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An efficient 1D OCCAM's inversion algorithm using analytically computed first- and second-order derivatives for DC resistivity soundings☆

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Abstract

An efficient algorithm has been developed for 1D resistivity inversion problem using both first- and second-order derivatives, which are computed analytically. The second-order derivative matrix, which is not used in the OCCAM's inversion, has been incorporated into the algorithm employing analytical expressions. Computation of complicated second-order derivatives in each iteration is circumvented by a new algorithm. These modifications result in stable convergence of the OCCAM's inversion and in general, better misfit can be achieved specially for smoothing parameter, $\mu < 1$. The modified inversion algorithm, coded in MATLAB was tested using two synthetic Schlumberger resistivity sounding examples. Its application has been illustrated with field data from south India.

Keywords: Hessian matrix; Jacobian matrix; Schlumberger sounding; Newton's method; Smoothing parameter

1. Introduction

The OCCAM's inversion algorithm was first introduced by Constable et al. (1987) to find the smoothest model that fits the magnetotelluric (MT) and Schlumberger geoelectric sounding data. The method gained popularity in inversion studies and was applied to many investigations (LaBrecque et al., 1996; Siripunvaraporn and Egbert, 1996; Qian et al., 1997). In this scheme a highly nonlinear problem is formulated in a linear fashion, which obviates the computation of second-order derivatives that carry useful curvature information of the objective function.

In this paper the 1D OCCAM's algorithm has been improved by inclusion of second-order derivative matrix known as Hessian that is computed analytically. This leads to a quadratic equation approximation of the objective function. The modified algorithm has been tested on synthetic and real field resistivity sounding data. It is found that the modified algorithm is more stable and convergent than OCCAM's inversion.

The computation of second-order derivatives in Schlumberger resistivity sounding involves cumbersome piece of algebra and therefore these derivatives are computed numerically using finite difference schemes. This introduces many unacceptable errors and requires more computational time, which results in inaccurate curvature information that decides the step of descent where as computation of the derivatives analytically

☆Code on server at http://www.iamg.org/CGEditor/index.htm.

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solves the problem. The analytic approach based on recursive formulation provides faster computation of the derivatives.

2. Formulation of the problem

The nonlinear resistivity inversion relates observed data and model parameters by equation

$$\Theta = g(x) + v, \tag{1}$$

where $\Theta = (\theta_1, \ldots, \theta_N,)$ is a vector representing observations at different half-electrode separations in Schlumberger sounding, N is number of half-electrode separations, $g(x) = (g_1(x), \ldots, g_N(x))$ represents predicted data at different half-electrode separations, and ν is the measurement noise.

Various schemes to treat this non-linear problem are described in detail by Dimri (1992). Terminology used here closely follows Chernoguz (1995) with some differences arising due to Constable et al. (1987). Following Constable et al. (1987) the inverse problem is posed as a constrained optimization problem, set forth to minimize misfit $X = ||W\Theta - Wg(x)||$, subject to the constraint that roughness $R = ||\partial x||$ is also minimized. This can be converted to an unconstrained problem by the use of Lagrange parameter μ as follows:

$$U = \frac{1}{2}||\partial x||^2 + \frac{1}{2\mu}\{(W\,\Delta\Theta(x))^{\mathrm{T}}(W\,\Delta\Theta(x) - \chi_*^2)\}, \tag{2}$$

where ∂ is $N \times N$ matrix defined by Constable et al. (1987) as

$$\partial = \begin{pmatrix} 0 & 0 & \ldots & \ldots & 0 \\ -1 & 1 & \ldots & \ldots & 0 \\ 0 & -1 & 1 & \ldots & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & \ldots & -1 & 1 \end{pmatrix}.$$

W is weighting matrix, χ_* is acceptable misfit value and, μ is a Lagrange parameter used to optimize the constrained functional 'U' (Smith, 1974) and $\Delta\Theta(x) = W\Theta - Wg(x)$. If we expand the functional in Taylor's series at $x = x_k$ (say) we get

$$U(x_k + \delta, \mu, \Theta) = U(x_k, \mu, \Theta) + J_k^{\mathrm{T}}\delta + \frac{1}{2}\delta^{\mathrm{T}} Q_k \delta,$$

where

$$J_k = \nabla x U = \partial^{\mathrm{T}}\partial x - \frac{1}{\mu}(WG(x))^{\mathrm{T}} W\,\Delta\Theta(x)$$

and

$$Q_k = \nabla^2 x U = \partial^{\mathrm{T}}\partial - \frac{1}{\mu}\nabla_x\{(WG(x))^{\mathrm{T}} W\,\Delta\Theta(x)\}.$$

Using the identity

$$\nabla x\{WG(x))^{\mathrm{T}} W\,\Delta\Theta(x)\} = (WH(x))^{\mathrm{T}} W\,\Delta\Theta(x) - (WG(x))^{\mathrm{T}} WG(x)$$

the Q_k becomes

$$Q_k = \nabla^2 x U = \partial^{\mathrm{T}}\partial - \frac{1}{\mu}\{(WG(x))^{\mathrm{T}} WG(x) - (WH(x))^{\mathrm{T}} W\,\Delta\Theta(x)\}$$

where $G(x)$ is Jacobian of $g(x)$ and $H(x)$ is Hessian of $g(x)$.

If we define

$$(WH)^{\mathrm{T}} W\,\Delta\Theta = \sum_j WH_j W\,\Delta\Theta_j \text{ as } q,$$

where in H_j is Hessian of $g(x)$ evaluated at jth data point and $\Delta\Theta_j = \theta_j - g_j(x)$, q is the nonlinear part of the Hessian, then minimization of the functional (2) using Newton's method for ith iteration step δ_i yields

$$\delta_i = -\left[\partial^{\mathrm{T}}\partial + \mu^{-1}\{WG(x)^{\mathrm{T}} WG(x) - q\}\right]^{-1} \times \left[\partial^{\mathrm{T}}\partial_x - \mu^{-1} WG(x)^{\mathrm{T}} W\,\Delta\Theta(x)\right]_{x=x_i}. \tag{3}$$

Thus $x_{i+1} = x_i + \delta_i$ forms the iterative basis for the optimization of functional (2). Eq. (3) gives generalized OCCAM's correction steps. By setting q as a null matrix, the equation gives the model correction of the popular OCCAM's inversion algorithm. The OCCAM's optimization in Eq. (3) can be viewed as two sub-algorithms, where primary optimizes the functional U for different values of x and μ and secondary optimizes only misfit function. The difficulty may arise when the primary suggests corrections in the direction of decreasing U and secondary moves in search of decreasing misfit without regarding the roughness. Thus due to lack of curvature information in the OCCAM's inversion, secondary algorithm becomes blind in the direction of true minimum of χ^2, when the requirement of the primary algorithm to reduce U is overpowering. Another problem in OCCAM's inversion is the choice of Lagrange's parameter μ. If we take $\mu < 1$ for minimization of functional used in standard OCCAM's inversion, the algorithm tends to be blind to minimize misfit function in the absence of the curvature information. Hence, there is need to incorporate curvature information in terms of Hessian matrix. If we take $\mu \leqslant 1$ in Eq. (3) the nonlinear part carrying curvature information, will contribute to the convergence. In our work we include the curvature information in the OCCAM's model correction steps. From Newton–Gauss method we have,

$$x_{i+1} = x_i + \alpha_i \delta_i, \tag{4}$$