$ and $j=1,\ldots,m)$ is given by

$$\boldsymbol{C}_v=\chi^2/(\boldsymbol{A}^T\boldsymbol{A}). \quad (10)$$

An estimate for the standard deviation of each parameter can be derived from the square root of the corresponding diagonal element of $\boldsymbol{C}_v$. Besides, the parameter correlation matrix $\boldsymbol{C}_r$ $(c^r{}_{ij},\ i=1,\ldots,m$ and $j=1,\ldots,m)$ can be obtained from the covariance matrix:

$$c^r_{ij}=c^v_{ij}/(c^v_{ii}c^v_{jj})^{1/2}. \qquad (11)$$

A linear relationship between two parameters is implied by a correlation coefficient with an absolute value near 1.0. In the resistivity inversion, a thin layer frequently produces a correlation very close to 1.0.

Cholesky's decomposition

The normal equation (3) or (8) can be solved by the Gaussian eliminate method. Since the coefficient matrix $\boldsymbol{A}^T\boldsymbol{A}$ or $(\boldsymbol{A}^T\boldsymbol{A}+v^2\boldsymbol{I})$ is symmetric and positive-definite, the solution of (3) or (8) can be obtained by symmetric Cholesky's decomposition with about half efforts compared with the Gaussian eliminate method. Details for the Cholesky's decomposition are given by Martin and Wilkinson (1965).

The Cholesky's decomposition is widely used in the least-squares fitting. When the number of parameters to be determined becomes large, however, the method using the Cholesky's decomposition is sometimes numerically unstable. Such an unstableness is demonstrated by solving the following example:

$$\begin{bmatrix} 1.0 & 0.5 & 0.333 & 0.25 \\ 0.5 & 0.333 & 0.25 & 0.2 \\ 0.333 & 0.25 & 0.2 & 0.167 \\ 0.25 & 0.2 & 0.167 & 0.143 \\ 0.2 & 0.167 & 0.143 & 0.125 \end{bmatrix} \boldsymbol{X}= \begin{bmatrix} 2.083 \\ 1.283 \\ 0.95 \\ 0.143 \\ 0.635 \end{bmatrix}. \qquad (12)$$

An accurate procedure of least-squares should produce $\boldsymbol{X}$ as

$$\boldsymbol{X}=[1.0,\ 1.0,\ 1.0,\ 1.0]^T. \qquad (13)$$

However the Cholesky's method gives

$$\boldsymbol{X}=\begin{bmatrix} 1.01097 \\ .888553 \\ 1.25500 \\ .839367 \end{bmatrix}. \qquad (14)$$

Although the solution (14) contains the maximum error of 25.5%, a substitution (14) into (12) shows that (14) is accurate in six significant decimal figures and all residuals are less than 10^{-6}. This result shows that, in the case of ill-conditioned matrix, the Cholesky's method may not give the correct solution even though the residuals are very small.

Householder's transformation

The Householder's orthogonal transformation is usually used in eigenvalue problems, and it can be also used in least-squares problems. The Householder's method usually gives more numerically stable solutions than the Cholesky's method. The Householder's method dose not solve the observation equation but the normal equation (Ralston, 1965).

Let's transform the coefficient matrix and the observed vector $\boldsymbol{Y}$ as

$$\boldsymbol{Q}^T\boldsymbol{A}=\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{0} \end{bmatrix}, \text{ or } \boldsymbol{A}=\boldsymbol{Q}\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{0} \end{bmatrix}, \qquad (15)$$

and

$$\boldsymbol{Q}^T\boldsymbol{Y}=\boldsymbol{Z}, \text{ or } \boldsymbol{Y}=\boldsymbol{QZ}, \qquad (16)$$

where

$$\boldsymbol{Q}^T\boldsymbol{Q}=\boldsymbol{I}, \qquad (17)$$

and $\boldsymbol{U}$ is the $m\times m$ upper triangular matrix, and $\boldsymbol{O}$ the $(n-m)\times m$ zero matrix. Form these the residual vector $\boldsymbol{R}$ is written by

$$\boldsymbol{R}=\boldsymbol{Y}-\boldsymbol{AX}=\boldsymbol{Q}\left(\boldsymbol{Z}-\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{O} \end{bmatrix}\boldsymbol{X}\right). \qquad (18)$$

Then the condition of least-squares is

$$\|\boldsymbol{R}\|^2=\boldsymbol{R}^T\boldsymbol{R}=\left\|\boldsymbol{Z}-\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{O} \end{bmatrix}\boldsymbol{X}\right\|^2, \qquad (19)$$

where $\|\ \|^2$ denotes the norm of argument. Here let's divide $\boldsymbol{Z}$ into two parts of $\boldsymbol{Z}_1$ and $\boldsymbol{Z}_2$ as

$$\boldsymbol{Z}=[\boldsymbol{Z}_1|\boldsymbol{Z}_2]^T=[z_1,\dots,z_m|z_{m+1},\dots,z_n]^T. \qquad (20)$$

Since

$$\boldsymbol{Z}-\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{O} \end{bmatrix}\boldsymbol{X}=\begin{bmatrix} \boldsymbol{Z}_1-\boldsymbol{UX} \\ \boldsymbol{Z}_2 \end{bmatrix}, \qquad (21)$$

(19) becomes

$$\|\boldsymbol{R}\|^2=\|\boldsymbol{Z}_1-\boldsymbol{UX}\|^2+\|\boldsymbol{Z}_2\|^2. \qquad (22)$$

Thus the condition of least-sequares becomes

$$\|\boldsymbol{Z}_1-\boldsymbol{UX}\|^2=\min, \text{ or } \boldsymbol{UX}=\boldsymbol{Z}_1. \qquad (23)$$

The residual of the least-squares solution $\boldsymbol{X}$ is given by

$$\|\boldsymbol{R}\|^2=\boldsymbol{R}^T\boldsymbol{R}=\|\boldsymbol{Z}_2\|^2, \qquad (24)$$

and the covariance matrix is obtained from (15) as

$$A^TA=[U^T,O]Q^TQ\begin{bmatrix}U\\O\end{bmatrix}=[U^T,O]\begin{bmatrix}U\\O\end{bmatrix}$$
$$=U^TU. \qquad (25)$$

Note that the Householder's method does not need to know $\boldsymbol{Q}$ explicitly. A detail procedure to compute $\boldsymbol{U}$ and $\boldsymbol{Z}$ is given by Ralston (1965).

The least-squares solution of (12) by means of the Householder's method is

$$X=\begin{bmatrix}.999999\\1.00002\\.999961\\1.00003\end{bmatrix}. \qquad (26)$$

This solution coincides with the true solution (13) in four significant decimal figures, and all residuals are less than 10^{-6}. Note that the Householder's method requires about two times more computations than the Cholesky's one.

RESISTIVITY INVERSION

In this section, I present a brief summary of the resistivity inversion with Householder's transformation used in this paper. Since the error in measurements of apparent resistivity (ρ_a) is usually a fixed percentage (2~3%) of ρ_a, it is expedient to transform immediately from ρ_a to log (ρ_a). The logarithmic tranformation then eliminates the requirement for a weight vector with elements inversely proportional to the magnitude of each measurement.

A further useful result is achieved by determining logarithmic resistivity and thickness instead of resistivity and thickness of each layer in the inversion process. This parameterization has the useful effect to exclude negative resistivity and thickness completely in possible solutions.

After transforming to logarithmic apparent resistivities $\boldsymbol{G}$ and logarithmic parameters $\boldsymbol{P}$, an approximate linear expression relating in $\boldsymbol{G}$ and $\boldsymbol{P}$ has the same form as (1), i.e.,

$$\Delta G=A\Delta P+R, \qquad (27)$$

where ΔG and ΔP are the changes in $\boldsymbol{G}$ and $\boldsymbol{P}$, respectively, $\boldsymbol{R}$ the residual vector and $\boldsymbol{A}$ the Jacobian matrix of derivatives with respect to parameters, i.e.,

$$a_{ij}=\frac{\partial g_i}{\partial p_j}\Big|_{P_0}, \qquad (28)$$

where P_0 is the initial guess. The solution of damped least-squares is given by (8), and it is expressed as

$$(A^TA+v^2I)\Delta P=A^T\Delta G \qquad (29)$$

As mentioned above, (29) is solved efficiently by the Cholesky's decomposition, but this procedure is sometimes numerically unstable.

In order to use the Householder's transformation, we must return to the observation equation. The least-squares problem equivalent to (29) can be written as

$$\begin{bmatrix}\Delta G\\O\end{bmatrix}=\begin{bmatrix}A\\vI\end{bmatrix}\Delta P+\begin{bmatrix}R\\O\end{bmatrix}. \qquad (30)$$

This equation is solved by Householder's transforming $\begin{bmatrix}A\\vI\end{bmatrix}$, and its solution is usually numerically more stable than the solution obtained from the Cholesky's method.

NUMERICAL EXPERIMENT

In this section, the method of resistivity inversion with Householder's transformation is illustrated by using a theoretical Schlumberger sounding curve. Fig. 1 shows the theoretical Schlumberger curve and its associated four-layer model. The theortical four-layer model is made by modifying the model of Inman (1975, Fig. 8).

Fig. 2 shows the partial derivatives of logarithmic apparent resistivities with respect to logarithmic parameters of the four-layer model. Since the third layer is too thin, the curves of $\partial\ln\rho_a/\partial\ln\rho_3$ and $\partial\ln\rho_a/\partial\ln d_3$ are nearly similar over the whole range. This means that the corresponding two column vectors in $\boldsymbol{A}$ become

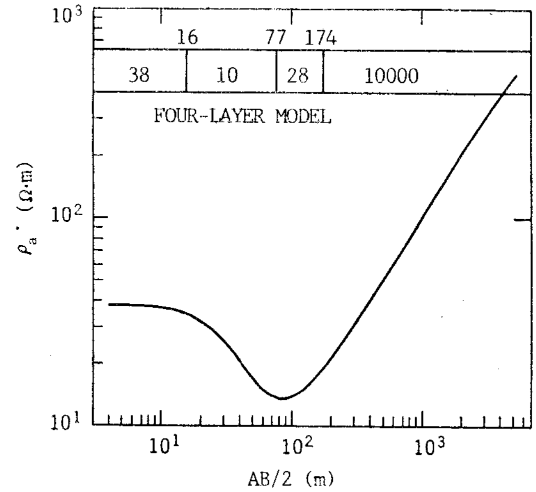

Fig. 1 A theoretical Schlumberger sounding curve and its associated four-layer model.

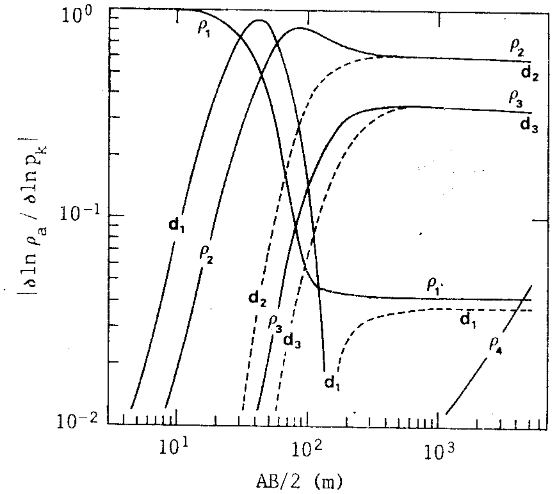

Fig. 2 Partial derivatives of apparent resistivity with respect to the parameters of four-layer model. The parameter p_k consists of ρ_1, ρ_2, ρ_3, ρ_4, d_1, d_2 and d_3. The solid and dashed lines represent positive and negative values, respectively.

almost linearly dependent. Hence the $(A^TA)^{-1}$ may be contaminated easily by round-off errors. Moreover, the maximum value of $\partial \ln\rho_a/\partial \ln\rho_4$ is much smaller than that of other curves. This means that the contribution of ρ_4 to ρ_a is very small. In other words, a small change of ρ_a leads a large change in the estimation of ρ_4, so that a noise involved in data significantly affects the estimation of ρ_4. As a result, the Jacobian matrix A is an ill-conditioned matrix.

Table 1 Relative errors between $(A^TA)^{-1}$ calculated by the Cholesky's method and that by the Householder's method for a four-layer model: $E_{ij}=(C_{ij}-H_{ij})/H_{ij}\times 100(\%)$, where E is the relative error, and C and H represent the $(A^TA)^{-1}$ calculated by the Cholesky's and Householder's methods, respectively.

i	*j*						
	1	2	3	4	5	6	7
1	.0000	.0704	.2397	−.1205	−.0471	.1697	.7210
2		.1402	.2086	−29.76	.1570	.1635	.2669
3			.1981	.2099	.2193	.2052	.1884
4				.0181	−4.582	.3430	.0687
5					.0939	.1827	.3025
6						.1365	.2253
7							.1837

Table 1 shows the relative error matrix between $(A^TA)^{-1}$ calculated by the Cholesky's method and that by the Householder's method for the four-layer model. An element of the relative error, E_{ij}, is calculated by

$$E_{ij}=(C_{ij}-H_{ij})/H_{ij}\times 100(\%), \qquad (31)$$

where C and H indicate the element of $(A^TA)^{-1}$ calculated by Cholesky's and the Householder's methods, respectively. Here the Cholesky's method is the one which solves the normal equation derived from the observation equation using the Cholesky's decomposition, and the Householder's method is the one which directly solves the observation equation using the Householder's transformation. From this table, one can find that the maximum relative error reaches to about 30%. As mentioned above, the Householder's method is numerically more stable than the Cholesky's method.

Based on the theoretical four-layer model, the Schlumberger sounding curve was calculated at 22 data points, and then approximately two percent Gaussian noise was added. This sounding curve is analyzed by the resistivity inversion

Table 2 Results of the interpretation of a data set with 2% normal noise for a four-layer model.

	Given value	Initial guess	Estimated value	Relative error (%)	Standard deviation (%)
ρ_1	8	40	37.61	−1.0	0.6
ρ_2	10	6	9.68	−3.2	8.6
ρ_3	28	50	30.59	9.3	134.7
ρ_4	10000	5000	13521	35.2	52.5
d_1	16	20	16.34	2.1	3.6
d_2	61	50	59.48	−2.5	54.3
d_3	97	150	106.4	9.7	28.0

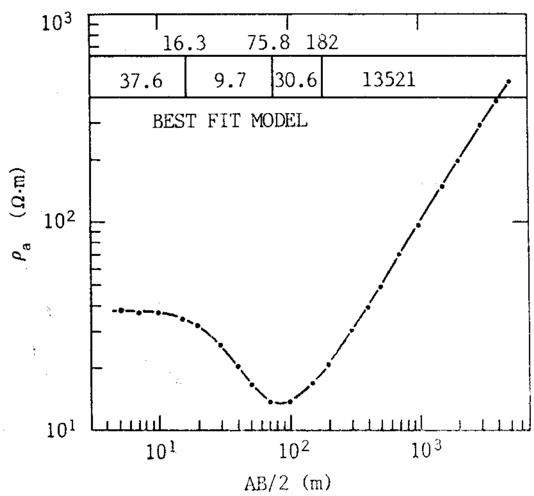

Fig. 3 Theoretical data, best fit curve and interpreted four-layer model.

Table 3 Correlation matrix for the solution in Table 2.

	ρ_1	ρ_2	ρ_3	ρ_4	d_1	d_2	d_3
ρ_1	1.0	.26	.11	.01	−.41	.16	.03
ρ_2		1.0	.87	.28	−.96	.94	.69
ρ_3			1.0	.40	−.79	.98	.94
ρ_4				1.0	−.25	.36	.52
d_1					1.0	−.87	−.61
d_2						1.0	.87
d_3							1.0

technique with Householder's transformation.

Table 2 shows results of the resistivity inversion for a given initial guess. The initial guess was obtained from rough interpretation with conventional curve-matching method, and it has a 50 percent error in maximum. The final estimated model is close to the original model except for estimation which has a reatively large error of about 35%. The residual variance estimated by Eq. (9) is 1.4×10^{-4}, which indicates an estimated error of 1.2 percent in the final fit. This value shows that the final fit is fairly good. Fig. 3 shows the curve of final fit and its associated best fit model. The standard deviations given by the square roots of the diagonal terms of the parameter covariance matrix, Eq. (10), are also shown in Table 2. Since a large resistivity jump exists between third and fourth layers, the standard deviation of ρ_3 is quite large.

Table 3 shows the correlation matrix for the parameters of the estimated model. The correlation matrix indicates a strong correlation between ρ_3 and d_2. Finally, it should be noted that a final model for the same example cannot be obtained by the inversion method using Cholesky's decomposition due to round-off errors.

DISCUSSION AND CONCLUSION

The Cholesky's decomposition is widely used in resistivity inversion problems because of its computational efficiency. When the number of parameters to be determined becomes large, however, the method using the Cholesky's decomposition is sometimes numerically unstable due to round-off errors. The method using the Householder's orthogonal transformation, however, is numerically more stable than that using Cholesky's decomposition. Such a stableness was demonstrated by solving the ill-conditioned matrix (12).

The Householder's method is less efficient than the Cholesky's one. In the resistivity inversion, however, the length of time for solving an observation equation is negligibly small compared with that for constructing it. In other words, time consuming parts are not backward process but forward process. Since a typical resistivity inversion requires several thousand forward problem evaluations, the length of time required to calculate one apparent resistivity is very important. Therefore, digital linear filter methods (Ghosh, 1971a and 1971b) is usually applied to estimate the apparent resistivity. In this paper, Anderson's adaptive J_1 filter (Anderson, 1979; Kim, 1985) was used to compute the Schlumberger apparent resistivity.

It is preferable to evaluate the derivative matrix from the analytical expression for each derivative. Although this approach may produce more accurate entries in $\boldsymbol{A}$, it involves a considerable increase in programming (Johansen, 1975; Kim, 1981). Rijo et al. (1977) showed that the logarithmic transformation and parameterization result in a sufficient linearization of the problem such that the derivatives may be evaluated numerically, by taking only first forward difference, with minimal loss in accuracy. In my procedure, two kinds of numerical differences are adopted to increase accuracy further: forward differences in early stage of iterations and central differences in late stage. This approach not only excludes additional routines for evaluating the integral encountered in the analytical derivative, but also has a sufficient accuracy.

Using the resistivity inversion method, it is possible to find a model that fits the data, to measure the accuracy of the fit by indicating relative level of noise in the data, and to predict the accuracy with which each parameter is estimated. This is certainly an improvement over most other methods because they are rarely able to indicate the range of models that will fit the data with a given degree of confidence. It is important to note that the resistivity inversion method always requires some geologic informations: an initial guess.

Although the one-dimensional resistivity inversion was discussed in this paper, the technique using the Householder's transformation can be applied to two and three-dimensional resistivity inversions. In the two-dimensional inversion, numerical solutions for the forward problem are based on the finite-element method (Sasaki, 1981), the finite-difference method (Smith and Vozoff, 1984), and the transmission-surface analogy (Tripp *et al.*, 1984). Good initial estimates of model parameters are also crucial for the success of two-dimensional interpretation, but it is more difficult to obtain them than in the case of one-dimensional ones.

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Householder 변환을 이용한 비저항반전

김 희 준*

요약 : Householder변환을 비저항반전 문제에 응용하여 해의 안정성을 조사하였다. 비저항탐사의 데이터를 해석할 때, 정규방정식을 통하여 지하구조모델을 구하는 종래의 비저항반전법은 수치적으로 불안정성을 야기시킬 경우가 간혹 있다. 이에 반하여 관측방정식의 해를 직접 구하는 Householder변환을 이용한 비저항반전법은 종래의 방법보다 수치적으로 더 안정하다. 본 논문에서는 Householder변환을 이용한 비저항반전법이 종래의 방법으로는 안정된 지하구조모델을 구할 수 없을 정도로 잡음이 포함된 이론적인 Schlumberger탐사 데이터의 경우에도 안정된 모델을 구할 수 있음을 보여 주었다.

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