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METHODS FOR CALCULATING FRÉCHET DERIVATIVES AND SENSITIVITIES FOR THE NON-LINEAR INVERSE PROBLEM: A COMPARATIVE STUDY[1]

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ABSTRACT

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A fundamental step in the solution of most non-linear inverse problems is to establish a relationship between changes in a proposed model and resulting changes in the forward modelled data. Once this relationship has been established, it becomes possible to refine an initial model to obtain an improved fit to the observed data. In a linearized analysis, the Fréchet derivative is the connecting link between changes in the model and changes in the data. In some simple cases an analytic expression for the Fréchet derivative may be derived. In this paper we present three techniques to accomplish this and illustrate them by computing the Fréchet derivative for the 1D resistivity problem. For more complicated problems, where it is not possible to obtain an expression for the Fréchet derivative, it is necessary to parameterize the model and solve numerically for the sensitivities – partial derivatives of the data with respect to model parameters. The standard perturbation method for computing first-order sensitivities is discussed and compared to the more efficient sensitivity-equation and adjoint-equation methods. Extensions to allow for the calculation of higher order, directional and objective function sensitivities are also presented. Finally, the application of these various techniques is illustrated for both the 1D and 2D resistivity problems.

INTRODUCTION

Linearized analysis, traditionally employed in solving non-linear inverse problems, demands that either the Fréchet derivative or the first-order sensitivities be computed to evaluate quantitatively how a change in the model affects a datum. Literature in various fields illustrates how these quantities can be computed; however, there does not exist a detailed comparison of the various approaches which are available. As such, when faced with solving an inverse problem, there is often indecision about what options exist and how best to find an analytic expression for the

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Fréchet derivative or how to compute the sensitivities numerically. The goal of this paper is to fill that void. Our hope is that at least one of the techniques offered here will be of use to any practitioner faced with inverting geophysical data.

We begin with a general discussion of the forward and inverse problems, which involve mappings between 'model space' and 'data space'. For the work presented here, model space is a Hilbert space of functions defined over a suitable interval and data space is an N-dimensional Euclidean vector space whose elements are real or complex numbers.

We can represent the forward mapping mathematically by

$$e_j = F_j(m), \qquad j = 1, 2, \ldots, N \tag{1}$$

where $F_j(m)$ is a functional which relates a given model $m(x)$ to the jth datum e_j. If the problem is linear then (1) can be expressed as

$$e_j = \int_D K_j(\mathbf{x}) m(\mathbf{x})\, \mathrm{d}^3\mathbf{x}, \qquad j = 1, 2, \ldots, N, \tag{2}$$

where $K_j(\mathbf{x})$ is the kernel function associated with the jth datum and D is the domain of the problem.

In many cases the physics of the experiment leads to a description of the forward problem in terms of a differential equation and a set of boundary conditions, which together define a mathematical boundary-value problem. The steady-state diffusion problem, for example, is described by the differential equation

$$Lu = -\nabla \cdot (p(\mathbf{x})\nabla u) + q(\mathbf{x})u = Q(\mathbf{x}), \tag{3a}$$

valid over the domain D, and the boundary condition

$$Mu = \alpha(\mathbf{x})u + \beta(\mathbf{x}) \frac{\partial u}{\partial n} = g(\mathbf{x}), \tag{3b}$$

valid on the boundary ∂D of D. In (3), $u(\mathbf{x})$ is the response function to be solved for, $p(\mathbf{x})$ and $q(\mathbf{x})$ jointly specify the model, and $Q(\mathbf{x})$ and $g(\mathbf{x})$ describe the source distribution (or system excitation). Although for simple geometries it may be possible to find a closed-form solution to (3), generally one is forced to appeal to numerical techniques.

In the inverse problem we seek to find a model $m^*(\mathbf{x})$ such that

$$e_j^{\text{obs}} = F_j(m^*), \qquad j = 1, 2, \ldots, N \tag{4}$$

where e_j^{obs} is the jth observation. If the forward problem is linear then a variety of standard techniques can be used to solve the set of equations in (4) for $m^*(\mathbf{x})$ (e.g. Parker 1977b; Menke 1984; Oldenburg 1984); the particular technique used defines the inverse mapping. Although non-iterative inverse mappings can be found for non-linear problems (e.g. Gel'fand–Levitan approaches for inverse scattering problems), the techniques are often unstable in the presence of noise. Also, for many non-linear problems encountered in geophysics, no direct inverse mapping has been found. The usual strategy in these cases is to start with an estimated solution, $m_{\text{est}}(\mathbf{x})$, and to solve the forward problem to obtain the predicted data. A perturbation $\delta m(\mathbf{x})$ is sought which, when added to $m_{\text{est}}(\mathbf{x})$, yields a model which reproduces the observed data.

To derive equations which accomplish this, we write the jth observation in terms of the expansion

$$e_j^{\text{obs}} = F_j(m_{\text{est}}) + F_j^{(1)}(m_{\text{est}})\delta m + \frac{1}{2!} F_j^{(2)}(m_{\text{est}})\delta m^2 + \ldots, \tag{5}$$

where the operator $F_j^{(n)}(m)$ is called the nth order Fréchet derivative of $F_j(m)$ (Griffel 1981; Zeidler 1985). The first-order derivative $F_j^{(1)}(m)$ is referred to simply as the Fréchet derivative.

Letting $\delta e_j = e_j^{\text{obs}} - F_j(m_{\text{est}})$ be the misfit for the jth observation, then (5) can be written as

$$\delta e_j = F_j^{(1)}(m_{\text{est}})\delta m + \mathrm{O}(\|\delta m\|^2). \tag{6}$$

If the higher-order terms represented by $\mathrm{O}(\|\delta m\|^2)$ are neglected, then (6) can be written as

$$\delta e_j \approx \int_D K_j(\mathbf{x}, m_{\text{est}})\delta m(\mathbf{x})\, \mathrm{d}^3\mathbf{x}, \tag{7}$$

where $K_j(\mathbf{x}, m)$ is the Fréchet kernel associated with the jth observation. It is this kernel which establishes the relationship between a small (first-order) perturbation in the model and the corresponding change in the datum. Since (7) is linear, the perturbation $\delta m(\mathbf{x})$ can be readily computed using standard techniques once an analytic expression for the Fréchet kernel has been derived.

Rather than deriving an expression for the Fréchet derivative, an alternate approach to the solution of the inverse problem is first to represent the model by a finite set of parameters m_k, $k = 1, 2, \ldots, M$. The model is then a Euclidean vector $\mathbf{m}$ and the Taylor series expansion for the jth datum is

$$e_j^{\text{obs}} = F_j(\mathbf{m}_{\text{est}}) + \sum_{k=1}^{M} \frac{\partial F_j(\mathbf{m}_{\text{est}})}{\partial m_k}\delta m_k + \frac{1}{2!}\sum_{k=1}^{M}\sum_{l=1}^{M} \frac{\partial^2 F_j(\mathbf{m}_{\text{est}})}{\partial m_k\, \partial m_l}\delta m_k \delta m_l + \cdots, \tag{8}$$

where $\partial^n F_j(\mathbf{m})/\partial m_k\, \partial m_l \ldots$, is the nth order sensitivity of $F_j(\mathbf{m})$ with respect to the kth, lth, $\ldots$, parameters. Equation (8) can also be written as

$$\delta e_j = \sum_{k=1}^{M} \frac{\partial F_j(\mathbf{m}_{\text{est}})}{\partial m_k}\delta m_k + \mathrm{O}(\|\delta \mathbf{m}\|^2). \tag{9}$$

If the higher-order terms encompassed by $\mathrm{O}(\|\delta \mathbf{m}\|^2)$ are neglected, one obtains the matrix equation

$$\delta \mathbf{e} \approx \mathbf{J}\delta \mathbf{m}, \tag{10}$$

where $\mathbf{J}$ is the $N \times M$ Jacobian matrix whose elements $J_{jk} = \partial F_j/\partial m_k$ are the first-order sensitivities. Practical formulations for finding the model perturbation $\delta \mathbf{m}$ make use of a generalized inverse for $\mathbf{J}$ (Jackson 1972; Wiggins 1972; Jupp and Vozoff 1975; Menke 1984).

The specific methods used to solve (7) or (10) will differ among inverse practitioners. Also, each problem is best tackled by introducing an appropriate weighted norm to be minimized and often different regularization schemes are implemented. Nevertheless, almost all linearized inversion methods make use of one of these two equations and thus the calculation of Fréchet derivative kernels and parameter sensitivities is of fundamental importance to the solution of the non-linear inverse problem.

Derivation of Analytic Fréchet Derivatives

The usual approach for deriving an expression for the Fréchet derivative is to perturb the governing differential equation and thereby formulate a new problem which relates the change in the forward response to a small perturbation in the model. Let the forward problem be described by

$$Lu = Q(\mathbf{x}). \tag{11}$$

Then the response perturbation $\delta u(\mathbf{x})$ satisfies, to first order, the problem

$$L\delta u + \delta L u = 0, \tag{12}$$

or

$$L\delta u = R(\mathbf{x}), \tag{13}$$

where δL is a new operator obtained by perturbing the model, and $R(\mathbf{x}) = -\delta L u$. The solution of (13), evaluated at an observation location $\mathbf{x}_0$, yields the Fréchet derivative for that observation.

Adjoint Green's function approach

A general way of solving (13) for the Fréchet derivative is to make use of an adjoint Green's function solution (Lanczos 1960; Roach 1982). We begin by defining an adjoint operator L^* and considering the problem

$$L^*G^* = \delta(\mathbf{x} - \mathbf{x}_0), \tag{14}$$

where $G^*(\mathbf{x}, \mathbf{x}_0)$ is the adjoint Green's function. Multiplying (13) by G^* and (14) by δu and subtracting, yields the expression

$$G^*L\delta u - \delta u L^*G^* = G^*R(\mathbf{x}) - \delta u(\mathbf{x})\delta(\mathbf{x} - \mathbf{x}_0). \tag{15}$$

Integrating both sides of (15) over the domain D, and making use of the properties of the Dirac delta function, yields

$$\int_D (G^*L\delta u - \delta u L^*G^*)\, \mathrm{d}^3\mathbf{x} = \int_D G^*(\mathbf{x}, \mathbf{x}_0)R(\mathbf{x})\, \mathrm{d}^3\mathbf{x} - \delta u(\mathbf{x}_0). \tag{16}$$

If the operator L^* and the adjoint boundary conditions are chosen such that

$$\int_D (G^*L\delta u - \delta u L^*G^*)\, \mathrm{d}^3\mathbf{x} = 0, \tag{17}$$

for all G^* and δu, then the Fréchet derivative is given by

$$\delta u(\mathbf{x}_0) = \int_D G^*(\mathbf{x}, \mathbf{x}_0) R(\mathbf{x}) \, \mathrm{d}^3\mathbf{x}. \tag{18}$$

Requiring the adjoint problem to satisfy (17) establishes a form of reciprocity between the response perturbation and adjoint problems. This makes it possible to compute the response perturbation $\delta u(\mathbf{x}_0)$ due to a unit source at $\mathbf{x}$ by placing a unit source at $\mathbf{x}_0$ and calculating the value of the adjoint Green's function at $\mathbf{x}$. Equation (18) then uses the linearity of the problem to obtain the response perturbation due to the complete source term $R(\mathbf{x})$ by superposition. In many cases it is much easier to solve for the adjoint Green's function and perform the required integrations than to solve (13) directly.

To illustrate the adjoint approach, we derive the Fréchet derivative for the d.c. resistivity problem. The general governing equations are

$$\nabla \cdot (\sigma(\mathbf{x}) \nabla \phi) = 0, \tag{19a}$$

$$\frac{\partial}{\partial z} \phi(x, y, 0) = -\frac{I}{\sigma(0)} \delta(x)\delta(y), \tag{19b}$$

$$\phi(x, y, z)|_{z \to \infty} = 0, \tag{19c}$$

where $\phi(\mathbf{x})$ is the potential due to a single current electrode located at $\mathbf{x}_s = (0, 0, 0)$ and $\sigma(\mathbf{x})$ is the subsurface conductivity distribution. When the conductivity varies only with depth, (19) can be written as

$$\frac{\sigma(z)}{r} \frac{\partial}{\partial r}\left(r \frac{\partial \phi}{\partial r}\right) + \frac{\mathrm{d}\sigma(z)}{\mathrm{d}z} \frac{\partial \phi}{\partial z} + \sigma(z) \frac{\partial^2 \phi}{\partial z^2} = 0, \tag{20a}$$

$$\frac{\partial}{\partial z} \phi(r, 0) = -\frac{I}{2\pi\sigma(0) r} \delta(r), \tag{20b}$$

$$\phi(r, z)|_{z \to \infty} = 0, \tag{20c}$$

where r is the radial distance from the current electrode.

Symmetry suggests taking the Hankel transform of ϕ

$$\tilde{\phi}(\lambda, z) = \int_0^\infty r \phi(r, z) \mathrm{J}_0(\lambda r) \, \mathrm{d}r, \tag{21}$$

where $\mathrm{J}_0(\lambda r)$ is a Bessel function of the first kind of order 0. The transformed response $h(\lambda, z) = \lambda \tilde{\phi}(\lambda, z)$ can then be shown to satisfy the forward problem

$$\frac{\mathrm{d}^2 h}{\mathrm{d}z^2} - w(z) \frac{\mathrm{d}h}{\mathrm{d}z} - \lambda^2 h = 0, \tag{22a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z} h(\lambda, 0) = -\frac{\lambda I}{2\pi\sigma(0)}, \tag{22b}$$

$$h(\lambda, z)|_{z \to \infty} = 0, \tag{22c}$$

where

$$w(z) = -\frac{1}{\sigma(z)}\frac{\mathrm{d}\sigma(z)}{\mathrm{d}z} = \frac{1}{\rho(z)}\frac{\mathrm{d}\rho(z)}{\mathrm{d}z}.$$

As a final transformation it is convenient to define the normalized response $\tilde{S}(\lambda, z) = h(\lambda, z)/h'(\lambda, 0)$ which satisfies

$$\frac{\mathrm{d}^2\tilde{S}}{\mathrm{d}z^2} - w(z)\frac{\mathrm{d}\tilde{S}}{\mathrm{d}z} - \lambda^2\tilde{S} = 0, \tag{23a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\tilde{S}(\lambda, 0) = 1, \tag{23b}$$

$$\tilde{S}(\lambda, z)\,|_{z\to\infty} = 0. \tag{23c}$$

Equations (23a, b, c) are the desired governing differential equation and boundary conditions for which the Fréchet derivative will be calculated.

Since $\rho(z)$ is expected to vary over several orders of magnitude and is strictly positive it is convenient to consider either $m(z) = \ln\rho(z)$ or $w(z) = (\mathrm{d}/\mathrm{d}z)\ln\rho(z)$ as the model. In many cases $w(z)$ is the appropriate choice since it will lead to smoother estimates of $\ln\rho(z)$. If $w(z)$ is selected as the model, then a perturbed system is obtained by letting $w(z) \to w(z) + \delta w(z)$ in (23). Subtracting the unperturbed from the perturbed system yields an equation for the response perturbation $\delta\tilde{S}(\lambda, z)$:

$$\frac{\mathrm{d}^2\delta\tilde{S}}{\mathrm{d}z^2} - w(z)\frac{\mathrm{d}\delta\tilde{S}}{\mathrm{d}z} - \lambda^2\delta\tilde{S} = \delta w(z)\frac{\mathrm{d}\tilde{S}}{\mathrm{d}z}, \tag{24a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\delta\tilde{S}(\lambda, 0) = 0, \tag{24b}$$

$$\delta\tilde{S}(\lambda, z)\,|_{z\to\infty} = 0. \tag{24c}$$

The adjoint problem which satisfies the reciprocity relationship in (17) can be found by multiplying (24a) by the adjoint Green's function $G^*(\lambda, z, \xi)$ and integrating over z. We obtain

$$\int_0^\infty G^*\left[\frac{\mathrm{d}^2\delta\tilde{S}}{\mathrm{d}z^2} - w(z)\frac{\mathrm{d}\delta\tilde{S}}{\mathrm{d}z} - \lambda^2\delta\tilde{S}\right]\mathrm{d}z = \int_0^\infty G^*\frac{\mathrm{d}\tilde{S}}{\mathrm{d}z}\delta w(z)\,\mathrm{d}z. \tag{25}$$

The first two terms on the left are then integrated by parts to yield

$$\frac{\mathrm{d}\delta\tilde{S}}{\mathrm{d}z}G^*\Big|_0^\infty - \delta\tilde{S}\left(\frac{\mathrm{d}G^*}{\mathrm{d}z} + wG^*\right)\Big|_0^\infty + \int_0^\infty \delta\tilde{S}\left[\frac{\mathrm{d}^2G^*}{\mathrm{d}z^2} + \frac{\mathrm{d}}{\mathrm{d}z}(w(z)G^*) - \lambda^2G^*\right]\mathrm{d}z$$

$$= \int_0^\infty G^*(\lambda, z, 0)\frac{\mathrm{d}\tilde{S}(\lambda, z)}{\mathrm{d}z}\delta w(z)\,\mathrm{d}z. \tag{26}$$

If we choose the adjoint problem to be

$$\frac{d^2G^*}{dz^2} + \frac{d}{dz}(w(z)G^*) - \lambda^2 G^* = \delta(z - \xi), \tag{27a}$$

$$\frac{d}{dz} G^*(\lambda, 0, \xi) + w(0)G^*(\lambda, 0, \xi) = 0, \tag{27b}$$

$$G^*(\lambda, z, \xi)|_{z \to \infty} = 0, \tag{27c}$$

then the Fréchet derivative $\tilde{S}^{(1)}(\lambda, 0)$ is given by

$$\delta\tilde{S}(\lambda, 0) = \tilde{S}^{(1)}(\lambda, 0)\delta w = \int_0^\infty G^*(\lambda, z, 0) \frac{d\tilde{S}(\lambda, z)}{dz} \delta w(z)\, dz \tag{28}$$

Note that in this case the problem is not self-adjoint (i.e. the response perturbation $\delta\tilde{S}$ and the Green's function G^* do not satisfy the same governing equations and boundary conditions). An analytic solution to (27),

$$G^*(\lambda, z, 0) = \frac{\rho(0)}{\rho(z)} \tilde{S}(\lambda, z), \tag{29}$$

can be found using standard techniques (e.g. Parker 1977a). The Fréchet derivative is then given by

$$\tilde{S}^{(1)}(\lambda, 0)\delta w = \int_0^\infty \frac{\rho(0)}{\rho(z)} \frac{h(\lambda, z)h'(\lambda, z)}{[h'(\lambda, 0)]^2} \delta w(z)\, dz. \tag{30}$$

The adjoint Green's function approach has also been used in a number of other 1D inverse problems in geophysics. Parker (1977a), for example, used this approach to derive the Fréchet derivative for the 1D magnetotelluric problem, while Chave (1984) used it to obtain the Fréchet derivative for the general 1D electromagnetic induction problem.

Series expansion approach

The second method for calculating the Fréchet derivative is based upon writing the response of a perturbed system in terms of a Taylor series expansion. In fact, this method is not fundamentally different from the adjoint Green's function approach but it does show how higher-order Fréchet derivatives can also be evaluated. The method will be illustrated by applying it to the 1D resistivity problem. Let the general model perturbation be $\delta w(z) = \varepsilon\eta(z)$, where $\eta(z)$ is an arbitrary function. The perturbed response $\tilde{S}_{\mathrm{pert}}(\lambda, z)$ can be written in terms of the Taylor series expansion

$$\tilde{S}_{\mathrm{pert}}(\lambda, z) = \tilde{S}(\lambda, z) + \varepsilon\tilde{S}_1(\lambda, z) + \frac{\varepsilon^2}{2!}\tilde{S}_2(\lambda, z) + \dots, \tag{31}$$

where

$$\tilde{S}_n(\lambda, z) = \frac{\partial^n}{\partial\varepsilon^n} \tilde{S}(\lambda, z).$$

The perturbed response satisfies

$$\frac{d^2}{dz^2}\left[\tilde{S} + \varepsilon\tilde{S}_1 + \frac{\varepsilon^2}{2!}\tilde{S}_2 + \cdots\right] - (w + \varepsilon\eta)\frac{d}{dz}\left[\tilde{S} + \varepsilon\tilde{S}_1 + \frac{\varepsilon^2}{2!}\tilde{S}_2 + \cdots\right] - \lambda^2\left[\tilde{S} + \varepsilon\tilde{S}_1 + \frac{\varepsilon^2}{2!}\tilde{S}_2 + \cdots\right] = 0. \tag{32}$$

Collecting terms involving the same power of ε, one obtains the series of equations

$$\frac{d^2\tilde{S}_k}{dz^2} - w(z)\frac{d\tilde{S}_k}{dz} - \lambda^2\tilde{S}_k = k\eta\frac{d\tilde{S}_{k-1}}{dz} \qquad k = 1, 2, \ldots. \tag{33}$$

For $k \geq 1$, the surface boundary condition is $(d/dz)\tilde{S}_k(\lambda, 0) = 0$ and all solutions are required to decay to zero as $z \to \infty$. For $k = 1$, $\tilde{S}_0(\lambda, z) = \tilde{S}(\lambda, z)$ is the field due to the unperturbed system. We note that each of the problems in (33) has the same form and is identical to that given in (24). $\tilde{S}_1(\lambda, 0)$ can be found using the adjoint Green's function approach and hence the Fréchet derivative $\tilde{S}^{(1)}(\lambda, 0)\delta w = \varepsilon\tilde{S}_1(\lambda, 0)$ will again be given by (30). Higher-order Fréchet derivatives may be calculated using the same adjoint Green's function.

Riccati equation approach

The third method for computing the Fréchet derivative is less general than the adjoint method in that it is restricted to governing equations of the form

$$u''(z) + A(z)u'(z) + B(z)u(z) = 0, \tag{34}$$

that is, to second-order homogeneous linear equations in one-dimension. Nevertheless, the pervasiveness of this equation in physical problems means that special solution methods tied to this equation can still have general usefulness (e.g. Oldenburg 1978 and 1979). To compute the Fréchet derivative, we first transform (34) to a Riccati equation by making the substitution $y(z) = -u'(z)/a(z)u(z)$ or $y(z) = -a(z)u(z)/u'(z)$ (Bender and Orszag 1978). The Riccati equation for δy, obtained by perturbing the model, is then solved using standard techniques.

To illustrate the method, we apply it to the 1D resistivity problem. Following Oldenburg (1978) let $S(\lambda, z) = h(\lambda, z)/h'(\lambda, z)$. Substituting into (22a) yields the Riccati equation

$$\frac{dS}{dz} + w(z)S + \lambda^2 S^2 - 1 = 0. \tag{35}$$

Perturbing $w(z)$ by $\delta w(z)$ generates a response perturbation $\delta S(\lambda, z)$ which satisfies, to first order, the equation

$$\frac{d\delta S}{dz} + (w(z) + 2\lambda^2 S)\delta S = -S\delta w(z). \tag{36}$$

This may also be written as

$$\frac{\mathrm{d}\delta S}{\mathrm{d}z} + \left(\frac{\mathrm{d}}{\mathrm{d}z} \ln \left[\frac{\mathrm{d}h}{\mathrm{d}z}\right]^2 - \frac{\mathrm{d}}{\mathrm{d}z} \ln \rho\right)\delta S = -S\delta w(z). \tag{37}$$

Making use of the integrating factor

$$\exp\left\{\int_0^z \frac{\mathrm{d}}{\mathrm{d}z}\left(\ln \frac{1}{\rho}\left[\frac{\mathrm{d}h}{\mathrm{d}z}\right]^2\right) \mathrm{d}z\right\} = \frac{\rho(0)}{\rho(z)}\left[\frac{h'(\lambda, z)}{h'(\lambda, 0)}\right], \tag{38}$$

we obtain an expression for the Fréchet derivative $S^{(1)}(\lambda, 0)$ given by

$$S^{(1)}(\lambda, 0)\delta w = \int_0^\infty \frac{\rho(0)}{\rho(z)} \frac{h'(\lambda, z)h(\lambda, z)}{[h'(\lambda, 0)]^2} \delta w(z)\, \mathrm{d}z. \tag{39}$$

This is identical to that obtained using the adjoint Green's function approach for the $\tilde{S}(\lambda, 0)$ response.

The Riccati-equation approach is particularly interesting because it allows one to compute Fréchet derivatives for a response or for its reciprocal. For example, we could have chosen the response

$$R(\lambda, z) = \frac{h'(\lambda, z)}{h(\lambda, z)}. \tag{40}$$

This leads to the Riccati equation

$$\frac{\mathrm{d}R}{\mathrm{d}z} - w(z)R + R^2 - \lambda^2 = 0, \tag{41}$$

and to a Fréchet derivative $R^{(1)}(\lambda, 0)$ given by

$$R^{(1)}(\lambda, 0)\delta w = -\int_0^\infty \frac{\rho(0)}{\rho(z)}\left[\frac{h(\lambda, z)}{h(\lambda, 0)}\right]^2 \frac{h'(\lambda, z)}{h(\lambda, z)} \delta w(z)\, \mathrm{d}z. \tag{42}$$

At the surface of the earth, either $S(\lambda, 0)$, or its reciprocal $R(\lambda, 0)$, is measured. For use in a linearized inverse solution one would like to choose the datum and its corresponding Fréchet derivative which leads to the most linear problem possible. This choice of data is also encountered in electromagnetic problems where both electric (E) and magnetic (B) fields are measured and their ratio, either E/B or B/E can be regarded as data. An analysis, making use of the Fréchet derivative for both data choices, can resolve which datum should be used for linearization.

Parameterization of the Forward and Inverse Problems

In a parametric formulation of a forward or inverse problem, the model can be written as

$$m(\mathbf{x}) = \sum_{k=1}^{M} m_k \psi_k(\mathbf{x}), \tag{43}$$

where $\{\psi_k\}$ is a set of basis functions. The choice of basis functions determines the type of model to be considered. For example, the model domain D can be divided into subdomains D_k with the kth basis function defined to be unity over the kth subdomain and zero elsewhere. The kth parameter m_k is then the value of the model over the corresponding subdomain. This parameterization permits 'blocky' models which are well suited to problems where large changes in the model are expected over short distances. Another approach is to define a grid of nodes over D and to let the kth parameter be the value of $m(\mathbf{x})$ at the location of the kth node. $\{\psi_k\}$ is determined by the interpolation method used to define the model between nodes. A third possibility is to choose $\{\psi_k\}$ as a set of regional basis functions (e.g. sinusoidal functions used in a Fourier expansion).

Regardless of the parameterization selected, the model is completely specified in terms of the vector $\mathbf{m} = (m_1, m_2, \ldots, m_M)$. In solving the inverse problem, the goal is to find values for these parameters which will acceptably reproduce the observations. Although there are many ways in which this problem can be approached – for example, using the steepest descent, conjugate gradient, or Gauss–Newton method (Gill, Murray and Wright 1981) – the inversion will generally require the computation of the sensitivity or partial derivative matrix in (10).

When the forward problem is expressed as a boundary-value problem, the sensitivities can be computed by solving another boundary-value problem which is either identical, or closely related to, the original problem. Many standard algorithms are available for the numerical solution of boundary-value problems – the most commonly used being the finite-difference, finite-element and boundary-element methods (e.g. Lapidus and Pinder 1982). These algorithms make use of a discretization to reduce the governing differential equation and boundary conditions to a system of algebraic equations. For a general forward problem, this system can be expressed as

$$\mathbf{Au} = \mathbf{q}, \tag{44}$$

where $\mathbf{u}$ is the solution at a set of discrete points in the domain. The entries of the coefficient matrix $\mathbf{A}$ depend on the material properties of the model and on the discretization scheme adopted. This means that a new coefficient matrix must be formed each time the forward problem is to be solved using a new model. The entries of the vector $\mathbf{q}$, on the other hand, are independent of the material properties of the model and depend only on the source distribution and discretization scheme.

Because of the need to solve (44) for many different source distributions, a direct solver based on some kind of factorization of $\mathbf{A}$ is generally used to obtain $\mathbf{u}$. One possible factorization is given by

$$\mathbf{A} = \mathbf{LU} \tag{45}$$

where $\mathbf{L}$ and $\mathbf{U}$ are respectively lower and upper triangular matrices (Golub and Van Loan 1983). The system in (44) becomes

$$\mathbf{LUu} = \mathbf{q}. \tag{46}$$

Letting $\mathbf{Uu} = \mathbf{v}$, the vector $\mathbf{v}$ can be computed by solving $\mathbf{Lv} = \mathbf{q}$ by forward substitution; $\mathbf{u}$ may be recovered by solving $\mathbf{Uu} = \mathbf{v}$ by back substitution. Once the factors of **A** have been computed, they can be used repeatedly to solve the forward problem for different source configurations at little additional expense.

Calculation of Differential Sensitivities

Given that the forward problem can be expressed as a boundary-value problem, there are three ways to obtain the sensitivities. In the first method, the sensitivities are computed from their finite-difference approximations, each requiring the solution of the forward problem with the corresponding parameter slightly perturbed. In the second method, a new boundary-value problem is derived for each of the sensitivities, and the sensitivities are solved for directly. In the third, the sensitivities are computed using the solution to an adjoint Green's function problem.

Perturbation approach

The most straightforward way to calculate the differential sensitivities is to approximate them using the one-sided finite-difference formula

$$\frac{\partial F_j(\mathbf{m})}{\partial m_k} \approx \frac{F_j(\mathbf{m} + \Delta\mathbf{m}_k) - F_j(\mathbf{m})}{\Delta m_k}. \tag{47}$$

The perturbed forward response $F_j(\mathbf{m} + \Delta\mathbf{m}_k)$ is obtained by re-solving the forward problem after the kth parameter has been perturbed by an amount Δm_k. Since the model must be altered to compute the perturbed responses, each sensitivity requires the solution of a completely new problem. As such, this 'brute force' method is inefficient, but it can nevertheless yield useful results (e.g. Edwards, Nobes and Gómez-Treviño 1984).

Sensitivity equation approach

In the sensitivity-equation method, a new forward problem is derived whose solution is the desired sensitivity function $\phi_k(\mathbf{x})$. Problems which have been addressed using this approach include the 2D magnetotelluric problem (Rodi 1976; Jupp and Vozoff 1977; Cerv and Pek 1981; Hohmann and Raiche 1988), the 2D electromagnetic problem (Oristaglio and Worthington 1980) and computer-aided design problems (Brayton and Spence 1980). Vemuri *et al.* (1969), McElwee (1982) and Townley and Wilson (1985) use the approach to address problems in groundwater flow.

To illustrate the technique, we consider the steady-state diffusion problem given in (3). Taking $p(\mathbf{x})$ to be the model, and assuming the parameterization $p(\mathbf{x}) = \sum_{l=1}^{M} p_l \psi_l(\mathbf{x})$, we obtain

$$-\nabla \cdot \left(\sum_{l=1}^{M} p_l \psi_l(\mathbf{x}) \nabla u \right) + q(\mathbf{x})u = Q(\mathbf{x}) \qquad \text{in } D, \tag{48a}$$

$$\alpha(\mathbf{x})u + \beta(\mathbf{x}) \frac{\partial u}{\partial n} = 0 \qquad \text{on } \partial D. \tag{48b}$$

Differentiating (48) with respect to p_k, and substituting for $u_k(\mathbf{x}) = \partial u(\mathbf{x})/\partial p_k$, yields the sensitivity problem

$$-\nabla \cdot (p(\mathbf{x})\nabla u_k) + q(\mathbf{x})u_k = \nabla \cdot (\psi_k(\mathbf{x})\nabla u) \qquad \text{in } D, \tag{49a}$$

$$\alpha(\mathbf{x})u_k + \beta(\mathbf{x}) \frac{\partial u_k}{\partial n} = 0 \qquad \text{on } \partial D. \tag{49b}$$

To compute the sensitivities for a model $p(\mathbf{x})$, the forward problem (3) is first solved to obtain $u(\mathbf{x})$ at all points $\mathbf{x}$ in D. For each parameter p_k, the corresponding sensitivity problem is solved to obtain $u_k(\mathbf{x})$ which is then evaluated at each of the observation locations. Note that the source term $\nabla \cdot (\psi_k(\mathbf{x})\nabla u)$ differs for each k, so that a total of $M + 1$ forward problems must be solved to obtain all of the sensitivities. Since the sensitivity problems and the original forward problem differ only in terms of their right-hand sides, they can be solved efficiently if a direct method such as the LU decomposition is used. Only a single matrix factorization is then required to solve all $M + 1$ forward problems.

The sensitivity-equation method is easily extended to the calculation of other kinds of sensitivities. For example, the directional sensitivity $u_\alpha(\mathbf{x})$, given by

$$u_\alpha(\mathbf{x}) = \sum_{k=1}^{M} \alpha_k u_k(\mathbf{x}), \tag{50}$$

where $\boldsymbol{\alpha}$ is a unit vector in parameter space, can be computed by first multiplying (49) by α_k and then summing over k to obtain the new problem

$$-\nabla \cdot (p(\mathbf{x})\nabla u_\alpha) + q(\mathbf{x})u_\alpha = \nabla \cdot \left(\sum_{k=1}^{M} \alpha_k \psi_k(\mathbf{x})\nabla u \right) \qquad \text{in } D, \tag{51a}$$

$$\alpha(\mathbf{x})u_\alpha + \beta(\mathbf{x}) \frac{\partial u_\alpha}{\partial n} = 0 \qquad \text{on } \partial D. \tag{51b}$$

$u\phi_\alpha(\mathbf{x})$ may then be solved for directly. Directional sensitivities are useful for determining an optimum model perturbation once a direction for the perturbation has been selected (e.g. Townley and Wilson 1985).

The sensitivity-equation method can also be extended to the calculation of higher-order sensitivities. For example, differentiating (49) with respect to the new parameter p_l yields a new problem whose solution is the second-order sensitivity function $u_{kl}(\mathbf{x}) = \partial^2 u(\mathbf{x})/\partial p_k \partial p_l$. Several parameter-estimation schemes that make use of these higher-order sensitivities to achieve rapid convergence are available (e.g. Brayton and Spence 1980; Gill *et al.* 1981). The use of second-order sensitivities in the estimation of parameter uncertainty has also been described (Townley and Wilson 1985).

Adjoint equation approach

The third method for calculating sensitivities is based on the adjoint Green's function concept discussed earlier. Some of the problems to which the adjoint-equation approach has been applied include the seismic problem (Tarantola 1984;

Chen 1985), the resistivity problem (Smith and Vozoff 1984), the magnetotelluric problem (Weidelt 1975; Park 1987), the groundwater flow problem (Neuman 1980; Carrera and Neuman 1984; Sykes and Wilson 1984; Sykes Wilson and Andrews 1985; Townley and Wilson 1985), the reservoir evaluation problem (Carter *et al.* 1974), and various problems in computer-aided design (Director and Rohrer 1969; Branin 1973; Brayton and Spence 1980). An equivalent approach, based on a reciprocity relationship for transmission networks, has also been described (Madden 1972; Tripp, Hohmann and Swift 1984).

As an illustration of the approach, consider again the steady-state diffusion problem given in (3). Having obtained the sensitivity problem in (49), the appropriate adjoint problem is found by constructing an operator L^* and boundary conditions such that (17) is satisfied. We obtain

$$L^*G^* = -\nabla \cdot (p(\mathbf{x})\nabla G^*) + q(\mathbf{x})G^* = \delta(\mathbf{x} - \mathbf{x}_j) \qquad \text{in } D, \tag{52a}$$

$$\mathrm{a}(\mathbf{x})G^* + \beta(\mathbf{x}) \frac{\partial G^*}{\partial n} = 0 \qquad \text{on } \partial D. \tag{52b}$$

Forming the expression

$$G^*Lu_k - u_k L^*G^* = G^*\nabla \cdot (\psi_k \nabla u) - u_k \delta(\mathbf{x} - \mathbf{x}_j), \tag{53}$$

and integrating over D yields

$$u\phi_k(\mathbf{x}_j) = \int_D G^*\nabla \cdot (\psi_k \nabla u) \, \mathrm{d}^3 z. \tag{54}$$

To compute the sensitivities, (52) must be solved for each observation location $\mathbf{x}_j$. The integration in (54) is then carried out for each parameter. Since the source term in (52a) differs for each observation location, a total of $N + 1$ forward problems must be solved (although again this can be done efficiently if an LU decomposition or other factorization is used).

In some cases, the sensitivity of an objective function is desired. For example, if a steepest-descent method is to be used to minimize the objective function

$$\phi(\mathbf{m}) = \sum_{j=1}^{N} [e_j^{\text{obs}} - e_j]^2 \tag{55}$$

where $e_j = F_j(\mathbf{m})$, then sensitivities of the form

$$\frac{\partial \phi}{\partial m_k} = -2 \sum_{j=1}^{N} (e_j^{\text{obs}} - e_j) u_k(\mathbf{x}_j) \tag{56}$$

must be calculated. Although this could be done by solving for each $u_k(\mathbf{x}_j)$, a more practical method can be arrived at by solving the modified adjoint problem

$$L^*\bar{G}^* = -\nabla \cdot (p(\mathbf{x})\nabla \bar{G}^*) + q(\mathbf{x})\bar{G}^* = -2 \sum_{j=1}^{N} (e_j^{\text{obs}} - e_j)\delta(\mathbf{x} - \mathbf{x}_j) \qquad \text{in } D, \tag{57a}$$

$$\alpha(\mathbf{x})\bar{G}^* + \beta(\mathbf{x}) \frac{\partial \bar{G}^*}{\partial n} = 0 \qquad \text{on } \partial D. \tag{57b}$$

The objective function sensitivities can then be computed from

$$\frac{\partial \phi}{\partial m_k} = -2 \sum_{j=1}^{N} (e_j^{\text{obs}} - e_j) u_k(\mathbf{x}_j) = \int_D \bar{G}^* \nabla \cdot (\psi_k(\mathbf{x}) \nabla u) \, d^3\mathbf{x}. \tag{58}$$

Using this approach only two forward problems need be solved to obtain all required sensitivities.

Example: 1D Resistivity Problem

To illustrate the numerical computation of sensitivities, we consider the 1D resistivity problem given in (22). Let $m(z) = \ln \rho(z)$ be the model and represent the earth by a sequence of layers of constant conductivity. Then

$$w(z) = \sum_{l=1}^{M} m_l \frac{d\psi_l(z)}{dz}, \tag{59}$$

where

$$\psi_l(z) = \begin{cases} 1 & \text{for } z_l < z < z_{l+1} \\ 0 & \text{otherwise} \end{cases}$$

and z_l is the depth to the top of the lth layer.

The reference model for this example, shown in Fig. 1a, consists of a 100 Ωm conductive zone buried within a more resistive 1000 Ωm half-space. The interval between $z = 0$ m and $z = 400$ m was divided into 20 m thick layers and the log resistivities of all but the first layer were taken to be parameters. (The log resistivity of the surface layer was not considered to be a parameter since if it were, the dependence of the boundary condition (22b) on the surface conductivity would unnecessarily complicate the example.) The transformed potentials for different values of λ

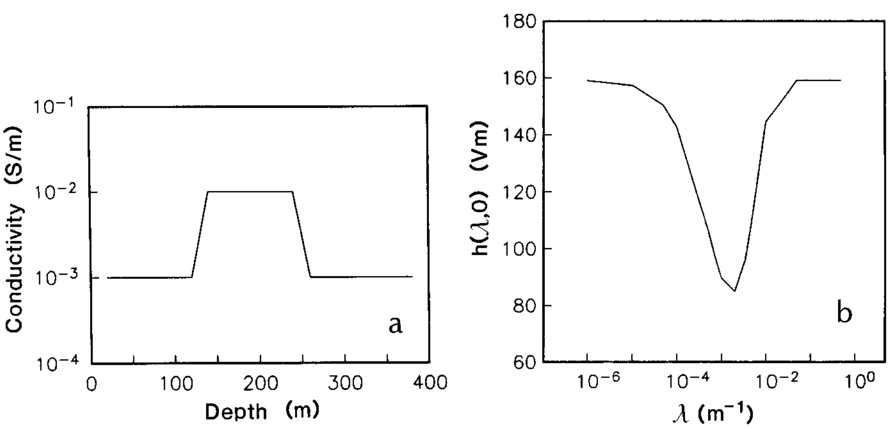


FIG. 1. (a) Conductivity model used in the 1D resistivity example. (b) Transformed surface potential $h(\lambda, 0)$ computed for the model shown in (a).

were computed using the propagator matrix algorithm described in Appendix A. Those results are shown in Fig. 1b. The presence of the conductive zone is indicated by the anomalously low value of the transformed potential.

Taking the transformed potential for $\lambda = 0.005\ \mathrm{m}^{-1}$ to be the single datum for this example, the differential sensitivities $h_k(\lambda, 0) = \partial h(\lambda, 0)/\partial m_k$ were computed using each of the three methods described in this paper.

First, making use of the perturbation approach and the approximation given in (47), the sensitivities for each layer were computed using conductivity perturbations of 1.0%, 10.0% and 100.0%. The sensitivities were computed using different perturbations so that the effect of perturbation size on the accuracy of the approximation could be examined. The results, plotted as functions of depth, are shown in Fig. 2a. As expected, the transformed potential is found to be most sensitive to changes in the near-surface conductivity, and a rapid decrease in sensitivity is observed at the top of the conductive zone. The shielding effect of the conductive layer is also apparent, resulting in the transformed potential being insensitive to changes in the conductivity below the layer. A comparison of the sensitivities obtained for the three different perturbation steps indicates that this approach is reasonably accurate except when large perturbations are used. The computational work involved, however, is great for problems that involve a large number of parameters relative to the number of data available. For this example a total of 20 forward problems had to be solved to obtain the sensitivities for only one datum.

The sensitivity-equation formulation is obtained by differentiating (22) with respect to m_k. This yields

$$\frac{\mathrm{d}^2 h_k}{\mathrm{d}z^2} - w(z)\frac{\mathrm{d}h_k}{\mathrm{d}z} - \lambda^2 h_k = \frac{\mathrm{d}\psi_k}{\mathrm{d}z}\frac{\mathrm{d}h}{\mathrm{d}z} = [\delta(z - z_{k-1}) - \delta(z - z_k)]\frac{\mathrm{d}h}{\mathrm{d}z}, \tag{60a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z} h_k(\lambda, 0) = 0, \tag{60b}$$

$$h_k(\lambda, z)|_{z \to \infty} = 0. \tag{60c}$$

The current source represented by the non-homogeneous boundary condition (22b) in the original problem must be replaced by two buried sources – one on either side of the kth layer. Although $\mathrm{d}h/\mathrm{d}z$ is discontinuous at each of the layer boundaries, the right hand side of (60a) can still be evaluated using

$$\delta(z - z_l)\frac{\mathrm{d}h}{\mathrm{d}z} = \frac{1}{2}\,\delta(z - z_l)\left[\left.\frac{\mathrm{d}h}{\mathrm{d}z}\right|_{z_l+} + \left.\frac{\mathrm{d}h}{\mathrm{d}z}\right|_{z_l-}\right]. \tag{61}$$

The sensitivity function $h_k(\lambda, z)$ is obtained by using the propagator matrix algorithm to solve (60) for each layer. The sensitivity-vs-depth relationship is shown in Fig. 2b. A total of 20 forward problems again had to be solved to compute the sensitivities for the one value of λ. Comparing Figs 2a and 2b, it is found that the sensitivities computed using this method correspond to those found by the perturbation approach for $\Delta\sigma/\sigma \to 0$.

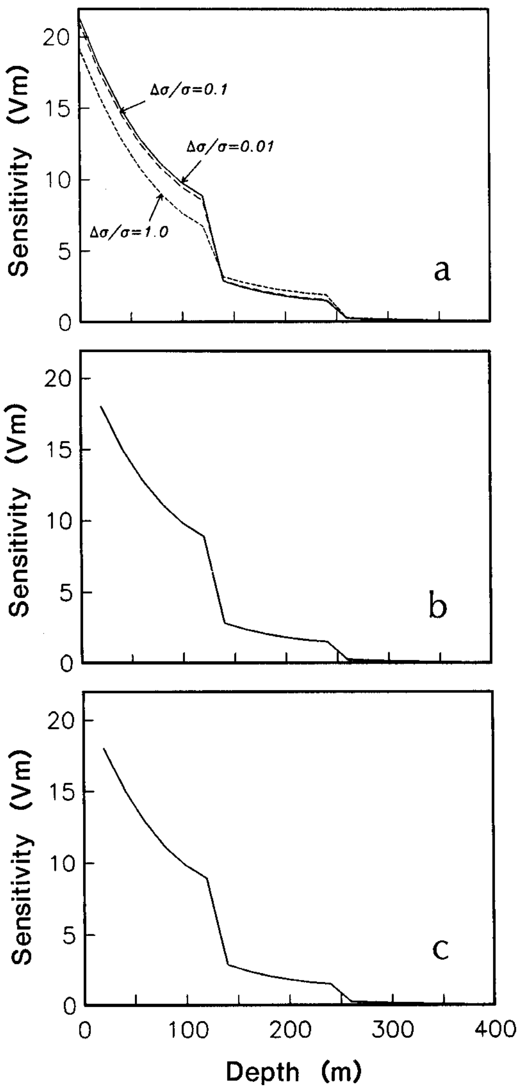


FIG. 2. Sensitivity as a function of depth for $\lambda = 0.005\ \mathrm{m}^{-1}$ computed using (a) the perturbation method, (b) the sensitivity-equation method, and (c) the adjoint-equation method.

To solve for the sensitivities using the adjoint-equation approach, we require the solution of the adjoint problem

$$\frac{\mathrm{d}^2 G^*}{\mathrm{d}z^2} + \frac{\mathrm{d}}{\mathrm{d}z}(wG^*) - \lambda^2 G^* = \delta(z), \tag{62a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z} G^*(\lambda, 0) + w(0)G^*(\lambda, 0) = 0, \tag{62b}$$

$$G^*(\lambda, z)|_{z\to\infty} = 0. \tag{62c}$$

The sensitivity $h_k(\lambda, 0)$ is then given by

$$h_k(\lambda, 0) = \int_0^\infty G^*(\lambda, z)[\delta(z - z_k) - \delta(z - z_{k+1})] \frac{\mathrm{d}}{\mathrm{d}z} h(\lambda, z)\, \mathrm{d}z. \tag{63}$$

The adjoint problem can also be solved (after some manipulation) using the propagator matrix algorithm, although a simple relationship can be found which allows $G^*(\lambda, z)$ to be calculated directly from $h(\lambda, z)$. Note that if a new function $\hat{G}^* = G^*\rho$ is defined, then $\hat{G}^*(\lambda, z)$ is found to satisfy the same forward problem as $h(\lambda, z)$ except that the current source is scaled by $-\lambda I/2\pi$. Since the original governing differential equation is linear, the Green's function $G^*(\lambda, z)$ required in (63) can be related to $h(\lambda, z)$ by

$$G^*(\lambda, z) = -\frac{2\pi}{\lambda I} \frac{h(\lambda, z)}{\rho(z)}. \tag{64}$$

Once the forward problem has been solved for $h(\lambda, z)$, then (64) is used to obtain $G^*(\lambda, z)$ and the integrations in (63) are carried out to compute the sensitivities. The results, shown in Fig. 2c, are identical to those found using the sensitivity-equation method. Only a single forward solution is required to generate all of the sensitivities using this approach.

Example: 2D Resistivity Problem

To illustrate the sensitivity and adjoint equation methods for a more complicated situation, consider the 2D resistivity problem described by the differential equation

$$\frac{\partial}{\partial x}\left(\sigma(x, z)\frac{\partial \phi}{\partial x}\right) + \sigma(x, z)\frac{\partial^2 \phi}{\partial y^2} + \frac{\partial}{\partial z}\left(\sigma(x, z)\frac{\partial \phi}{\partial z}\right) = -I\delta(x - x_s)\delta(y)\delta(z - z_s), \tag{65a}$$

and the boundary conditions

$$\frac{\partial}{\partial n}\phi(x, y, z)|_{\partial D} = 0, \tag{65b}$$

$$\phi(x, y, z)|_{R\to\infty} = 0, \tag{65c}$$

where $\phi(x, y, z)$ is the potential due to a single current electrode located at $\mathbf{x}_s = (x_s, 0, z_s)$ and $R = [(x - x_s)^2 + y^2 + (z - z_s)^2]^{1/2}$. The second current electrode is assumed to be located at infinity. Because of the 2D nature of the conductivity structure, it is convenient to consider the Fourier cosine transform of ϕ given by

$$\tilde{\phi}(x, K_y, z) = \int_0^\infty \phi(x, y, z) \cos(K_y y)\, \mathrm{d}y. \tag{66}$$

The transformed response $\tilde{\phi}$ then satisfies

$$\frac{\partial}{\partial x}\left(\sigma(x, z)\frac{\partial \tilde{\phi}}{\partial x}\right) - K_y^2\sigma(x, z)\tilde{\phi} + \frac{\partial}{\partial z}\left(\sigma(x, z)\frac{\partial \tilde{\phi}}{\partial z}\right) = -\frac{I}{2}\delta(x - x_s)\delta(z - z_s), \quad (67a)$$

$$\frac{\partial}{\partial n}\tilde{\phi}(x, K_y, z)|_{\partial D} = 0, \quad (67b)$$

$$\tilde{\phi}(x, K_y, z)|_{r\to\infty} = 0, \quad (67c)$$

where $r = [(x - x_s)^2 + (z - z_s)^2]^{1/2}$.

The forward problem given in (67) can be solved using an integrated finite-difference algorithm (Narasimhan and Witherspoon 1976; Dey and Morrison 1979) to yield transformed potentials over a finite-difference mesh for any particular value of K_y. The forward responses in the spatial domain can be obtained by numerically evaluating the inverse cosine transform

$$\phi(x, y, z) = \frac{2}{\pi}\int_0^\infty \tilde{\phi}(x, K_y, z)\cos(K_y y)\, dK_y. \quad (68)$$

Numerical computations proceed by representing the conductivity model $\sigma(x, z)$ by a set of rectangular prisms of constant conductivity which extend to infinity in the y-direction. The parametrized model is then given by

$$\sigma(x, z) = \sum_{j=1}^{M_z}\sum_{k=1}^{M_x}\sigma_{jk}\psi_{jk}(x, z), \quad (69)$$

where

$$\psi_{jk}(x, z) = \begin{matrix} 1 & \text{for } x_k < x < x_{k+1}, \quad z_j < z < z_{j+1}, \\ 0 & \text{otherwise.} \end{matrix}$$

The sensitivity problem, obtained by differentiating (67) with respect to σ_{jk}, is

$$\frac{\partial}{\partial x}\left(\sigma(x, z)\frac{\partial \tilde{\phi}_{jk}}{\partial x}\right) - K_y^2\sigma(x, z)\tilde{\phi}_{jk} + \frac{\partial}{\partial z}\left(\sigma(x, z)\frac{\partial \tilde{\phi}_{jk}}{\partial z}\right)$$
$$= K_y^2\psi_{jk}\tilde{\phi} - \frac{\partial}{\partial x}\left(\psi_{jk}\frac{\partial \tilde{\phi}}{\partial x}\right) - \frac{\partial}{\partial z}\left(\psi_{jk}\frac{\partial \tilde{\phi}}{\partial z}\right), \quad (70a)$$

$$\frac{\partial}{\partial n}\tilde{\phi}_{jk}(x, K_y, z)|_{\partial D} = 0, \quad (70b)$$

$$\tilde{\phi}_{jk}(x, K_y, z)|_{r\to\infty} = 0, \quad (70c)$$

where $\tilde{\phi}_{jk}(x, K_y, z) = \partial/\partial\sigma_{jk}\,\tilde{\phi}(x, K_y, z)$ is the desired sensitivity in the transformed domain.

The adjoint Green's function problem corresponding to (70) is

$$\frac{\partial}{\partial x}\left(\sigma(x, z)\frac{\partial G^*}{\partial x}\right) - K_y^2\sigma(x, z)G^* + \frac{\partial}{\partial z}\left(\sigma(x, z)\frac{\partial G^*}{\partial z}\right) = \delta(x - x_0)\delta(z - z_0), \quad (71a)$$

$$\frac{\partial}{\partial n} G^*(x, K_y, z, x_0, z_0)|_{\partial D} = 0, \tag{71b}$$

$$G^*(x, K_y, z, x_0, z_0)|_{r \to \infty} = 0. \tag{71c}$$

Since the form of (71) is identical to that of the original transformed forward problem in (67), the same finite-difference algorithm can be used to solve both. This takes advantage of the computational savings associated with decomposing the original matrix.

Note that for the 2D resistivity problem it will often be the case that an electrode used to make one or more potential measurements will have also been used at some point in the survey as a current electrode. If this occurs, then (71) need not be solved since $G^*(x, K_y, z, x_0, z_0)$ can always be computed directly from the forward modelled response $\tilde{\phi}(x, K_y, z)$ due to the current electrode at (x_0, z_0).

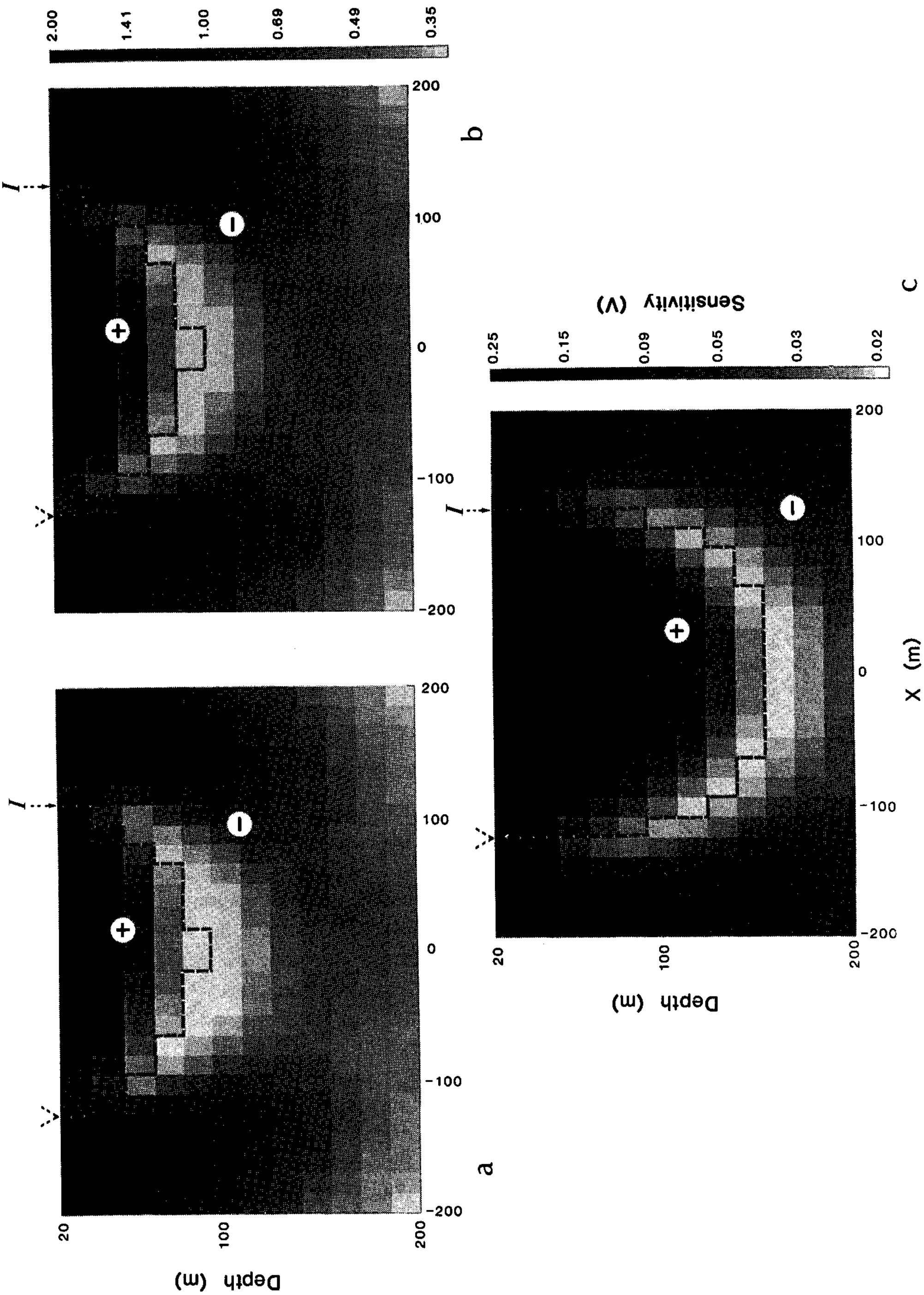
Once the adjoint Green's function has been obtained, the sensitivity of the corresponding transformed potential can be computed from

$$\tilde{\phi}_{jk}(x_0, K_y, z_0) = \int_D \left[K_y^2 \psi_{jk} \tilde{\phi} - \frac{\partial}{\partial x}\left(\psi_{jk} \frac{\partial \tilde{\phi}}{\partial x}\right) - \frac{\partial}{\partial z}\left(\psi_{jk} \frac{\partial \tilde{\phi}}{\partial z}\right)\right] \cdot G^*(x, K_y, z, x_0, z_0)\, \mathrm{d}^2\mathbf{x}. \tag{72}$$

An inverse cosine transform is then required to obtain the sensitivity of the potential in the spatial domain

$$\phi_{jk}(x_0, y_0, z_0) = \frac{2}{\pi} \int_0^\infty \tilde{\phi}_{jk}(x_0, K_y, z_0) \cos(K_y y_0)\, \mathrm{d}K_y. \tag{73}$$

As an illustration of the adjoint-equation method we compute the sensitivities for a half-space of 1000 Ωm. For this example we concentrate on a limited region of the model (i.e. -200 m $< x <$ 200 m and 20 m $< z <$ 200 m). The parametrization of this region is indicated on the cross-sections shown in Figs 3 and 5. Having placed a current electrode at $\mathbf{x}_s = (125, 0, 0)$ m and a potential electrode at $\mathbf{x}_0 = (-125, 0, 0)$ m, the sensitivity of the measured potential to changes in the conductivity of each prism was computed. A total of two forward solutions for each of the nine K_y values used in the inverse transform were needed to obtain all 312 sensitivities. The absolute value of the resulting sensitivities, displayed in cross-section form, are shown in Fig. 3a. These numerically-generated sensitivities compare well with those computed from the analytic solutions for the potential and Green's function, shown in Fig. 3b. We see from the results for the half-space that the sensitivity is largest at those blocks which are near to either of the electrodes. We notice also that the sensitivity can be either positive or negative. There is a region of positive sensitivity at shallow depths in a semicircle between the current and potential electrode; outside this region the sensitivity is negative which means that the potential at the measuring site will decrease when the conductivity increases.



2.00
1.41
1.00
0.69
0.49
0.35
I
V
+
-
200
100
0
-100
-200
20
100
200
Depth (m)
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Sensitivity (V)
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0.02
X (m)
c

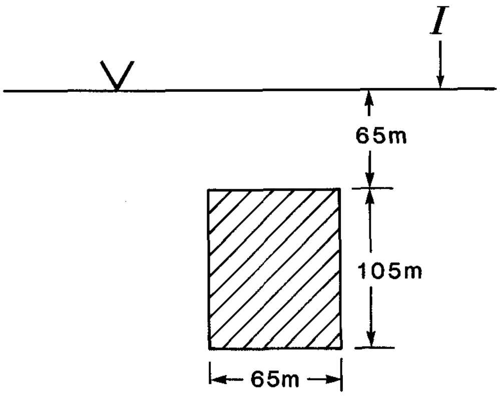

FIG. 4. Cross-section showing a 100 Ωm conductive prism buried in a 1000 Ωm halfspace.

In any inverse problem, one attempts to acquire data which provide complementary information about the earth structure. In the d.c. resistivity problem, we expect different sensitivities if the potential is measured at a different offset in either the x- or y-direction. The sensitivities resulting from changing the offset in the y-direction or strike direction are particularly easy to compute. Having obtained the transformed sensitivity $\tilde{\phi}_{jk}$ for enough values of K_y to allow for an accurate numerical evaluation of (73), one can compute the sensitivity of potentials for different points along the strike direction by simply re-evaluating the inverse transform using different values of y_0. Thus the sensitivities for off-line potentials can be obtained at little additional expense once the on-line sensitivities have been computed. Fig. 3c shows the sensitivity computed for a potential electrode located at $\mathbf{x}_0 = (-125, 200, 0)$ m.

As a final example, the adjoint method was used to compute the sensitivities for the more complicated situation of a conductive body buried in a half-space (Fig. 4). The sensitivities for the same current and on-line potential electrode as in Fig. 3 are shown in Fig. 5. There has been considerable change in the sensitivity pattern caused by the conductive prism. Overall, the amplitudes of the sensitivities have increased and the demarcation between positive and negative sensitivities has been greatly distorted in the region between the two electrodes where the prism lies.

FIG. 3. Absolute sensitivities computed for a 1000 Ωm half-space using (a) the adjoint-equation approach, and (b) the analytic expressions for the potential and Green's function. The current and potential electrodes were located at $\mathbf{x}_s = (125, 0, 0)$ m and $\mathbf{x}_0 = (-125, 0, 0)$ m respectively. (c) Absolute sensitivities computed using the adjoint-equation approach for an off-line potential electrode at $\mathbf{x}_0 = (-125, 200, 0)$ m. The dashed line is the demarcation between positive and negative values of the sensitivities.

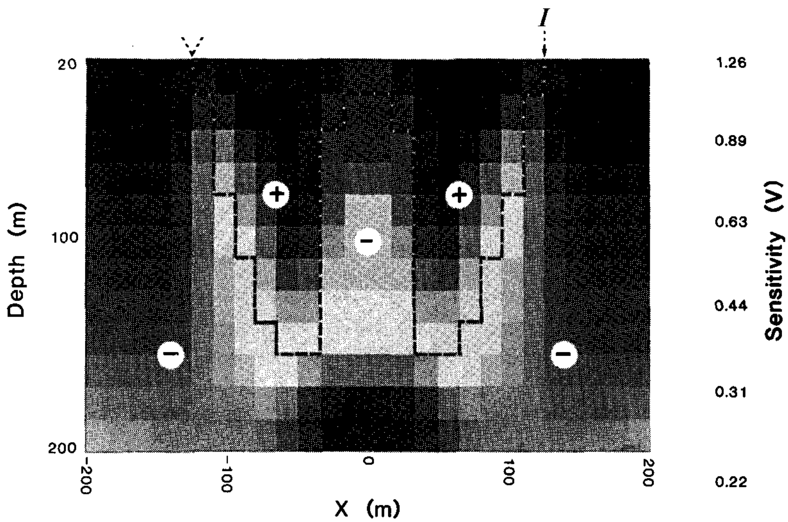

FIG. 5. Absolute sensitivities computed for the conductive prism model shown in Fig. 4 using the adjoint-equation approach.

SUMMARY

The efficient solution of the non-linear inverse problem requires that the dependence of the data on changes in the model be easily quantified. The most convenient way of quantifying this dependence is to derive the analytic Fréchet derivative using one of the three procedures described in this paper. In most cases, however, it is not possible to derive an analytic expression for either the forward responses or the Fréchet derivatives, so one must resort to a model parameterization to simplify the problem. The dependence of the data on changes in the model is then given by a set of partial derivatives or sensitivities. These sensitivities can be computed from their finite-difference approximation, although this requires the solution of a large number of forward problems. When dealing with boundary-value problems we can derive a new set of equations whose solution yields either the sensitivities themselves or quantities from which the sensitivities can be calculated. The similarity of these new equations and the original forward problem allows the sensitivities to be computed efficiently if a numerical solution based on a matrix factorization is used.

ACKNOWLEDGEMENTS

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APPENDIX A

Forward responses for the 1D resistivity problem

Let the earth be represented by a sequence of M_L layers of constant conductivity over a half-space. Within any of the layers or the half-space, the governing differential equation for the 1D resistivity problem reduces to

$$\frac{\mathrm{d}^2 h}{\mathrm{d}z^2} - \lambda^2 h = 0. \tag{A1}$$

The general solution to (A1) for the kth layer can then be written as

$$h(\lambda, z) = U_k \mathrm{e}^{-\lambda(z_{k-1} - z)} + D_k \mathrm{e}^{\lambda(z_{k-1} - z)}, \tag{A2}$$

and for the half-space, as

$$h(\lambda, z) = D_{M_L} + 1\, \mathrm{e}^{\lambda(z_{M_L} - z)}. \tag{A2b}$$

Making use of the continuity relationship

$$h(\lambda, z_k^+) - h(\lambda, z_k^-) = 0, \tag{A3}$$

and the conservation of charge relationship

$$\frac{\sigma_{k+1}}{\lambda}\frac{\mathrm{d}}{\mathrm{d}z} h(\lambda, z_k^+) - \frac{\sigma_k}{\lambda}\frac{\mathrm{d}}{\mathrm{d}z} h(\lambda, z_k^-) = \begin{cases} \dfrac{I}{2\pi} & \text{for } k = k_s \\ 0 & \text{otherwise,} \end{cases} \tag{A4}$$

one can solve for the coefficients U and D for the kth layer in terms of those for the $(k+1)$th layer. This leads to the propagator matrix expression

$$\begin{pmatrix} U_k \\ D_k \end{pmatrix} = \mathbf{A}_k \begin{pmatrix} U_{k+1} \\ D_{k+1} \end{pmatrix} + \mathbf{s}_k, \tag{A5}$$

where

$$\mathbf{A}_k = \begin{bmatrix} \mathrm{e}^{-\lambda d_k} & 0 \\ 0 & \mathrm{e}^{\lambda d_k} \end{bmatrix} \frac{1}{t_k} \begin{bmatrix} 1 & r_k \\ r_k & 1 \end{bmatrix}$$

and

$$t_k = \frac{2\sigma_k}{\sigma_k + \sigma_{k+1}}, \qquad r_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_k + \sigma_{k+1}}.$$

The source vector $\mathbf{s}_k$ is given by

$$\mathbf{s}_k = \begin{cases} \dfrac{I}{4\pi\sigma_k} \begin{pmatrix} \mathrm{e}^{-\lambda d_k} \\ -\mathrm{e}^{\lambda d_k} \end{pmatrix} & \text{for } k = k_s \\ \mathbf{0} & \text{otherwise.} \end{cases}$$

Combining the propagator matrix expressions for each layer yields

$$\begin{pmatrix} U_1 \\ D_1 \end{pmatrix} = \mathbf{A}_1\mathbf{A}_2 \cdots \mathbf{A}_{M_L}\begin{pmatrix} 0 \\ D_{M_L+1} \end{pmatrix} + \mathbf{A}_1\mathbf{A}_2 \cdots \mathbf{A}_{k_s-1}\mathbf{s}_{k_s}. \tag{A6}$$

U_1 and D_1 can be related using the boundary condition at $z = 0$ which requires that $h(\lambda, z)$ satisfy

$$-\frac{\sigma_1}{\lambda}\frac{\mathrm{d}}{\mathrm{d}z}h(\lambda, 0^+) = -\sigma_1(U_1 - D_1) = \begin{cases} \dfrac{I}{2\pi} & \text{for surface electrode,} \\ 0 & \text{for buried electrode.} \end{cases} \tag{A7}$$

The solution $h(\lambda, 0) = U_1 + D_1$ is then obtained from (A6) and (A7).

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