Rapid least-squares inversion of apparent resistivity pseudosections by a quasi-Newton method

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Abstract

A fast inversion technique for the interpretation of data from resistivity tomography surveys has been developed for operation on a microcomputer. This technique is based on the smoothness-constrained least-squares method and it produces a two-dimensional subsurface model from the apparent resistivity pseudosection. In the first iteration, a homogeneous earth model is used as the starting model for which the apparent resistivity partial derivative values can be calculated analytically. For subsequent iterations, a quasi-Newton method is used to estimate the partial derivatives which reduces the computer time and memory space required by about eight and twelve times, respectively, compared to the conventional least-squares method. Tests with a variety of computer models and data from field surveys show that this technique is insensitive to random noise and converges rapidly. This technique takes about one minute to invert a single data set on an 80486DX microcomputer.

Introduction

Electrical tomography surveys can be used to map areas with complex subsurface geology where conventional resistivity sounding or profiling surveys are inadequate (Griffiths and Barker 1993). Such surveys normally employ a number (25 or more) of electrodes laid out on a straight line with a constant spacing (Fig. 1). A computer-controlled system is then used to select automatically the active electrodes used for each measurement (Griffiths, Turnbull and Olayinka 1990). The data from these surveys are commonly arranged and contoured in the form of a pseudosection (Hallof 1957), which gives an approximate picture of the subsurface resistivity. However, an inversion of the data is required to obtain a more accurate model of the subsurface resistivity.
One approach used to interpret the data is trial-and-error forward modelling with two-dimensional (2D) earth models using the finite-difference or finite-element method. However, this approach is time consuming and requires an experienced geophysicist. Furthermore, the model obtained could suffer interpreter bias.

Thus much research has been carried out on the use of automatic inversion techniques (Smith and Vozoff 1984; Tripp, Hohmann and Swift 1984). These commonly use a non-linear optimization technique to improve a simple starting model. The Gauss–Newton least-squares optimization method has been widely used and it has proved to be a robust technique which converges rapidly (deGroot-Hedlin and Constable 1990; Sasaki 1992). However, the main disadvantage of this technique is the large amount of computing time required. For this reason, it is commonly carried out on mainframe or workstation computers. The computing resources needed are often not conveniently available, particularly to small geophysical companies involved in mineral, hydrological and engineering surveys, and so it is not practical to carry out this type of 2D modelling in the field during the course of a survey. Thus, for 2D resistivity surveys to be more widely used, an inversion technique which is sufficiently fast when used on commonly available microcomputers is needed.

The least-squares and other gradient-based optimization techniques require the calculation of the apparent resistivity partial derivatives (Lines and Treitel 1984). The calculation of the partial derivatives can be time consuming. The use of a quasi-Newton technique (Broyden 1972) which avoids the direct calculation of the partial derivatives is examined in this paper.

Brief descriptions of the Gauss–Newton least-squares and quasi-Newton methods are given in the following section. This is followed by a discussion on ways to reduce the computational time required by the finite-difference or finite-
element method to calculate the apparent resistivity values. A simple inversion scheme using the quasi-Newton method is then described. The proposed technique is completely automatic and it does not even require the user to supply a starting model. Finally, the results from several tests with this technique, including comparisons with the conventional least-squares method, are given.

**Method**

*Smoothness-constrained least-squares method*

The model used, which consists of a number of 2D rectangular blocks, is shown in Fig. 2. We have adopted the model used by Barker (1992), where the blocks are equal in number to the data points in the apparent resistivity pseudosection and are arranged in a similar manner. The depths to the centres of the interior blocks are placed at the median depth of investigation (Edwards 1977) for the different electrode spacings used. The median depth of investigation is about 0.5 times the electrode spacing for the Wenner array. In some cases, slightly better results can be obtained by using a model with thinner blocks near the surface and thicker blocks near the bottom (Loke 1994).

The conventional Gauss-Newton least-squares method (Lines and Treitel 1984) can be used to determine the resistivity of the rectangular blocks (the model parameters) that will minimize the differences between the calculated and measured apparent resistivity values. We start with an initial model for the subsurface and try to improve this model in an iterative manner. The smoothness-constrained modification to the Gauss–Newton method (deGroot-Hedlin and Constable 1990) leads to the following system of normal equations:

\[
\left( J_i^T J_i + \lambda_i C^T C \right) \rho_i = J_i^T g_i,
\]

(Fig. 2) Arrangement of rectangular blocks used in the 2D model.
where $i$ is the iteration number, $\mathbf{J}_i$ is the Jacobian matrix of partial derivatives, $\mathbf{g}_i$ is the discrepancy vector which contains the differences between logarithms of the measured and calculated apparent resistivity values, $\lambda_i$ is the damping factor and $\mathbf{p}_i$ is the perturbation vector to the model parameters for the $i$th iteration. The 2D flatness filter $\mathbf{C}$ is used to constrain the smoothness of the perturbations to the model parameters to some constant value (Sasaki 1992). The logarithms of the apparent and model resistivity values are normally used in resistivity problems.

The value of the damping factor $\lambda$ depends on the level of random noise present in the data (Sasaki 1992). A larger value of $\lambda$ is used for higher levels of noise. For blocks of equal size, the partial derivatives associated with a block become smaller with increasing depth of the block. The amplitude of the elements of the flatness filter matrix $\mathbf{C}$ are increased by about 10% for each deeper row to stabilize the inversion process. The matrix $\mathbf{C}^T \mathbf{C}$ is symmetric and very sparse. The computing time and memory space required can be significantly reduced by storing the elements of this matrix in a sparse matrix format (George and Liu 1981).

The conventional least-squares inversion method may be divided into three main steps. The first step is to calculate the apparent resistivity values for the present model. The second step is to calculate the Jacobian matrix $\mathbf{J}$ of partial derivatives. The apparent resistivity and partial derivative values can be calculated using the finite-difference or finite-element methods (Smith and Vozoff 1984; Tripp et al. 1984). The third step is to solve the above system of linear equations. A number of numerical techniques, such as the modified Gram-Schmidt, Cholesky decomposition and singular value decomposition methods (Golub and van Loan 1989) can be used. The time taken to calculate the partial derivatives can be much longer than that taken by the other steps when there is a moderate (less than 500) number of data points.

**Quasi-Newton methods**

The Jacobian matrix $\mathbf{J}$ must be recalculated in each iteration in the conventional Gauss–Newton method. Quasi-Newton methods avoid the recalculation of the Jacobian matrix by using an updating method. The Jacobian matrix for subsequent iterations can be estimated by using an updating formula if the Jacobian matrix $\mathbf{J}_0$ for the starting model in the first iteration is available. The partial derivatives can be calculated analytically by using a homogeneous earth model as the starting model (McGillivray and Oldenburg 1990; Park and Van 1991). A very fast technique to obtain an approximate initial model for the subsurface with one iteration of the least-squares method by using a homogeneous earth starting model is described by Loke and Barker (1995). A detailed description of the calculation of the partial derivatives for the homogeneous earth model is also given in the same paper.

The Jacobian matrix $\mathbf{J}_i$ for the $i$th iteration is replaced by an approximation $\mathbf{B}_i$. 

The quasi-Newton method (Broyden 1965) uses the following updating equation:

\[ \mathbf{B}_{i+1} = \mathbf{B}_i + \mathbf{u}_i \mathbf{p}_i^T, \]  

(2)

where

\[ \mathbf{u}_i = \frac{\Delta \mathbf{y}_i - \mathbf{B}_i \mathbf{p}_i}{\mathbf{p}_i^T \mathbf{p}_i}, \]

\[ \Delta \mathbf{y}_i = \mathbf{y}_{i+1} - \mathbf{y}_i, \]

and \( \mathbf{y}_i \) is the model response for the \( i \)th iteration. The approximation of the Jacobian matrix \( \mathbf{B}_{i+1} \) for the \((i + 1)\)th iteration is calculated using the Jacobian matrix approximation \( \mathbf{B}_i \), the parameter perturbation vector \( \mathbf{p}_i \) and the change in the model response \( \Delta \mathbf{y}_i \) for the \( i \)th iteration. The updating matrix \( \mathbf{u}_i \mathbf{p}_i^T \) is a rank-one matrix and Broyden’s method is a rank-one quasi-Newton method (Scales 1985). The flop count for this updating method is proportional to \( n^3 \) (we use the definition by Sheriff (1991) where one flop is equal to one floating point multiplication and addition), where \( n \) is the number of data points. Thus it is much faster than the direct recalculation of the Jacobian matrix where the flop count is proportional to \( n^3 \). However, the convergence rate of Broyden’s method is slower than the Gauss–Newton method. It has a super-linear convergence rate compared to the quadratic convergence of the Gauss–Newton method (Burden, Faires and Reynolds 1981). In many applications the decrease in the convergence rate is more than compensated for by the reduction in the computational time for each iteration.

In order to calculate the parameter perturbation vector for the \( i \)th iteration using the quasi-Newton method, the following system of normal equations is used:

\[ (\mathbf{B}_i^T \mathbf{B}_i + \lambda \mathbf{C}_i^T \mathbf{C}_i) \mathbf{p}_i = \mathbf{B}_i^T \mathbf{g}_i. \]

(3)

It should be noted that several other quasi-Newton updating techniques, some of which might be more efficient than Broyden’s method for the 2D inversion of resistivity data, have been proposed (Dennis and Schnabel 1983). Broyden’s method was chosen because it has been widely used, it is stable and has a reasonably fast convergence rate for many non-linear problems (Broyden 1972; More and Trangenstein 1976).

The time taken to solve the system of normal equations can also be reduced by using matrix updating techniques (Golub and Van Loan 1989). The solution of the system of equations must be recalculated after each iteration in the conventional Gauss–Newton method. As an example, the Cholesky method (Schwarz et al. 1973) uses the decomposition

\[ \mathbf{J}^T \mathbf{J} = \mathbf{R}^T \mathbf{R}, \]

(4)

where \( \mathbf{R} \) is an upper triangular matrix. The estimated Jacobian matrix \( \mathbf{B}_{i+1} \) differs from the matrix \( \mathbf{B}_i \) for the previous iteration by a rank-one matrix. In this case, it is possible to calculate the matrix \( \mathbf{R}_{i+1} \) for the \((i + 1)\)th iteration from the \( \mathbf{R}_i \) matrix in...
the $i$th iteration (Golub and van Loan 1989). The flop count of the matrix updating technique is proportional to $n^2$, whereas the Cholesky method requires about $2n^3/3$ flops.

However, in most non-linear optimization schemes, the damping factor $\lambda$ is normally changed after each iteration (Scales 1985), especially during the first few iterations. Standard matrix updating techniques cannot be used if the damping factor is changed since the flatness filter matrix $C$ in the smoothness-constrained least-squares equation (3) has off-diagonal elements. The following updating method was used when the damping factor changes by making use of the fact that the solution of the least-squares equation by the Cholesky method consists of two main parts. In the first part, the matrix product

$$H = B^T \cdot B$$

is calculated. This operation requires about $n^3/2$ flops when the number of data points and model parameters are the same. We can make use of Broyden's updating formula to construct an updating formula for $H$ as follows:

$$B_{i+1}^{T} \cdot B_{i+1} = (B_{i}^{T} \cdot u_{i} \cdot p_{i}^{T})^{T} \cdot (B_{i}^{T} \cdot u_{i} \cdot p_{i}^{T})$$

$$= B_{i}^{T} \cdot B_{i} + (B_{i}^{T} \cdot u_{i}) \cdot p_{i}^{T} + p_{i}^{T} \cdot (B_{i}^{T} \cdot u_{i})^{T} + (u_{i}^{T} \cdot u_{i}) \cdot p_{i} \cdot p_{i}^{T}$$

which can be rewritten as

$$H_{i+1} = H_{i}^{T} + (B_{i}^{T} \cdot u_{i}) \cdot p_{i}^{T} + p_{i} \cdot (B_{i}^{T} \cdot u_{i})^{T} + (u_{i}^{T} \cdot u_{i}) \cdot p_{i} \cdot p_{i}^{T}.$$  

Thus the $H_{i+1}$ matrix can be calculated from the $H_{i}$ matrix in the previous iteration. The flop count for this updating method is proportion to $n^2$. This method is much faster than the direct calculation of $B_{i+1}^{T} \cdot B_{i+1}$ when $n$ is large. The second part of the Cholesky method, i.e. the factorization of $B_{i+1}^{T} \cdot B_{i+1}$ to determine $R_{i+1}$, involves $n^3/6$ flops. This updating method reduces the time taken by the Cholesky method by nearly three times. A similar partial updating scheme can also be devised for the modified Gram-Schmidt method.

Some care must be taken in using the Cholesky method when the number of data points and model parameters is large. The round-off errors for the Cholesky method are much larger than those for the modified Gram-Schmidt or singular value decomposition methods if the variables are stored in arrays with the same precision (such as single precision arrays). The elements of the $B^{T} \cdot B$ matrix are stored in an 8-byte double precision array (Lawson and Hanson 1974) to ensure that the Cholesky method has the same order of accuracy as the other methods. Only slightly more than half the elements are stored in the array since the matrix $B^{T} \cdot B$ is symmetric. The Cholesky method is used for most data sets where the sparsity of the flatness filter matrix product $C^{T} \cdot C$ can be more easily exploited. The calculations are repeated for some data sets using the modified Gram-Schmidt method to ensure that round-off errors are not a serious problem. The differences
in the results obtained by the two methods are less than 0.1%, which is not significant.

**Optimizing the finite-difference method**

When the partial derivatives are not required, the number of floating-point operations required by the finite-difference or finite-element technique can be reduced to a bare minimum so that the results are just sufficient to calculate the apparent resistivity values. The potential distribution $\phi(x,y,z)$ due to a current source $I(x,y,z)$ in a 2D earth model is given by Poisson’s equation

$$-\nabla \cdot [\sigma(x,z) \nabla \phi(x,y,z)] = I(x,y,z).$$  \hfill (8)

While the conductivity distribution $\sigma(x,z)$ is 2D, the current source is 3D (point). The 3D potential distribution $\phi(x,y,z)$ is reduced to a 2D transformed potential $\tilde{\phi}(x,k_y,z)$ by taking the Fourier transform of the above equation in the $y$-direction. This gives the equation

$$-\nabla \cdot [\sigma(x,z) \nabla \tilde{\phi}(x,k_y,z)] + k_y^2 \sigma(x,z) \tilde{\phi}(x,k_y,z) = I(x,k_y,z),$$  \hfill (9)

where $k_y$ is the Fourier transform variable. The finite-difference discretization (Dey and Morrison 1979) of (9) for each node in the 2D mesh (Fig. 3) gives rise to the matrix equation

$$A \tilde{\phi} = \nu,$$  \hfill (10)

where the capacitance matrix $A$ is an $N \times N$ symmetric sparse banded matrix ($N$ is the number of nodes), $\tilde{\phi}$ is a column vector with the transformed potentials and $\nu$ is the current vector. Equation (10) can be solved using the band-Cholesky method (Martin and Wilkinson 1965). This method first carries out the decomposition,

$$A = R^T R.$$  \hfill (11)
In order to determine the potential vector $\tilde{\phi}$, (10) is solved by using the forward substitution step

$$R^Tq = v$$

followed by the backward substitution step

$$R\tilde{\phi} = q.$$  \hspace{1cm} (13)

The transformed potential $\phi(x, k_y, z)$ is obtained for a number (usually five to ten) of $k_y$ values and an inverse Fourier transform is used to obtain the potential $\phi(x, y, z)$. When the electrodes are placed along a single profile, the inverse Fourier transform reduces to the integral

$$\phi(x, 0, z) = \frac{1}{\pi} \int_0^\infty \phi(x, k_y, z) \, dk_y,$$

which is evaluated by numerical quadrature. The partial derivative of the potential $\phi'$ is obtained by differentiating (10) with respect to the conductivity of the block, say $\sigma_j$, which gives

$$A^\prime \phi' = w,$$

where

$$w = -A^\prime \phi.$$  \hspace{1cm} (15)

The vector $w$ may be viewed as a fictitious current vector given by the product of the capacitance matrix differential $A'$ and the potential vector $\phi$ (Sasaki 1989).

Figure 3 shows part of a mesh used in this research to discretize the subsurface. The electrodes are placed 4 horizontal nodes apart. The nodes are numbered along columns (Dey and Morrison 1979) starting from the top left node. To the left of the first electrode there are 11 horizontal nodes where the spacing between the nodes is progressively increased so that the left edge of the mesh is sufficiently far from the first electrode. A similar arrangement is used to the right of the last electrode. The mesh used has 18 nodes in the vertical direction. Thus for a survey with 30 electrodes, the mesh has 139 by 18 nodes giving a total of 2502 nodes. To determine the apparent resistivity values measured with a multielectrode survey, it is most convenient to calculate first the potentials due to a single current electrode at the first electrode $E_1$. After that, the potentials due to a current electrode at $E_2$ are determined. This process is repeated for the other electrodes. The Cholesky decomposition in (11) is only carried out once since the capacitance matrix $A$ does not depend on the location of the current electrode. The forward and backward substitution steps in (12) and (13) are repeated to calculate the potentials due to each electrode.

Only the potentials at the nodes where the electrodes are located are needed to calculate the apparent resistivity values. Thus, for a single current electrode in a 30-electrode array, it is only necessary to calculate the potentials at 29 nodes (out of
a total of 2502 nodes). As an example, consider the case when the current electrode is at E1 in Fig. 3 and the data level is one (Fig. 1). The current vector \( \mathbf{v} \) then only has a single non-zero element, \( v_{199} \). Since the first 198 elements of the auxiliary vector \( \mathbf{q} \) in (12) are zero, only the 199th to the 2502nd elements of the \( \mathbf{q} \) vector have to be directly calculated. For the backward substitution step in (13), it is only necessary to carry out the calculations for the 217th (where the electrode \( E_2 \) is located) to the 2502nd elements of the \( \phi \) vector. When the current electrode is at \( E_3 \), the backward substitution step is carried out for the 235th node (with the \( E_3 \) electrode) onwards. Only the potentials at the nodes with numbers higher than or equal to the first electrode to the right of the current electrode are needed. By using the principle of reciprocity, the calculation of the potentials at the electrodes to the left of the current electrode can be avoided. Thus the times taken for the forward and backward substitution steps are progressively reduced as the current electrode is further away from the first electrode. In comparison, to determine the partial derivatives, the time taken by the backward substitution step cannot be reduced since the potentials at all the nodes must be calculated. They are needed in the calculation of the elements of the fictitious current vector \( \mathbf{w} \) in (15) which further increases the computing time.

The times taken for the forward and backward substitution steps become shorter as the node number of the current electrode becomes larger. This property can be more fully exploited by a judicious use of sparse matrix techniques (George and Liu 1981) to renumber the nodes so that the nodes with the electrodes end up with even higher numbers. For example, by using the alternate-diagonal method (Woo et al. 1976) and placing the electrodes on the even columns of nodes, all the electrodes will have node numbers that are higher than 1251 (compared to 199 for \( E_1 \) in Fig. 3). Even larger reductions in the computing time can be achieved by using more sophisticated sparse matrix techniques such the one-way dissection and nested dissection methods (George and Liu 1981).

The number of inverse Fourier transforms needed to calculate all the partial derivatives is much larger than that required to calculate the apparent resistivity values only. For a survey with 30 electrodes using a Wenner array with 8 levels of data in the pseudosection, 435 inverse Fourier transforms are needed to calculate the apparent resistivity values. In comparison, 45408 inverse Fourier transforms are required to calculate the partial derivatives. An optimized finite-difference program takes about 14 seconds to calculate the apparent resistivity values on a 33 MHz 80486DX microcomputer. In comparison, if the partial derivatives are calculated as well, it takes about 130 seconds.

**Practical procedure**

The main steps in a simple but effective algorithm using the quasi-Newton inversion method are described below. It is assumed that the only data available are the measured apparent resistivity values.
Step (a). Firstly some parameters that will guide the inversion process have to be chosen. An initial damping factor $\lambda_0$ and a minimum damping factor $\lambda_m$ for the least-squares method have to be selected. We have found that values of 0.20 and 0.04 for $\lambda_0$ and $\lambda_m$ give satisfactory results for most field data sets. The maximum number of iterations for the quasi-Newton inversion method should also be selected.

Some type of convergence criterion, such as a minimum rms error value, should be set. For field data sets where the exact noise level is usually not known, it is more convenient to use the change in the rms error $e_i$. This is given by

$$e_i = \left( e_i - e_{i+1} \right) / e_i,$$

(16)

where $e_i$ and $e_{i+1}$ are the rms errors for the $i$th and $(i+1)$th iterations. Normally the inversion process is stopped when $e_i$ is less than 5%.

Step (b). A homogeneous earth model is used as the starting model for the first iteration. The logarithm of the resistivity $r_0$ of this model is calculated by taking the average of the logarithms of the measured apparent resistivity values $f_i$ using the equation

$$r_0 = \frac{1}{n} \sum_{i=1}^{n} f_i,$$

(17)

where $n$ is the number of data points.

The Jacobian matrix $B_0$ is then calculated for the electrode array used from the partial derivatives which have been precomputed and stored in a disc file (Loke and Barker 1995). The least-squares equation (3) is then solved to determine the model parameter perturbation vector $p_0$. An estimate $r_1$ of the resistivity of the blocks is given by

$$r_1 = r_0 + p_0.$$

(18)

The apparent resistivity values for the new model are then calculated using the finite-difference method.

Step (c). Broyden’s method is used to update the approximation of the Jacobian matrix $B_{i+1}$ for the next iteration. Normally if the rms error has decreased in the previous iteration, the damping factor is reduced by half if it is still larger than the minimum value $\lambda_m$ set in step (a). If the rms error is larger than that for the previous iteration, a line search using quadratic interpolation is used in an attempt to find the optimum step size for the model parameter perturbation vector $p_i$. This will usually result in a model with a lower rms error. If this still does not work, the damping factor is increased and the vector $p_i$ is recalculated.

Step (d). The parameter perturbation vector $p_{i+1}$ is calculated by using the estimated Jacobian matrix $B_{i+1}$ in (3), after which a new model is obtained.

Steps (c) and (d) are repeated until the program converges or the maximum number of iterations is reached. A fairly simple strategy is used to change the damping factor after each iteration in this algorithm. This algorithm has worked
Figure 4. (a) Wenner array pseudosection due to a wide rectangular block. Inverse models obtained with (b) the Gauss–Newton method and (c) the quasi-Newton method. Note that a different contour interval is used for the apparent resistivity pseudosection. The depths to the centre of each row of the model blocks are shown in (b) and (c). The outline of the block is also shown for comparison.
fairly well in all the tests that we have carried out with computer-generated and field data sets. More sophisticated algorithms (Scales 1985) could be used for more problematical data sets.

Applications

Some of the results from the tests that we have carried out are given in this section. A comparison between the models obtained (as well as the computer time and memory required) by the conventional Gauss–Newton method and the quasi-Newton method is made in the first two examples. The tests were carried out on a 33 MHz 80486DX IBM PC compatible microcomputer with 4 megabytes of memory.

Example 1: Rectangular block model

Figure 4a shows the apparent resistivity pseudosection due to a wide rectangular block model with a resistivity of 500 $\Omega$m embedded in a medium of 100 $\Omega$m. The initial and minimum damping factors were set at 0.05 and 0.01, respectively, in the quasi-Newton method (5% noise) and the Gauss-Newton method (0% noise). The results are shown in Figure 5.

Figure 5. Error curves for the inversion of the rectangular block pseudosection data using the Gauss–Newton and quasi-Newton methods.
Table 1. A comparison of the number of iterations and the time taken by the Gauss-Newton (GN) and quasi-Newton (QN) methods to converge for different data sets. The exact rms error of the final model and the memory required by the finite-difference subroutine are also shown.

<table>
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<th>Data set</th>
<th>Inversion method</th>
<th>No. of iterations</th>
<th>rms error (%)</th>
<th>Time taken (s)</th>
<th>Memory required (Kilobytes)</th>
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</table>

inversion of this data set. Rather small damping factors can be used since this data set is noise free. The rms error convergence limit was set at 1%. The models obtained by the Gauss-Newton and quasi-Newton methods are shown in Figs 4b and c, respectively. There are no significant differences between the two models. The shapes of both models agree reasonably well with the actual shape of the block. The highest model resistivity value near the centre of the rectangular block is about 250 Ωm, which is less than the true value of 500 Ωm. This is partly a result of equivalence (Keller and Frischknecht 1966), where a thicker body with a lower resistivity contrast can give rise to the same anomaly as a thinner block with a higher resistivity contrast.

The quasi-Newton method takes 5 iterations to converge compared to 4 iterations for the Gauss-Newton method. Figure 5 shows the error curves for both methods in the inversion of this data set. In the first 3 iterations the Gauss-Newton converges at a slightly faster rate than the quasi-Newton method. However, after the 4th iteration the difference in the rms errors of the two methods is less than 0.2%. The slightly slower convergence rate of the quasi-Newton method is more than offset by the shorter time per iteration that it requires. The computer time and memory required by the two methods are shown in Table 1. The quasi-Newton method takes about 91 seconds to reduce the rms error to less than 1% compared to 691 seconds for the Gauss-Newton method. The finite-difference subroutine for the quasi-Newton program requires about 210 kilobytes to store all the arrays involved. In comparison, a similar subroutine for the Gauss-Newton program (which also calculates the partial derivatives) requires about 2370 kilobytes.

Gaussian noise (Press et al. 1988) with an amplitude of 5% was added to the apparent resistivity data to study the effect of noise on the inversion results. The resulting pseudosection (Fig. 6a) shows severe distortions. Since this data set has some noise, larger values of 0.20 and 0.04 were used for the initial and minimum
Figure 6. (a) Wenner array pseudosection due to a wide rectangular block with 5\% random noise. Models obtained with (b) the Gauss–Newton method and (c) the quasi-Newton method. The outline of the block is also shown for comparison.

The error curves (Fig. 5) show that the convergence rates for both methods are
Figure 7. (a) Stud Farm survey apparent resistivity pseudosection. Models obtained with (b) the Gauss–Newton and (c) the quasi-Newton methods. Locations of boreholes and observed depths to weathered microdiorite are indicated. Almost the same for the noisy data. There are no significant differences between the rms errors for the two methods from the 3rd iteration onwards. However, the quasi-Newton method requires only about one-ninth of the time taken by the Gauss–Newton method (Table 1).
Example 2: Stud Farm survey

This survey was carried out to map the thickness of the clay overburden along a proposed tunnel route to join a new microdiorite quarry at Stud Farm to another quarry at Cliffe Hill (Leicester) which is about 2 km away. The microdiorite is expected to have a resistivity of the order of several hundred ohm-metres, whereas the overburden has a resistivity of 25 to 80 Ωm (Turnbull 1986).

Figure 7a shows the apparent resistivity pseudosection from this survey where an electrode spacing of 25 m was used. The initial and minimum damping factors were set at 0.20 and 0.04 for this data set (as well as for the following examples). The error curves of the Gauss–Newton and quasi-Newton methods in the inversion of this pseudosection are shown in Fig. 8. The rms error for the Gauss–Newton method at the 1st iteration is higher than that for the quasi-Newton method. This is probably caused by small differences between the homogeneous earth model partial derivatives calculated numerically in the Gauss–Newton method and those calculated analytically in the quasi-Newton method. The rms error decreases...
rapidly in the first 4 iterations for both methods. After the 5th iteration, the relative change in the rms error is less than 5%. The models obtained at the 5th iteration by the two methods (Fig. 8) do not show any significant differences.

Both models show an undulating bedrock with a resistivity of over 200 Ωm covered by overburden material with a resistivity of less than 80 Ωm (Figs 7b and 7a).

Figure 9. (a) Blue Farm survey apparent resistivity pseudosection. (b) Model section obtained at the 5th iteration with the quasi-Newton method. (c) Schematic diagram of the subsurface geology from surface and borehole surveys.

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c). The microdiorite is known to be deeply weathered in places, so a gradational increase in the resistivity from the overburden to the fresh bedrock is expected. The two regions with higher resistivity material near the surface at the 450 and 650 m marks are probably due to boulders and partially weathered material. The depths to the weathered bedrock at four boreholes near the survey line are also shown. There is good agreement between the microdiorite topography in the models and the borehole depths at locations BH1 and BH2. The model bedrock interface is significantly deeper than the borehole depths at BH3 and BH4. One possible reason is that the boreholes record the top of the very weathered microdiorite and not the higher resistivity bedrock shown in the sections. Another possible reason is that the boreholes were sunk into core boulders (Turnbull 1986). Furthermore, it is known from other boreholes in this area that the bedrock topography is not 2D which could also account for differences between the models and the boreholes.

![Figure 10. Borehole resistivity log from a survey at Blue Farm. The model resistivity obtained by the quasi-Newton method along the borehole is also shown for comparison.](image)

The quasi-Newton method requires only about one-ninth of the computing time needed by the Gauss–Newton method to converge (Table 1). Perhaps more importantly, the finite-difference subroutine in the quasi-Newton program requires only about 240 kilobytes of memory compared to 2700 kilobytes for the Gauss–Newton program. It is possible to reduce the memory space required by saving some of the arrays temporarily in a disc file but this would substantially increase the computing time. This pseudosection (with 35 electrodes) is about the largest that can be efficiently processed by the Gauss–Newton program in a computer with only 4 megabytes of memory. In comparison, we have successfully processed pseudosections with 64 electrodes using the quasi-Newton program.

Example 3: Blue Farm survey

Figure 9a shows the apparent resistivity pseudosection from one of the surveys by Andrews (1993) at Blue Farm, Cambridgeshire. This was part of a study of the Magusi River orebody.

Figure 11. (a) Dipole-dipole apparent resistivity pseudosection for the Magusi River orebody survey. (b) Model section obtained at the 6th iteration by the quasi-Newton method. Note that the apparent resistivity pseudosection uses a different contour interval. The boundaries of the orebody and overburden (Edwards 1977) are also shown.
movement of nitrates through chalk covered with thin soil. The apparent resistivity pseudosection shows several prominent areas with high resistivity values of up to 120 $\Omega$m which extend to the 5th data level. Between the high resistivity zones there are areas with lower apparent resistivity values.

The model produced by the quasi-Newton method at the 5th iteration (Fig. 9b) shows that the source of the zones of high and low apparent resistivity values lies near the surface. This agrees with the known surface geology and borehole measurements. The geological and borehole data indicate that the resistivity anomalies are caused by variations in the thickness of a sand layer (with a maximum thickness of 2 m) overlying an undulating chalk bedrock (Andrews 1993). A schematic diagram of the subsurface geology is shown in Fig. 9c. Figure 10 shows the resistivity log obtained in a borehole at the 18 m mark. The borehole measurements were made using a Wenner array with a spacing of 0.3 m. The subsurface resistivity reaches a maximum value of about 120 $\Omega$m at a depth of about 3 m after which it slowly decreases with depth. The model resistivity values at the borehole location show the same general trend but with a smaller resistivity range. This is probably because the borehole measurements are mainly affected by the subsurface material within a distance of 0.5 m from the borehole. However, the model gives the average resistivity for a much larger volume of the subsurface.

Example 4: Magusi River orebody

The apparent resistivity data for the Magusi River orebody survey (Edwards 1977) is used as an example of the inversion of a dipole-dipole array field data set. A resistivity and IP survey was carried out over a massive sulphide orebody using dipole lengths of 100, 200 and 300 feet (30, 60 and 90 m). Figure 11 shows the apparent resistivity pseudosection for the data collected with a dipole length of 30 m and the model obtained by the quasi-Newton method at the 6th iteration (after which there is only a small change in the rms error). Although the minimum electrode spacing of 30 m (and thus the expected resolution of the model) is about the same as the width of the ore body, there is good agreement between the inverse model and the true shape of the ore body (Edwards 1977). The orebody has a much lower resistivity (about 10 $\Omega$m) compared to the country rocks (over 100 $\Omega$m).

Conclusions

A fast and powerful technique using a quasi-Newton optimization method is presented for the automatic inversion of resistivity pseudosections. The computer time and memory space required to produce a satisfactory 2D subsurface model are reduced by about eight and twelve times respectively, by avoiding the direct calculation of the partial derivatives. It has proved to be a robust method which converges rapidly. This method is able to resolve complex geological structures which cause overlapping anomalies in the pseudosection. The inversion of a single
data set takes about one minute on an 80486DX microcomputer. This makes it possible to carry out the interpretation of the data during the course of a survey using a field laptop microcomputer.

Research is being carried out into different ways to improve the inversion method further, using more sophisticated quasi-Newton techniques (Dennis and Schnabel 1983) and different schemes to determine the optimum damping factor and step size for the model perturbation vector (Scales 1985; deGroot-Hedlin and Constable 1990). The reduction in the computer time and memory required achieved by using the quasi-Newton method might ultimately prove to be an even more important factor in the inversion of 3D resistivity data which involves thousands of data points.

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