Applied geophysical inversion

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SUMMARY

Using the 2-D DC-resistivity tomography experiment as an example, we examine some of the difficulties inherently associated with constructing a single maximally smooth model as a solution to a geophysical inverse problem. We argue that this conventional approach yields at best only a single model from a myriad of possible models and at worst produces a model which, although having minimum structure, frequently has little useful relation to the earth that gave rise to the observed data. In fact in applied geophysics it is usual to have significant prior information which is to be supplemented by further geophysical experiments. With this perspective we suggest an alternate approach to geophysical inverse problems which emphasizes the prior information and includes the data from the geophysical experiment as a supplementary constraint. To this end we take all available prior information and construct an inversion algorithm which, given an arbitrary starting model and the absence of any data, will produce a preconceived earth model and then introduce the observed data into the inversion to determine how the prior earth model is influenced by the supplementary geophysical data.

Key words: inversion, tomography.

1 INTRODUCTION

Geophysical inverse problems are notoriously ill-posed (Tikhonov & Arsenin 1977), primarily because of the non-uniqueness resulting from sparse noisy data and the need to finely parameterize the earth so that sufficient variation is allowed in the solution. In order to overcome this ill-posedness, many regularizing schemes have been invented, and sometimes re-invented, all under the guise of various physical, mathematical or empirical motivations e.g. Marquardt (1970), maximum likelihood (Tarantola & Valette 1982), Occam's razor (Constable, Parker & Constable 1987), etc. While the practitioners of a particular regularization scheme often advocate their favourite technique with almost religious zeal, it must be remembered that all these techniques are simply different forms of regularization of an ill-posed inverse problem. The common perspective in these schemes is that the data is given and geophysical inversion should produce a single model which fits the data. Unfortunately, experience shows that this conventional approach can be of limited value in applied geophysical problems, as we shall illustrate in Section 3.

The main difficulty with the conventional approach is that it is attempting the impossible. By producing a single model to a fundamentally non-unique inverse problem the bias of the geophysicist is inevitably introduced. The sentiment of may geophysicists is echoed by Menke (1984, p. 49) 'There is something unsatisfying about having to add *a priori* information to an inverse problem to single out a solution'. One alternative is to give up the idea of generating a single model, perhaps using appraisal and inference methods (e.g. Backus & Gilbert 1976) or the method of funnel functions (Oldenburg 1983). While these methods are highly recommended they are computationally cumbersome for realistic applied inverse problems.

In this paper we advocate an alternative to the conventional approach. Our approach looks at the inverse problem from a different perspective. In applied geophysics we often have significant prior knowledge about the earth under investigation. Such information may come, for example, from the local geology or other geophysical experiments. In fact, it seems rather rare for a geophysical survey to be conducted over a region about which *nothing* is known. Consequently, we suggest looking at the applied geophysical inverse problem from the following perspective: given certain prior information about the earth then how does the observed geophysical data constrain or modify that prior information? This perspective can be converted into an inversion algorithm by minimizing an objective function based on prior model character with an additional

data-misfit constraint. Such an inversion algorithm is briefly outlined in Section 2 and its utility is shown in Sections 4 and 5

In order to put our advocacy in context with existing methods, it is useful to classify conventional inverse theory into three categories (Menke 1984); length methods, generalized inverse methods, and maximum likelihood methods. The perspective that we advocate falls under the category of length methods and what makes it distinct from the conventional length method is the amount of emphasis placed on the prior information, or equivalently, the model-weighting function. The examples presented later will clarify this distinction.

A primary motivation for our work has been the need to be able to incorporate prior information from geological or geotechnical constraints, often of a geometric nature, into an inversion scheme. For example, if a conductivity variation is known to be constrained geometrically, this information must be incorporated into the inversion. The naive 'smoothest' model is usually rather unsatisfactory.

2 THE INVERSION ALGORITHM

We have advocated that applied geophysical inversion should be approached from the perspective of prior information constrained by observed data rather than the more usual approach of observed data inverted with a regularization scheme. In order to solve an inverse problem in this manner it is frequently convenient to begin by parameterizing the model space using a set of M basis vectors. The 'model', \mathbf{m} , is then simply an element of R^M .

In the absence of any geophysical data, we require that the inversion algorithm takes an arbitrary starting model and produces a model consistent with the prior information. This can be accomplished by defining an objective function,

$$\phi_{\mathbf{m}}[\mathbf{m}] = \|\mathbf{W}_{\mathbf{m}}(\mathbf{m} - \mathbf{m}_{0})\|^{2} \tag{1}$$

where \mathbf{m}_0 is a base model and \mathbf{W}_m is a weighting matrix which is designed so that a model is produced with specific characteristics consistent with prior information. The matrix \mathbf{W}_m and the base model, \mathbf{m}_0 , contain the prior information and, in realistic applied problems, will be extremely complicated requiring a major effort to be expended at the beginning of the inversion. For example, some of the considerations which must be addressed at this stage are:

- (1) generating a base model. A base model may come from analysis of other geophysical data, from drill-hole logs, from geological constraints, etc.
- (2) Determining regions where the true earth is likely to be close to the base model and regions where the discrepancies might be large.
- (3) Deciding what type of 'smoothness' is required, e.g. whether horizontal smoothness is required as might be the case for sedimentary basins, or vertical smoothness in heavily faulted regions. Further consideration should be given as to whether an l_1 -norm should be used to produce blocky models, or an l_2 -norm for smoother models, and whether first- or second-model derivatives should be used, etc.
- (4) Deciding if there are areas where smoothing should be relaxed, e.g. in a region near a fault.

(5) Determining the relative weights of the components of \mathbf{W}_{m} which allow a relative trade-off between the different components in the model norm.

The minimization of ϕ_m yields a model that is close to \mathbf{m}_0 with the metric defined by \mathbf{W}_m and so the characteristics of the recovered model are directly controlled by these two quantities. The minimization of ϕ_m is our primary objective and, in the absence of data constraints, should produce the prior model.

Data constraints can be incorporated in the following manner. In a typical geophysical inverse problem we are supplied with N observations d_j^{obs} and their estimated uncertainties, and we wish to use these observations as constraints on the minimization problem of eq. (1). The relationship between the jth datum and the model is $d_j = g_j[\mathbf{m}]$. The functionals g_j are assumed known. The data misfit may be characterized by

$$\phi_{d}(\mathbf{d}) = \|\mathbf{W}_{d}(\mathbf{d} - \mathbf{d}^{\text{obs}})\|^{2}$$
(2)

were $\mathbf{W}_{\rm d}$ is an $N \times N$ matrix. If the noise contaminating the jth observation is an uncorrelated Gaussian random variable, having zero mean and standard deviation σ_j then an appropriate form for $\mathbf{W}_{\rm d}$ is $\mathbf{W}_{\rm d} = {\rm diag}\{1/\sigma_1,\ldots,1/\sigma_N\}$. With such assumptions, $\phi_{\rm d}$ is a random variable distributed as chi-squared with N degrees of freedom. The expected value of $\phi_{\rm d}$ is therefore approximately equal to N and accordingly, the model sought from the inversion algorithm should reproduce the observations to about this value. The inverse problem then becomes

minimize
$$\phi_{\mathbf{m}}[\mathbf{m}] = \|\mathbf{W}_{\mathbf{m}}(\mathbf{m} - \mathbf{m}_0)\|^2$$

such that $\phi_{\mathbf{d}}^* = \|\mathbf{W}_{\mathbf{d}}(\mathbf{d} - \mathbf{d}^{\text{obs}})\|^2$ (3)

where ϕ_d^* represents the expected χ^2 data misfit.

The constrained minimization problem, eq. (3), may be solved using the method of Lagrange multipliers. The appropriate objective function to be minimized is

$$\phi[\mathbf{m}] = \phi_{\mathbf{m}}[\mathbf{m}] + \mu[\phi_{\mathbf{d}}[\mathbf{d}] - \phi_{\mathbf{d}}^*] \tag{4}$$

where μ is the Lagrange multipler. The inverse problem is non-linear and is attacked by linearizing eq. (4) about the current model $\mathbf{m}^{(n)}$ and iterating. If $\delta \mathbf{m}$ is a model perturbation, then a Taylor expansion that has terms only up to second order is

$$\phi[\mathbf{m}^{(n)} + \delta \mathbf{m}] = \phi_{\mathbf{m}} + \gamma_{\mathbf{m}} \cdot \delta \mathbf{m} + \frac{1}{2} \delta \mathbf{m}^{\mathrm{T}} \mathbf{H}_{\mathbf{m}} \delta \mathbf{m} + \mu \{ \phi_{\mathbf{d}} + \gamma_{\mathbf{d}} \cdot \delta \mathbf{m} + \frac{1}{2} \delta \mathbf{m}^{\mathrm{T}} \mathbf{H}_{\mathbf{d}} \delta \mathbf{m} - \phi_{\mathbf{d}}^{*} \}$$
(5)

where $\gamma_{\rm m} = \nabla_{\rm m}\phi_{\rm m}$ and $\gamma_{\rm d} = \nabla_{\rm m}\phi_{\rm d}$ are gradient vectors, $\mathbf{H}_{\rm m} = \nabla_{\rm m}\nabla_{\rm m}\phi_{\rm m}$ and $\mathbf{H}_{\rm d} = \nabla_{\rm m}\nabla_{\rm m}\phi_{\rm d}$ are Hessian matrices and $\nabla_{\rm m}$ is the operator $(\partial/\partial m_1, \, \partial/\partial m_2, \, \dots, \, \partial/\partial m_M)^{\rm T}$. In eq. (5) $\phi_{\rm m}$ is understood to be $\phi_{\rm m} [\mathbf{m}^{(n)}]$ and $\phi_{\rm d} [\mathbf{d}^{(n)}]$.

The general solution proceeds by differentiating eq. (5) with respect to $\delta \mathbf{m}$ and μ to obtain an $M \times M$ system of equations to be solved for $\delta \mathbf{m}$, and a constraint equation used to evaluate the misfit and hence adjust the value of μ . Recent investigations have shown that the subspace method (Oldenburg, McGillivray & Ellis 1992; Kennett & Williamson 1988; Skilling & Bryan 1984) is an efficient method of solution for large-scale systems. In a subspace approach, the 'model' perturbation $\delta \mathbf{m} \in R^M$ is restricted to

lie in a q-dimensional subspace of R^M which is spanned by the vectors $\{\mathbf{v}_i\}$ i=1, q. The model perturbation can be written as

$$\delta \mathbf{m} = \sum_{i=1}^{q} \alpha_i \mathbf{v}_i \equiv \mathbf{V} \boldsymbol{\alpha} \tag{6}$$

and is therefore specified once the parameters α_i are determined. One particular advantage to this approach is that, by judicious choice of the basis vectors, prior information can be incorporated into the inversion. For example, if the basis vectors span only a subspace of the model space then the inversion result will be constrained to lie in that subspace. This type of control over the final-inversion result is a useful adjunct to control via the model norm $\mathbf{W}_{\mathbf{m}}$.

The equations for the subspace formulation are generated by substituting (6) into (5) to yield

$$\phi[\mathbf{m}^{(n)} + \mathbf{V}\alpha] = \phi_{\mathbf{m}} + \gamma_{\mathbf{m}}^{\mathbf{T}} \mathbf{V}\alpha + \frac{1}{2}\alpha^{\mathbf{T}} \mathbf{V}^{\mathbf{T}} \mathbf{H}_{\mathbf{m}} \mathbf{V}\alpha + \mu \{\phi_{\mathbf{d}} + \gamma_{\mathbf{d}}^{\mathbf{T}} \mathbf{V}\alpha + \frac{1}{2}\alpha^{\mathbf{T}} \mathbf{V}^{\mathbf{T}} \mathbf{H}_{\mathbf{d}} \mathbf{V}\alpha - \phi_{\mathbf{d}}^* \}.$$
(7)

This is a quadratic objective function to be solved for the parameter vector α . Differentiating (7) with respect to α and setting the resultant equation equal to zero yields

$$\mathbf{V}^{\mathrm{T}}(\mathbf{H}_{\mathrm{m}} + \mu \mathbf{H}_{\mathrm{d}})\mathbf{V}\alpha = -\mu \mathbf{V}^{\mathrm{T}} \mathbf{\gamma}_{\mathrm{d}} - \mathbf{V}^{\mathrm{T}} \mathbf{\gamma}_{\mathrm{m}}. \tag{8}$$

This system of equations is solved iteratively. At each iteration the solution of this system requires that a line search be carried out to find the value of the Lagrange multipler μ so that a specific target value ϕ_d^* is achieved. This involves an initial guess for μ , solving eq. (8) by SVD for the vector $\boldsymbol{\alpha}$, computing the perturbation $\boldsymbol{\delta m}$, carrying out the forward modelling to evaluate the true responses

and misfit, then adjusting μ . The estimation of an acceptable value of μ typically requires 3 or 4 forward modellings. Final convergence is reached when the data misfit equals the final target misfit and the model norm is minimized.

3 CONVENTIONAL FLATTEST MODEL INVERSION

The difficulties inherent in the conventional inversion perspective that take the observed data and invert it to find a 'flattest' model, are clearly illustrated by the following example which was motivated by tomographic DC-resistivity monitoring done in conjunction with an in situ vitrification (ISV) experiment (Oma, Farnworth & Russin 1982) conducted by ORNL and the University of Tennessee. As a 2-D simulation of the melt phase of the ISV experiment, let us consider a pole-pole DC-resistivity experiment over an earth model consisting of two conductors buried in a resistive host, see Fig. 1, with boreholes located at x = -5.5 m and x = +5.5 m. Electrodes are placed in the boreholes at depths z = 0.50, 1.72, 2.95, 4.15 and 5.95 m. Each electrode is used in turn as a current electrode and the potential is recorded at all other electrodes. This arrangement produces 90 potential measurements, to which 1 per cent unbiased Gaussian noise has been added; these noisy potentials form the observed data for the following inversions.

The observed data were inverted in the conventional sense to find the flattest model. This inversion embodies the spirit of the archetypal Occam inversion (Constable, Parker & Constable 1987, p. 293, above eq. 6)

minimize
$$\phi = \|\nabla(\mathbf{m} - \mathbf{m}_0)^2\| + \mu^{-1} \|\mathbf{W}_d(\mathbf{d} - \mathbf{d}^{\text{obs}})\|^2$$
. (9)

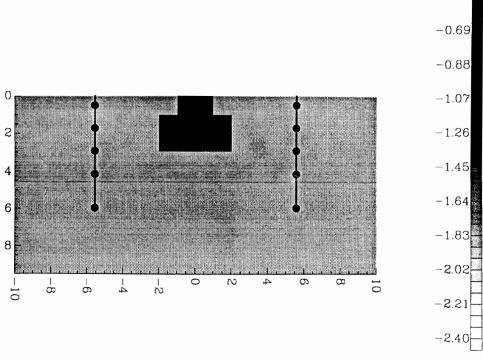


Figure 1. The true 2-D conductivity model used to generate the synthetic data. The resistive host has a conductivity of $0.01 \, \mathrm{S} \, \mathrm{m}^{-1}$ and the large and small conductors have conductivities 1. $\mathrm{S} \, \mathrm{m}^{-1}$ and $0.1 \, \mathrm{S} \, \mathrm{m}^{-1}$ respectively. The scale on the right-hand-side gives $\log_{10} \sigma$, the vertical and horizontal axes are in metres.

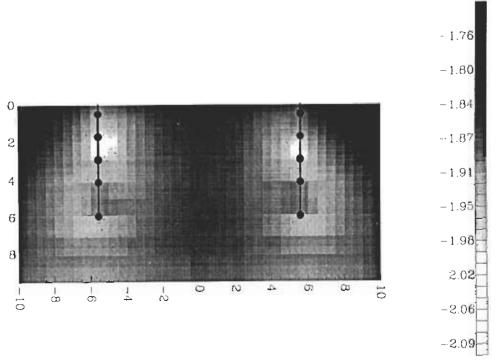


Figure 2. The result of the conventional flattest model inversion of data generated by 2-D forward modelling the model shown in Fig. 1. The scale on the right-hand-side gives $\log_{10} \sigma$, the vertical and horizontal axes are in metres.

The resulting model is shown in Fig. 2 and gives predicted data which have a $\chi^2 = 90$ misfit compared with the observed data. Note that $\chi^2 = 90$ corresponds to a global percentage rms error of 1 per cent. The desired misfit was achieved using a line search to find the appropriate value of the trade-off parameter μ^{-1} . The reference model was chosen to be a constant with the background conductivity, $m_0(x, z) = 0.01 \,\mathrm{S\,m^{-1}}$, however, the reference model has very little influence on the final-inversion result since it is annihilated by the operator ∇ . If the square root of the first term in the objective function, eq. (9), is used as a measure of the 'flatness' of the model, then the flatness of the original model which was used to generate the synthetic data is 663, while the 'flatness' of the model shown in Fig. 2 is 6.4. Whilst the flattest model is extremely flat, note that the conductivity variation is predominantly around the boreholes and that the conductivity distribution is bounded by $0.008 < \sigma(x, z) < 0.018 \,\mathrm{S\,m^{-1}}$. Clearly this inversion result shows very little resemblance to the true model. This is a demonstration of the limitation of producing a single model with minimum structure, in the face of the non-uniqueness inherent in most geophysical experiments with a finite number of noisy data and poor angular coverage. In particular, we emphasize that the result of this inversion is entirely subjective: an arbitrary (although plasuible) choice of regularization has been made which leads to an arbitrary (flat) model being produced.

4 INCORPORATING PRIOR INFORMATION USING MODEL NORMS

There are a number of ways of obtaining reliable information from noisy inaccurate data, for example, the work of Backus & Gilbert (1976) on appraisal and

inference, or the method of funnel functions (Oldenburg 1983), however, such methods are too numerically demanding to be applied to 2-D inverse problems. Yet, geophysicists must do more than simply computing the flattest model in the conventional style. This has led us to formulate an alternative perspective for the geophysical inverse problem, which we now apply to the DCtomography experiment. The first step is to collect prior information and to design a weighting matrix \mathbf{W}_{m} . To be specific we know that the ISV melt zone is confined to the region between the borehole and it is conjectured, on the basis of thermodynamic arguments, that the melt zone consists of a conducting core of molten material surrounded by a resistive halo of desiccated earth all enveloped by a warm moist conducting shell. Whether the overall response of the melt zone is conductive or a resistive is unknown. Hence we assume:

- (1) the conductivity should vary smoothly.
- (2) Conductivity variation is more likely to occur in the region centred between the boreholes.
- (3) The background conductivity is in the vicinity of $0.01\,\mathrm{S\,m^{-1}}$.

From this prior information a weighting matrix \mathbf{W}_{m} and a reference model m_0 are constructed. Since we will be working on a 2-D (x, z) inverse problem, it is convenient to restrict the objective function to be the sum of three terms

$$\phi_{\mathbf{m}} = \|\mathbf{W}_{\mathbf{m}}(\mathbf{m} - \mathbf{m}_{0})\|^{2}$$

$$= \phi_{s} + \phi_{x} + \phi_{z}$$

$$= \alpha_{s} \|\mathbf{W}_{s}(\mathbf{m} - \mathbf{m}_{0})\|^{2} + \alpha_{x} \|\mathbf{W}_{x}(\mathbf{m} - \mathbf{m}_{0})\|^{2}$$

$$+ \alpha_{z} \|\mathbf{W}_{z}(\mathbf{m} - \mathbf{m}_{0})\|^{2}$$

$$= (\mathbf{m} - \mathbf{m}_{0})^{T} \{\alpha_{s} \mathbf{W}_{s}^{T} \mathbf{W}_{s} + \alpha_{x} \mathbf{W}_{x}^{T} \mathbf{W}_{x} + \alpha_{z} \mathbf{W}_{z}^{T} \mathbf{W}_{z}\}$$

$$\times (\mathbf{m} - \mathbf{m}_{0})$$
(10)

where \mathbf{W}_{s} , \mathbf{W}_{x} , \mathbf{W}_{z} will be used to separately control smallness of the model relative to the reference model, the x-variation of the model, and the z-variation of the model, respectively. For this case, \mathbf{W}_{s} is a diagonal matrix with elements $f_{ij}^{s}\sqrt{\Delta x_{i}}\,\Delta z_{j}$ where Δx_{i} is the length of the ijth cell and Δz_{j} is its thickness, \mathbf{W}_{x} has elements $\pm f_{ij}^{s}\sqrt{\Delta z_{i}/dx_{j}}$ where dx_{i} is the distance between the centres of horizontally adjacent cells, and \mathbf{W}_{z} has elements $\pm f_{ij}^{s}\sqrt{\Delta x_{i}/dz_{j}}$ where dz_{j} is the distance between the centres of vertically adjacent cells.

In order to incorporate the prior information that the conductivity variation should be manifest between the boreholes we have incorporated spatial weighting functions $f_{ij}^{*,x,z}$ into W_{m} . If $f_{ij}^{*}=1$ then the deviation of the final model from the base model for any cell has the same penalty. Instead, for the ISV example, choosing f_{ij}^{*} given by

$$f_{ij}^{s} = \max \left\{ 0.02, \ 1 - 1.5 \exp\left(-\left[\left(\frac{x_{i} - x_{0}}{\Delta x}\right)^{2} + \left(\frac{z_{j} - z_{0}}{\Delta z}\right)^{2}\right]\right) \right\}$$
 (11)

corresponds to the likelihood of greater model deviation from the base model in the region surrounding x_0 , z_0 . The scale factors 0.02 and 1.5 control the amount of deviation and Δx , Δz , x_0 and z_0 control the geometry of the deviation from the prior model. For this example we choose Δx , $\Delta z = 3$, 3 and $(x_0, z_0) = (0., 2.)$ m corresponding to model deviation between the boreholes. Since we expect model variation to occur in the vicinity of model deviation we set $f^x = f^z = f^s$. It remains to choose a base model, and since the background conductivity is assumed to be 0.01 S m⁻¹ and the conductivity in the melt zone is too complex to model a priori, we set $m_0 = 0.01$ S m⁻¹. With these choices

any starting model will converge to the constant model $\sigma = 0.01 \, \text{S m}^{-1}$ in the absence of data constraints.

Using eq. (10), and incorporating data constraints in the inversion outlined in Section 2, gives the result shown in Fig. 3. This model gives predicted data which fits the observed data to $\chi^2 = 90$ with an objective function eq. (10) measure of $\sqrt{\phi_m} = 2.5$ which is to be compared with the $\sqrt{\phi}_{\rm m}$ = 25 for the true model. The contributions to the model norm and misfits are shown in Table 1. Notice that a major improvement has been achieved towards an inversion result, which in some general sense, reproduces the true model. What is more important is the following: we can conclude that, given the prior information listed above then a conducting zone between the borehole is implied by the observed data. This might be compared to the conventional flattest model inversion which implies that there exists at least one model that fits the data and has effectively no structure in the inter-borehole region.

By varying the weight function, f_{ij} , a variety of models with equal misfit may be constructed. For example, if the prior information is modified slightly so that the conductivity variation is expected anywhere in the region between the electrodes with equal likelihood, we could repeat the inversion with a model norm of the form

$$f_{ij} = \begin{cases} 1 & (x_i, z_j) \notin \mathcal{R} \\ 0.02 & (x_i, z_j) \in \mathcal{M} \end{cases} \quad \mathcal{R} = \{(x, z) : -2 \le x \le 2, z \le 3\}.$$
(12)

This choice of f_{ij} produces the model shown in Fig. 4 with the inversion statistics shown in Table 2.

We now have three models which give predicted data that

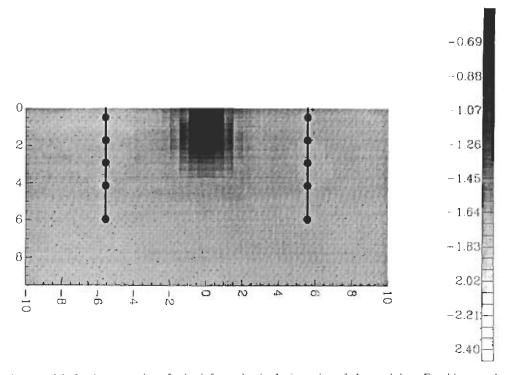


Figure 3. The resultant model after incorporation of prior information in the inversion of observed data. For this example a Δx , $\Delta z = 3$, 3 and $(x_0, z_0) = (0, ..., 2)$ Gaussian-model norm were used. The scale on the right-hand side gives $\log_{10} \sigma$, the vertical and horizontal axes are in metres.

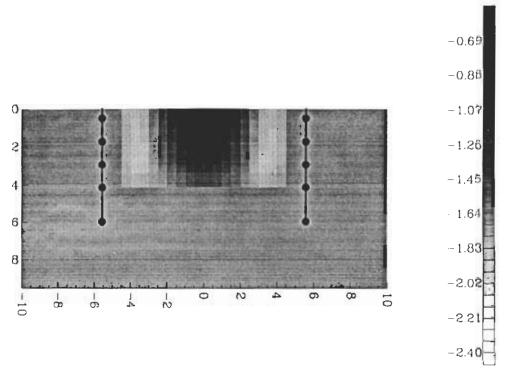


Figure 5. The results of the subspace inversion of data generated by 2-D forward modelling the model shown in Fig. 1. For this example a constant-model-norm weighting was used, with block-basis vectors in the inter-borehole zone. See Table 3. Notice that the model has structure in the melt zone, although comparison with Fig. 1 indicates that the structure is somewhat too shallow, too localized and does not reproduce the geometry of the true model. The scale on the right-hand side gives $\log_{10} \sigma$ and is the same as in Fig. 1. The vertical and horizontal axes are in metres.

Table 3. The χ^2 and model-norm measures for the model shown in Fig. 5.

Model	χ²	φ	ø,	ó _s	ϕ_t
inuc	87	663	1.76	186.	474.
(muerolon	90	66.1	1.24	40.5	24.4

inversion. Typically in the conventional approach, the need for prior information to regularize an inversion is regarded as an unfortunate but necessary fact of life. In this paper we have advocated attaching a much greater significance to prior information. In fact by looking at the inverse problem from the perspective of prior information constrained by observed data, we have shown that useful information can be extracted. In practical terms, it is rare for the applied geophysicist to be interested in knowing how the earth deviates from 'flatness', more often he or she already knows the earth is not 'flat' but rather, wishes to know whether the observed data modify or constrain a prior model. Given this perspective it is natural to construct an inversion algorithm with the prior information incorporated from the beginning and to include the observed data as constraints.

The inversion examples that we presented were based on the tomographic 2-D DC-resistivity inverse problem and were motivated by a geotechnical conductivity-monitoring experiment. The actual details of the field experiment are not relevant to the ideas presented in this paper and for clarity we have confined our attention to noisy synthetic data. Further we emphasize that our theme is not specific to the tomographic DC-resistivity inverse problem, but will apply to any ill-posed inverse problem.

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