# Practical methods for model uncertainty quantification in electromagnetic inverse problems

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## Practical methods for model uncertainty quantification in electromagnetic inverse problems

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**Summary**

Geophysical inverse problems are non-unique. Through regularization and the use of *a priori* information we can derive stable and geologically reasonable inversion models. Providing an analysis of the model uncertainty is necessary for the critical task of separating inversion artifacts from robust geological features. Bayesian inference is a widely used approach but is not tractable for large three-dimensional electromagnetic problems. However, another approach based on extremizing model parameters, which is called most squares, shows great promise for quantifying model uncertainty and is computationally feasible.

**Introduction**

Too often we focus almost entirely on the non-trivial task of finding one solution to a geophysical inverse problem that adequately explains the available data and is geologically reasonable without understanding the tradeoffs or uncertainty in the resulting model. Just finding one solution to a three-dimensional (3D) inverse problem is itself a computationally challenging and time-consuming effort. It is understandable, therefore, that attempts to map out model uncertainty include computing linearized covariance estimates (Duijndam, 1988) or invoking vague hand-waving arguments and the admission that it is a difficult problem that many smart people are working on.

Recently a great deal of effort has been put into developing efficient model uncertainty algorithms based on a Bayesian inference framework and using, for example, Markov chain Monte Carlo (MCMC) to sample the model space (e.g., Sambridge and Mosegaard, 2002; Malinverno, 2002; Chen and Hoversten, 2012). These algorithms are certainly practical for 1D, challenging yet reachable for 2D problems, but application to realistic 3D problems remains elusive, given how much computational effort is required to obtain even one solution. We believe that with increases in computational hardware and research into efficient sampling algorithms, these approaches will eventually be applicable to 3D inverse problems. However, even when the model space can be effectively sampled, the resulting models, which are often numerically interesting but geologically unreasonable, can be difficult to interpret (Tompkins et al, 2011).

In this abstract, we seek more practical ways to quantify model uncertainty for a geophysical inverse model. Furthermore, we wish to find a method that is computationally feasible and dovetails with our existing and extensive suite of numerical software, which are deterministic gradient-based algorithms. One such method that meets these requirements is called most squares and was developed by Jackson (1976) for linear inverse problems. The most squares method solves an optimization problem that is a simple extension from standard damped least squares algorithms and whose solutions are the extremal bounds for specified model parameters. Because compensating changes are simultaneously allowed elsewhere in the model, the method admits larger parameter ranges than would be obtained by simply varying one parameter at a time keeping the others fixed (Jackson, 1976). Although it is true that this method only finds model bounds around a linearized inverse model, typically that particular model is the result of many runs optimizing parameters, adding in all available *a priori* information such as well information and geology and therefore represents our best solution. The goal at this point is indeed to find the model bounds around that particular model.

The most squares method was later extended to nonlinear inverse problems by Meju and Hutton (1992) in which they applied the method to the 1D magnetotelluric problem. Subsequently, Meju (1994) showed how it could be used for finding extremal models for inverse problems including *a priori* information, and later for regularized inverse problems (Meju, 2009). Most squares was applied for model appraisal for 2D magnetotellurics (Meju and Sakkas, 2007), but only for amalgamations of model blocks due to the computational effort required at that time. It was applied in resolution analysis of 2D MT models by Kalscheuer and Pedersen (2007) in a linear approach and 1D seismic full-waveform inversion models by Fichtner and Trampert (2011). Since then, it seems to have found little notice in the geophysical community.

In this work, we explore further the utility of the nonlinear most squares method for quantifying uncertainty of models obtained by standard linearized iterative least squares methods, using 1D and 2D magnetotellurics for computational simplicity, before application to larger 3D problems. We briefly summarize the method and then show examples for 1D and 2D magnetotellurics to demonstrate its effectiveness.

**Most squares for nonlinear inverse problems**

The generic geophysical inverse problem can be written as

$$\mathbf{d} = F(\mathbf{m}) + \mathbf{e} \tag{1}$$

where $\mathbf{m}$ is the discrete model vector, $\mathbf{d}$ is the discrete data vector, $\mathbf{e}$ is the error vector, and $F(\mathbf{m})$ represents the forward function that predicts data for a given model $\mathbf{m}$. The geophysical inverse problem is to solve this equation for the unknown model parameters. The standard approach is by regularized iterative least squares in which the solution is taken to be the minimum of a Tikhonov objective function (Tikhonov and Arsenin, 1977)

$$\Psi(\mathbf{m}) = \left(\mathbf{d} - F(\mathbf{m})\right)^T \mathbf{W}\left(\mathbf{d} - F(\mathbf{m})\right) + \lambda \mathbf{m}^T \mathbf{K}\mathbf{m} \tag{2}$$

where $\mathbf{K}$ is the regularizing matrix, representing the spatial roughness of the model, $\mathbf{W}$ is a weighting matrix whose diagonal is specified to be the inverse of the data variances, and $\lambda$ is the regularization parameter, which is a tradeoff between model smoothness and the fit to the data. There are many ways to minimize this objective function including Gauss-Newton and nonlinear conjugate gradients (Rodi and Mackie, 2001). However, because the problem is nonlinear we must linearize around the current model, update the model parameters, and iterate until we have reached the minimum. The Gauss-Newton model update, for example, is given by

$$\mathbf{m}_{i+1} = \mathbf{m}_i - \mathbf{H}_i^{-1}\mathbf{g}_i \tag{3}$$

where $\mathbf{H}$ is the Hessian (ignoring second order terms) and $\mathbf{g}$ is the gradient.

The most squares method maximizes the linear objective function $\mathbf{m}^T\mathbf{b}$, where $\mathbf{b}$ is the parameter projection vector that contains zeros except at the locations for the model parameters that are being maximized where it is set to one. If the value of the normalized squared residuals (the first term of the objective function) is denoted as $q_0$, then we find the maximum of $\mathbf{m}^T\mathbf{b}$ subject to the constraint that the normalized squared residuals do not exceed some target value $q_t$. The minimization is straightforward, and owing to the non-linearity of the problem, we must iterate until we have reached or exceeded the target value. It can be easily shown (Meju and Hutton, 1992) that the model updates are given by

$$\mathbf{m}_{i+1} = \mathbf{m}_i - \mathbf{H}_i^{-1}(\mathbf{g}_i - \mu\mathbf{b}) \tag{4}$$

where $\mu$ is given by the formula

$$\mu = \pm\left(\frac{q_t - q_0}{\mathbf{b}^T\mathbf{H}^{-1}\mathbf{b}}\right)^{1/2} \tag{5}$$

and there are two solutions representing the min/max bounds or solution envelopes for those model parameters.

**Examples**

We begin from simple 1D models in order to evaluate this approach and because it is easier to visualize the results. We use a 1D model from Whittall and Oldenburg (1992) that was derived for their review of 1D MT inverse methods. This geologically plausible model comprises four layers over a half-space. Synthetic data were generated at 14 logarithmically spaced frequencies from 1000 to 0.0003 Hz. Random Gaussian noise of 5% magnitude was added to the data prior to inversion. The smooth inversion model had 54 layers with thickness increasing logarithmically with depth, starting from 10m for the first layer and growing by a factor of 1.2 thereafter.

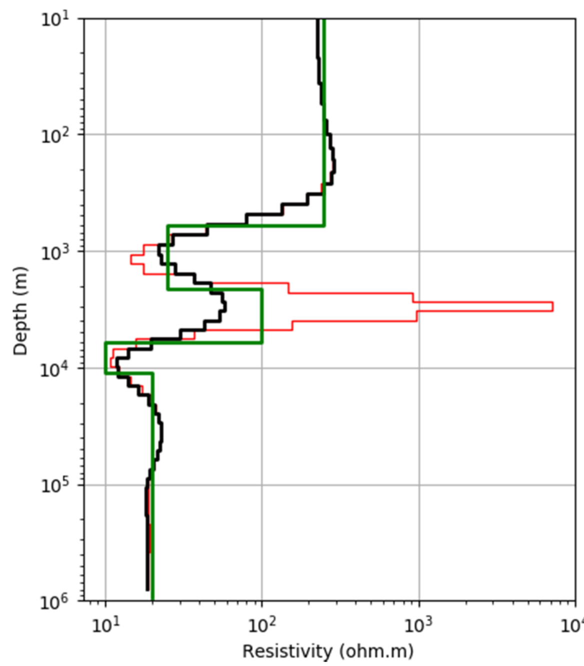


Figure 1: Smooth 1D inverse (least-squares) model shown in black, the true model in green, and one extremal (most-squares) model in red.

The starting model for the inversion was a 20 ohm-m half space; the data were fit to a normalized RMS of 1.056 in a few Gauss-Newton iterations. We then carried out an iterative nonlinear most squares analysis finding the two extremal values for each layer in the model where we set $q_t$ = 1.2 $q_0$, equivalent to a normalized RMS value of 1.156. An example of one such model is shown in Figure 1 where we have extremized layer 22 in the inverse model (2700-3200m depth) which is in the deeper resistive layer of the true model. This extremal model comports with the well-known fact that MT is generally insensitive to resistive zones.

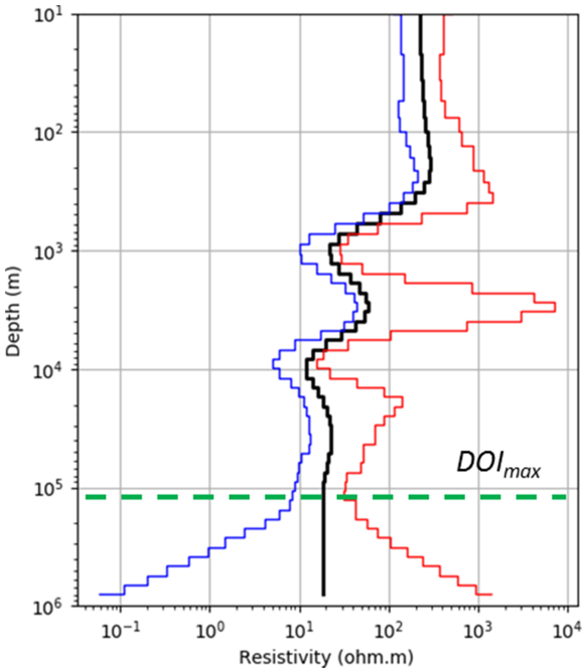


Figure 2: Smooth 1D inverse (least-squares) model shown in black with the lower and upper bounds of all the extremal (most-squares) models in blue and red. Also indicated by the green dashed line is the maximum depth of investigation where the extremal models diverge.

One can collect all the minimum and maximum values for each layer creating an envelope representing the bounds of extremal values for the inverse model. Such a result for the 1D model under discussion is shown in Figure 2. It is clear that the resistive layers can have larger variations with respect to the conductive zones. Furthermore, we can define the maximum depth of investigation (Oldenburg and Li, 1999) as the depth at which the two extremal bounding curves diverge. In other words, below this depth the model is not constrained by any data and should be excluded from interpretation. Overall, this approach gives reasonable model bounds that agree with our understanding of the physics of EM induction.

Alternatively, Meju and Hutton (1992) suggest that one could also set the projection vector **b**=1, that is extremizing all model parameters simultaneously, in order to provide a solution envelope. However, for 1D models we find that the regularization and the small number of model parameters strongly constrains the inverse model and the envelope solution tends to exclude large variations in the model parameters.

Next, we applied the nonlinear most squares method to a synthetic 2D MT dataset that was based on a real exploration problem. For this example, we created a 2D resistivity model (Figure 3, top panel) using a seismic tomography velocity model for structural information and a smooth MT inversion of real data in order to set resistivity values. Synthetic 2D MT data (TM and TE) were generated at 20 frequencies from 100 to 0.01 Hz and 30 sites and then 5% random Gaussian noise was added to the data before inversion.

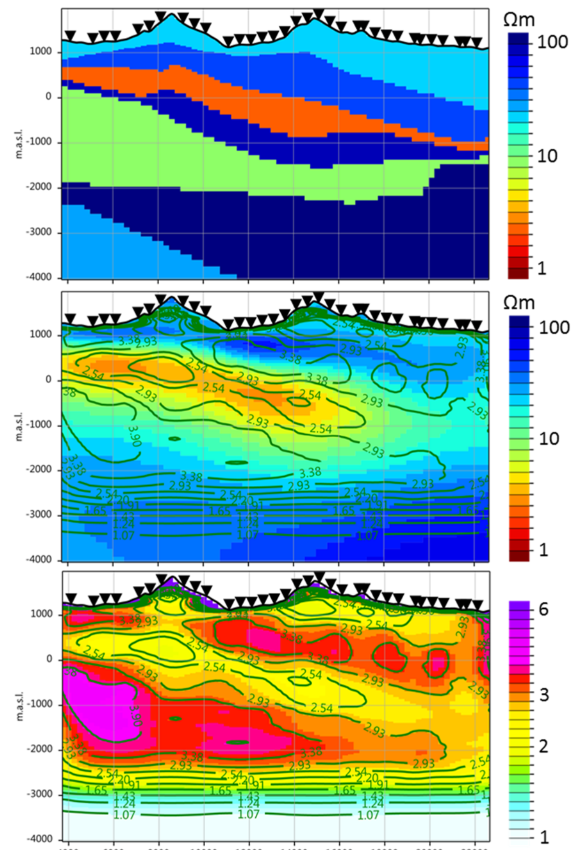


Figure 3: Top panel: true model used to generate synthetic data. Middle panel: smooth inversion model plotted using the color scale on the right, with the ratio of max/min extremal values plotted as contours. Lower panel: a color plot of the ratio of max/min extremal values also with contour lines.

The starting model for this inversion was a 20 ohm-m half space; the data were fit to a normalized RMS of 1.041 after 40 nonlinear conjugate gradient iterations (Rodi and Mackie, 2001). We then carried out an iterative nonlinear most squares analysis finding the two extremal values for each of the model parameters in the main part of the model (that is, excluding the padding on the sides and at depth) setting $q_t = 1.2\, q_0$, equivalent to a normalized RMS value of 1.140. We computed the ratio of the maximum and minimum values for each model parameter, which are shown as contour lines over the inversion model in the middle panel of Figure 3 and as a separate color plot in the lower panel. A plot of all extremal models as a function of depth at a site located at a horizontal model distance of 9000m is shown in Figure 4.

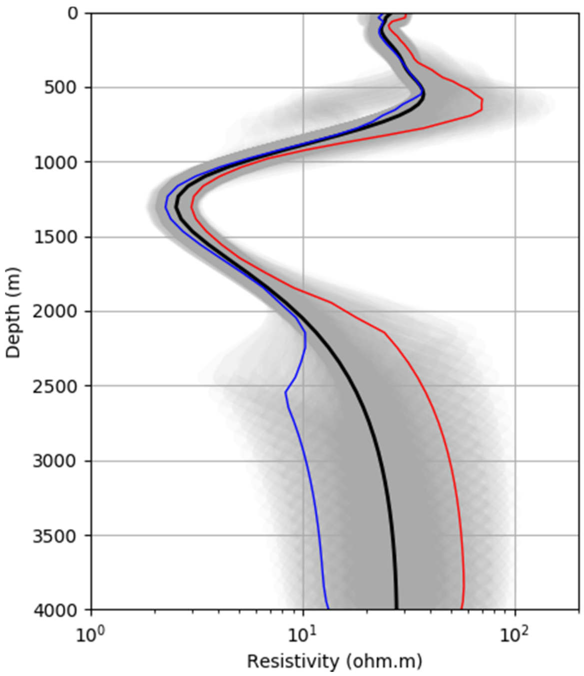


Figure 4: Variation in extremal models versus depth at a site located at a horizontal model distance of 9000m. All extremal models are plotted in light gray and the blue and red bounding represent the 1st and 99th percentile of all ensemble models. The central black line is the smooth 2D inverse model.

Similar to the 1D example, here we see that the conductive zone in general has smaller variations compared to more resistive zones and there is more variability at depth. Even though we have confined the area over which to compute extremal models, and even though we have parallelized the MT forward solutions over frequencies, this analysis still takes a significant amount of time. While certainly feasible for 2D problems, extrapolating to 3D indicates this could still be problematic.

It is reasonable to suggest, then, to extremize blocks of model parameters. We found, for example, that finding the extremal values for 10x10 blocks of model parameters and shifting the analysis by 5 blocks vertically each time significantly speeds up the computations while producing reasonable results (Figure 5). Here it is clear that the model variations are reduced by the effect of regularization over the model blocks being extremized.

The iterative nonlinear most squares optimization typically requires the equivalent computational cost of only 4 to 6 additional inversion iterations per parameter group. For a simple envelope analysis this is a negligible cost, if the added value of a confidence bound is taken into account. Using blocks of cells encourages the extension of this method to 3D problems, where we foresee the possibility for the geophysicist to select a region of interest where uncertainty quantification is desired.

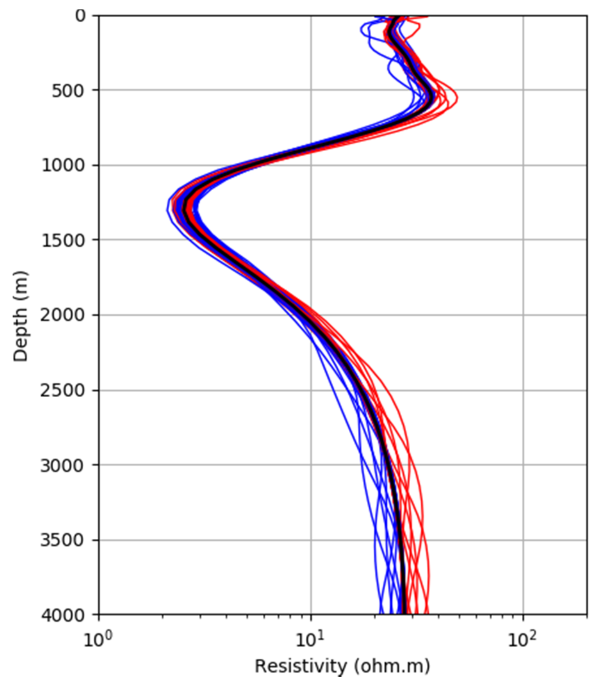


Figure 5: The variation in extremal models versus depth for the same location as shown in Figure 4. Here we have extremized small blocks of model parameters.

## Conclusions

We have implemented the nonlinear most squares optimization method in order to quantify model uncertainty for large scale electromagnetic inverse problems. Testing the method on 1D and 2D problems indicates it should be computationally feasible if applied to judicious choices of model parameters for 3D problems. Although the estimates of model uncertainty are about a linearized model, they would represent model uncertainty about our best inversion models and will help quantify the robustness of certain features in the inverse models. We believe that this will be an invaluable tool in analyzing large-size inverse modeling results and can be applied to any type of geophysical inverse problem.