Linearized model uncertainty analysis of 3D moderate- to large-scale MT inversion based on space transformation and efficient stochastic estimation

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SUMMARY

Geophysical inverse problems are unstable and non-unique. A meaningful solution should be composed of the preferred inversion model and its uncertainty estimates. However, almost all the current three-dimensional (3D) magnetotelluric (MT) inversion studies only offer the preferred model and ignore corresponding uncertainty estimates, which makes separating inversion artifacts from robust geological features impossible. One of the main bottlenecks is the huge computational cost, especially for large-scale 3D MT problems. Here, within the classical linearized model analysis framework, we try to demonstrate a relatively low-cost approach for accurately estimating the diagonal elements of the model covariance matrix by transforming the calculation domain from model space to data space with an efficient stochastic matrix diagonal estimator. The ability to estimate the diagonal of the covariance matrix thus facilitates the introduction of additional tools for model analysis, even for very large inverse problems, with storage and computational costs comparable to those required for obtaining inverse solutions.

Keywords: three-dimensional, magnetotellurics, uncertainty analysis, data-space, stochastic estimation

INTRODUCTION

MT, for example, continent-scale arrays, such as USArray (e.g. Schultz et al. 2023), and other deployments, along with increasingly large-scale inversions are dramatically improving our understanding of the crust, mantle, and whole Earth.

However, we often place excessive focus only on the non-trivial task of finding a single solution to a geophysical inverse problem that adequately explains the available data and is geologically plausible, without fully grasping the uncertainty inherent in the solution. It is understandable that just finding one solution to a 3D inverse problem is itself a computationally challenging and time-consuming effort, therefore, further attempts to figure out model uncertainty including computing linearized covariance estimates (Mackie et al. 2018; Ren and Kalscheuer 2020) is indeed a challenging topic.

Over the past decade, significant effort has been dedicated to advancing model uncertainty algorithms within the Bayesian inference framework (e.g. Peng et al. 2024). While these algorithms, termed as nonlinear global search algorithms, have proven practical for 1D applications and are becoming more attainable yet still challenging for 2D scenarios, their application to 3D moderate- to large-scale MT inversion problems remains elusive. In addition, although these approaches will definitely extended to 3D someday with advancing hardware and efficient sampling, the results are prone to mathematical interesting yet geologically unreasonable and therefore may be hard to interpret (Mackie et al. 2018).

Different from the Bayesian inference theory, linearized model analysis tools were designed mainly for the model analysis of the preferred inversion models which usually be termed “geologically reasonable result” by utilizing suitable regularization and (if applicable) the structural or petrophysical *a prior* information. Quantitative measures of model uncertainty can be computed in terms of the model covariance matrix (Backus and Gilbert 1968). The model covariance matrix describes how uncertainties in the true model, the reference model, and the data translate into uncertainties in the final solution (e.g. Ren and Kalscheuer 2020). The size of the model covariance matrix is $M \times M$, where M is the number of the model parameter. For 1D and 2D inversion problems, storage and direct computation of the generalized inverse matrix as well as the corresponding covariance matrix is not a big problem. However, for 3D moderate- to large-scale inversion problems, M can be easily excessed to more than a few tens of thousands, making computing the inverse of a dense matrix with $M \times M$ size challenging and impractical.

In this abstract, we seek a practical way to quantify model uncertainty for moderate- to large-scale 3D MT inversion problems. This work is mainly inspired by two brilliant ideas to reduce computational costs: (1) transforming the calculation domain from model space to data space (e.g. Siripunvaraporn and Egbert. 2000), and (2) efficient stochastic matrix diagonal elements estimator (Bekas et al. 2007) originally used in atomic density functional theory. This work facilitates the introduction of an additional tool to perform MT inversion analysis, even for very large inverse problems, with storage and computational costs comparable to those required for obtaining inverse solutions.

METHODOLOGY

Model covariance matrix

The iterative least-squares solution in the (k+1)th iteration of MT inversion can be expressed as (e.g. Kalscheuer et al. 2018):

$$\mathbf{m}_{k+1}(\alpha) = \left[\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}\mathbf{J} + \alpha^2\mathbf{W}_m^{\mathrm{T}}\mathbf{W}_m\right]^{-1}\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}\hat{\mathbf{d}}_k + \mathbf{m}_{\mathrm{r}}$$

$$= \mathbf{J}_{\mathbf{W}}^{-g}\mathbf{W}_{\mathrm{d}}\hat{\mathbf{d}}_k + \mathbf{m}_{\mathrm{r}} \qquad (1)$$

Here, $\mathbf{J}_{\mathbf{W}}^{-g} = \left[\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}\mathbf{J} + \alpha^2\mathbf{W}_m^{\mathrm{T}}\mathbf{W}_m\right]^{-1}\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}$ is the generalized inverse, $\hat{\mathbf{d}}_k = \mathbf{d} - \mathrm{F}[\mathbf{m}_{\mathrm{k}}] + \mathbf{J}(\mathbf{m}_{\mathrm{k}} - \mathbf{m}_{\mathrm{r}})$ is a data difference vector with the nonlinear forward response $\mathrm{F}[\mathbf{m}_{\mathrm{k}}]$, $\mathbf{J}, \mathbf{W}_{\mathrm{d}}, \mathbf{W}_m, \mathbf{m}_{\mathrm{r}}$ is sensitivity matrix, data weighting matrix, model regularizing matrix, and reference model, respectively.

The model covariance matrix that measures the stability of the inverse model can be expressed as (e.g. Kalscheuer et al. 2018):

$$\left[\mathrm{cov}\,\mathbf{m}_{k+1}\right] = E\left[(\mathbf{m}_{k+1} - E[\mathbf{m}_{k+1}])(\mathbf{m}_{k+1} - E[\mathbf{m}_{k+1}])^{\mathrm{T}}\right]$$

$$\approx (\mathbf{I} - \mathbf{R}_{\mathrm{M}})\left[\mathrm{cov}\,\mathbf{m}_r\right](\mathbf{I} - \mathbf{R}_{\mathrm{M}})^{\mathrm{T}} + (\mathbf{J}_{\mathbf{W}}^{-g})(\mathbf{J}_{\mathbf{W}}^{-g\mathrm{T}}) \quad (2)$$

where $\mathbf{R}_{\mathrm{M}} = (\mathbf{J}_{\mathbf{W}}^{-g})(\mathbf{J}_{\mathbf{W}})$ is the model resolution matrix. In the smoothness-constraint inversion schemes (e.g. Usui et al 2017), $\mathbf{m}_r$ has typically reckoned a fixed vector and, hence, [cov $\mathbf{m}_r$] = 0. More conservatively (e.g. Kalscheuer et al. 2018; Gallardo and Meju 2011), the model covariance matrix can be express as:

$$\left[\mathrm{cov}\,\mathbf{m}_{k+1}\right] = \left[\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}\mathbf{J} + \alpha^2\mathbf{W}_m^{\mathrm{T}}\mathbf{W}_m\right]^{-1} \qquad (3)$$

Since the diagonal elements of the model covariance matrix are the standard variances of model parameters (e.g. Ren and Kalscheuer 2020), they can be used as proxies in evaluating model uncertainty, and have big potential in decreasing calculation effort comparing inverting the whole covariance matrix.

Efficient diagonal estimator

For large-scale 2D problems and 3D model analysis cases, the stochastic algorithm originally applied to atomic density functional theory (Bekas et al. 2007) seems to be a good choice considering its high-efficiency nature in estimating the diagonal elements when the matrix is known only via its actions on arbitrary vectors.

Until now, however, fast estimation algorithms based on this efficient stochastic method are only used in seismic tomography problems (e.g. MacCarthy et al. 2011). We believe the MT (and other EM methods) could also expect benefits by using these methods in model resolution and uncertainty analysis. In this abstract, an effort is made for the first time to adapt it to the 3D MT model uncertainty analysis.

Consider a sequence of s M-length random vectors, $\mathbf{v}_1, \ldots, \mathbf{v}_s$, with independent elements drawn from a standard normal distribution. The estimate for the diagonal of an $M \times M$ square matrix $\mathbf{C}$ is then:

$$\mathbf{D}_s = \left[\sum_{k=1}^{s}\mathbf{v}_k \odot \mathbf{C}\mathbf{v}_k\right] \oslash \left[\sum_{k=1}^{s}\mathbf{v}_k \odot \mathbf{v}_k\right] \qquad (4)$$

where $\odot$, $\oslash$ signifies element-wise vector multiplication and division, respectively.

Here we briefly summarize the method:

Stochastic matrix diagonal estimator:

Step1. $\mathbf{t}_0$, $\mathbf{q}_0 = 0$

Step2. **for** k=1…s

(i) Generate a random vector $\mathbf{V}_k$

(ii) $\mathbf{t}_k = \mathbf{t}_{k-1} + \mathbf{v}_k \odot \mathbf{C}\mathbf{v}_k$

(iii) $\mathbf{q}_k = \mathbf{q}_{k-1} + \mathbf{v}_k \odot \mathbf{v}_k$

(iv) $\mathbf{D}_k = \mathbf{t}_k \oslash \mathbf{q}_k$

Step3. **End**

In practice, the choice of s will depend on the desired accuracy of the diagonal determination. MacCarthy et al. (2011) mentioned an s of 256–512 is adequate for many large geophysical inversions. When $\mathbf{C}$ is the covariance matrix, the above calculation can be computed by noting that a matrix-vector product $\mathbf{y} = \mathbf{C}\mathbf{v}_k$ can be rewritten in terms of the known matrices $\mathbf{J}, \mathbf{W}_m$:

$$\mathbf{y} = \left[\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}\mathbf{J} + \alpha^2\mathbf{W}_m^{\mathrm{T}}\mathbf{W}_m\right]^{-1}\mathbf{v}_k \qquad (5)$$

which can be termed as a solution of a linear equation system with a coefficient matrix $\left[\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}\mathbf{J} + \alpha^2\mathbf{W}_m^{\mathrm{T}}\mathbf{W}_m\right]$.

Different from seismic tomography, the coefficient matrix in MT is dense, therefore, the sparse matrix solver for tomography (e.g. LSQR) can't be successfully applied. Considering that in MT inversion, the number of data (*N*) is often much smaller than the number of models (*M*), converting the calculation of the above linear system to data-space seems to be an efficient path suitable for the MT method, similar to data-space inversion (e.g. Usui et al. 2017).

Linear equation system solved in data-space

In this work, we use the same manner as Usui et al. (2017) to apply the Sherman–Morrison–Woodbury formula (Golub and Van Loan 2013) to the inverse of the coefficient matrix:

$$\left[\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}\mathbf{J}+\alpha^{2}\mathbf{W}_{m}^{\mathrm{T}}\mathbf{W}_{m}\right]^{-1}$$

$$=(\alpha^{2}\mathbf{W}_{m}^{\mathrm{T}}\mathbf{W}_{m})^{-1}(\mathbf{I}-\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}}\boldsymbol{\Gamma}^{-1}\mathbf{W}_{\mathrm{d}}\mathbf{J}(\alpha^{2}\mathbf{W}_{m}^{\mathrm{T}}\mathbf{W}_{m})^{-1} \quad (6)$$

$$\boldsymbol{\Gamma}=\mathbf{I}+\mathbf{W}_{\mathrm{d}}\mathbf{J}(\alpha^{2}\mathbf{W}_{m}^{\mathrm{T}}\mathbf{W}_{m})^{-1}\mathbf{J}^{\mathrm{T}}\mathbf{W}_{\mathrm{d}}^{\mathrm{T}} \quad (7)$$

Transforming the computational domain from model space to data space can greatly reduce the computational cost when *M* is much larger than *N,* further making the model analysis practical.

VERIFICATION OF THE PROPOSED MODEL ANALYSIS TOOL

Due to the limited pages, here we only use one synthetic model (Figure 1) to verify the proposed model analysis tool.

Synthetic model setting

Here we simulate a moderate-scale MT model analysis case where one key profile has dense MT station coverage, while the other part of the study area is covered by regional sparse stations (Figure 1). The inverted data is full-component MT impedance tensors at 15 periods from 0.00316 to 3162 s. Gaussian random noises were added with a standard deviation of 3 percent. The total number of data is 4200, the total number of inverted parameters is 26912.

The preferred resistivity structure

The preferred model, shown in Figure 2, was obtained by the MT inversion module of joint inversion framework (Song et al. 2024) developed based on femtic (e.g. Usui et al. 2017) and fmtomo (Rawlinson and Sambridge 2003).

Uncertainty analysis of the preferred model

Although many interesting aspects need to be investigated since it is the first try to use the stochastic diagonal estimator transforming to the data space for moderate- to large-scale MT model uncertainty analysis, we mainly focus on one most straightforward and important aspect, i.e. the estimation stability and calculation time while using different numbers (*s*) of random vectors, in this abstract.

Here, referring to the recommended intervals for *s* (MacCarthy et al. 2011), we set *s* to 32, 256, 512, 1024, and 2048, and compare the corresponding estimated model uncertainty ($\log_{10}(\delta\rho)$, square root of diagonal elements). It is clear to see in Figure 3 that in the vicinity of the MT stations and the structure shallower than around 5km, the model uncertainty is relatively small (around 0.1- 0.2 in the logarithmic regime), while the uncertainty gradually increases with increasing depth and increasing distance to the MT station, which quantitively demonstrates the common qualitative sense of the uncertainty of geophysical inversion; moreover, with the increasing number of random vectors, the uncertainty value of each grid tends to be stable. Considering the calculation time shown in Table 1, we recommend that the number of random vectors should ideally be around 1024 in cases similar to this synthetic example.

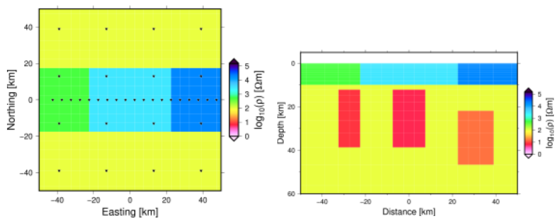

Figure 1. Synthetic model setting. The reversed black triangles are MT stations. The left figure is a horizontal cross-section at 5km depth, and the right is a vertical cross-section along the dense profile.

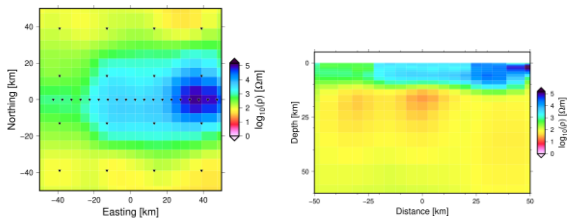

Figure 2. Preferred resistivity solution selected by L-curve criteria (Hansen, 1992). The setting of cross-sections are same as in Figure 1.

Table 1 Calculation time for preferred inversion result and corresponding uncertainty analysis

Task		time per iteration (s)	time total (s)
Full Inversion run		64	704
uncertainty analysis	s=32	5.13	164
	s=256	3.79	972
	s=512	3.82	1958
	s=1024	3.64	3727
	s=2048	3.63	7434

Conclusions

To reduce the huge computational cost that hinders model uncertainty analysis in 3D MT inversion problems, we propose a practical way by using an efficient stochastic matrix diagonal estimator to accurately estimate the diagonal of the model covariance matrix and transforming the calculation space from model space to data space. The synthetic example verified the effectiveness and efficiency of this method. The ability to quickly estimate the diagonal of the covariance matrix thus facilitates the introduction of additional tools for model analysis, with computational costs comparable to those required for obtaining inverse solutions. This work makes the model uncertainty analysis practical, especially for moderate- to large-scale MT studies when the exact expression of the covariance matrix is hard to obtain. This idea is easy to extend to MT model resolution analysis, and also model uncertainty and resolution analysis for joint inversion, which are our current works.

In addition to the synthetic verification shown here, more theoretical discussion will be presented in the meeting, as well as the application of the proposed uncertainty analysis tool to a large-scale MT inversion case using USArray data.

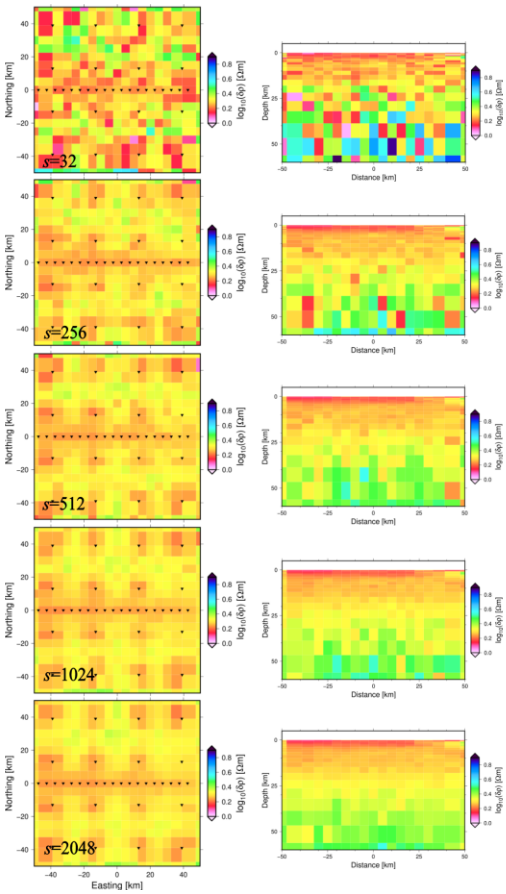

Figure 3. Uncertainty analysis for the preferred solution with the number (*s*) of random vectors equal to 32, 256, 512, 1024, 2048, respectively. The setting of cross-sections are same as in Figure 1.

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