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A trans-dimensional Bayesian Markov chain Monte Carlo algorithm for model assessment using frequency-domain electromagnetic data

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SUMMARY
A meaningful interpretation of geophysical measurements requires an assessment of the space of models that are consistent with the data, rather than just a single, ‘best’ model which does not convey information about parameter uncertainty. For this purpose, a trans-dimensional Bayesian Markov chain Monte Carlo (MCMC) algorithm is developed for assessing frequency-domain electromagnetic (FDEM) data acquired from airborne or ground-based systems. By sampling the distribution of models that are consistent with measured data and any prior knowledge, valuable inferences can be made about parameter values such as the likely depth to an interface, the distribution of possible resistivity values as a function of depth and non-unique relationships between parameters. The trans-dimensional aspect of the algorithm allows the number of layers to be a free parameter that is controlled by the data, where models with fewer layers are inherently favoured, which provides a natural measure of parsimony and a significant degree of flexibility in parametrization. The MCMC algorithm is used with synthetic examples to illustrate how the distribution of acceptable models is affected by the choice of prior information, the system geometry and configuration and the uncertainty in the measured system elevation. An airborne FDEM data set that was acquired for the purpose of hydrogeological characterization is also studied. The results compare favourably with traditional least-squares analysis, borehole resistivity and lithology logs from the site, and also provide new information about parameter uncertainty necessary for model assessment.

Key words: Inverse theory; Probability distributions; Electrical properties; Non-linear electromagnetics; Hydrogeophysics.

INTRODUCTION
Analysis of parameter uncertainty is a critical, but frequently overlooked, aspect of geophysical inverse problems. Estimated model parameters have both a value and uncertainty, which are inextricably linked to the acquisition geometry, measurement physics, data errors, inversion or estimation methods, parametrization and prior assumptions or constraints. In many cases, information about parameter uncertainty and non-uniqueness is just as important as the estimate of parameter values (Tarantola & Valette 1982). For example, some relevant questions in geophysical problems that require more than the estimation of ‘best’ parameter values might include: What is the likely range of depths to bedrock or the base of an aquifer? How well constrained is the near-surface resistivity (or other bulk geophysical property)? How are model parameters correlated? This work focuses on methodologies that aim to answer these questions, with specific application to frequency-domain electromagnetic (FDEM) data.

Multifrequency electromagnetic data are commonly acquired from airborne and ground-based systems to provide spatially continuous information about subsurface electrical resistivity variability. These data have widespread applications related to mineral exploration (Fraser 1978; Taylor 1990; Farquharson et al. 2003), geological mapping (Gabriel et al. 2003; Best et al. 2006), groundwater (Fitterman & Deszcz-Pan 1998; Roettger et al. 2005; Lipinski et al. 2008), agriculture (Alfred et al. 2005; Daniels et al. 2008; Sams et al. 2008) and environmental studies (Siemon et al. 2002; Al-Fouzan et al. 2004). The EM data are often presented as maps and cross-sections of apparent electrical resistivity (or conductivity) to highlight anomalous features of interest (Fraser 1978; Sengpiel 1988; Huang & Fraser 1996; Siemon 2001).

More recently, inversion algorithms have been developed that recover subsurface distributions of electrical conductivity and, optionally in some cases, magnetic susceptibility or dielectric permittivity. The majority of these inversion algorithms solve for 1-D layered-earth models using non-linear least-squares algorithms (Beard & Nyquist 1998; Farquharson et al. 2003; Huang & Fraser 2003; Tolbøl & Christensen 2006), though a simulated annealing approach was also introduced by Yin & Hodges (2007) that is less prone to being trapped in local minima. Siemon et al. (2009)
implemented a laterally constrained inversion (LCI) strategy for airborne FDEM data that was based on previous work applied to resistivity data (Auken & Christiansen 2004; Auken et al. 2005). The LCI approach produces 2-D models based on independent 1-D inversions that are subject to the additional constraint that they are laterally continuous. Similar work by Brodie & Sambridge (2006) solves for 3-D models by simultaneously inverting 1-D soundings on a 3-D conductivity model that is constrained spatially, and their algorithm also solves for system calibration parameters. Cox & Zhdanov (2008) describe an explicit 3-D inversion strategy for airborne FDEM data that incorporates localized 3-D sensitivities to better account for heterogeneity in the Earth.

While these algorithms are generally fast and provide useful estimates of subsurface properties, an analysis of parameter uncertainty, correlation and non-uniqueness is often left unaddressed. Analysis of uncertainty within the least-squares framework is typically assessed through the use of measures computed from the linearized Jacobian such as the posterior covariance or resolution matrices (e.g. Aster et al. 2005). This analysis can be useful for showing the approximate uncertainty in individual parameter estimates, but is often limited to a display of the diagonal elements of the posterior covariance matrix (Auken et al. 2005; Telbøll & Christensen 2006; Christensen et al. 2009), which does not account for strongly correlated parameters. Additionally, these sensitivity-based methods are limited by the linearization of the inverse problem.

In this study, a Bayesian Markov chain Monte Carlo (MCMC) approach is used to provide a direct assessment of parameter uncertainty, correlation and non-uniqueness for the FDEM parameter estimation problem. The method is adapted from the work of Malinverno (2002), who introduced a similar approach with dc resistivity data, and has also been adapted to seismic (Malinverno & Leaney 2005; Bodin & Sambridge 2009; Agostinetti & Malinverno 2010), gravity (Luo 2010), climate reconstruction (Hopcroft et al. 2007) and multimethod parameter estimation (Chen et al. 2007) problems. This approach involves sampling the space of model parameters that simultaneously fit the data and satisfy available a priori information. Instead of producing a single best-fit model, this approach produces many (typically hundreds of thousands) 1-D models that satisfy the data and prior information, which provides useful information for model assessment and interpretation.

In addition to adapting the method to FDEM data, this work also investigates how alternate types of prior information affect the posterior distribution of models; the effect of allowing the elevation of the FDEM system above the ground to be an unknown parameter; and how changes in the FDEM system parameters such as coil orientation, coil elevation, frequency range and data errors influence model uncertainty. Synthetic airborne and ground-based examples are provided, as well as the analysis of an airborne field data set.

**METHODOLOGY**

The methods implemented here are based on the work of Malinverno (2002), who introduced the use of a reversible-jump MCMC sampling strategy (Green 1995) to solve the 1-D electrical resistivity parameter estimation problem in a Bayesian framework. The reversible-jump algorithm is part of a class of transdimensional methods that allows the number of unknowns to vary. In this work, the number of layers for each sampled model is an unknown parameter, and models that contain fewer layers are implicitly favoured due to the naturally parsimonious aspect of this algorithm (Malinverno 2002; Sambridge et al. 2006). This provides a significant advantage over traditional algorithms that solve for either (1) models with a small (but pre-specified) number of layers with variable layer depths (e.g. Siemons et al. 2009) or (2) models with many fixed layers that are constrained to be smooth and/or close to a reference model (e.g. Farquharson et al. 2003). In the former case, it is often not known what number of layers is appropriate, or the best number of layers may vary over a survey area. In the latter overparametrized case, the regularization required to stabilize the inverse problem often results in blurred boundaries between layers. A summary of the basic algorithm is provided below, though the reader is referred to Malinverno (2002) for a more detailed discussion and theoretical background of the method.

**Parametrization**

A 1-D parametrization is used (Fig. 1), whereby the model, $\mathbf{m}$, is described by an unknown number of layers $k$; log-depths to each layer interface $z = \ln(z_1), \ldots, \ln(z_k)$; the log-electrical conductivity of each layer $\sigma = \ln(\sigma_1), \ldots, \ln(\sigma_k)$; and the EM sensor elevation above the ground surface, $h^\circ$.

$$\mathbf{m} = [k, \mathbf{z}, \mathbf{\sigma}, h^\circ].$$

Allowing the number of layers to vary provides a significant degree of flexibility in the model parametrization, as the appropriate number of layers is generally not known a priori. Instead, the number of layers that are required by the data is determined through the MCMC sampling algorithm described later. Because of the natural parsimony of this method (Malinverno 2002; Sambridge et al. 2006), models with fewer layers are favoured over those with many layers. Although the problem is formulated in terms of log-conductivity, this paper also refers to the electrical resistivity ($\rho = 1/\sigma$), which is used frequently in near-surface problems.

Following Malinverno (2002), layer interfaces are restricted to fall between user-specified minimum and maximum depths $z_{\text{min}}$ and $z_{\text{max}}$, which are typically based on the EM system geometry, frequencies and altitude. A maximum number of layers, $k_{\text{max}}$, is also specified, but is generally larger than the number of layers required to fit the data. Additionally, no layer can be added that produces a layer thinner than the minimum allowable thickness,

$$h_{\text{min}} = \frac{z_{\text{max}} - z_{\text{min}}}{2k_{\text{max}}}.$$  

Because the assumed instrument elevation and near-surface conductivity values are correlated, there is a range over which specific combinations of these parameters produce the same forward response. This non-uniqueness means that uncertainty in the instrument elevation is propagated to uncertainty in conductivity structure. This non-uniqueness is difficult to quantify using traditional linearized inversion strategies, but can be readily explored within the Bayesian framework presented here by incorporating the transmitter elevation ($h^\circ$) as an unknown parameter. Elevation errors can be due to instrument swing or false altimeter returns from vegetation when towed from an airborne platform (Fitterman & Yin 2004; Davis et al. 2009; Beamish & Leväniemi 2010), or more subtle changes in the height of ground-based instrument as it is carried or towed over irregular terrain. The sensitivity of the data to elevation errors increases with decreasing survey elevation and increasing ground conductivity; therefore, it is especially important to account for elevation errors under these conditions to limit the uncertainty in inferred conductivity values.
Incorporating these parameters will be the focus of future work.

The impact is expected to be measurable due to the extra computational effort involved in searching the higher dimensional parameter space.

Optionally, though not considered in this study, the model can be appended with magnetic susceptibility and/or electric permittivity parameters in addition to the conductivity for each layer. The $k$–1 layer interfaces are between user-specified minimum and maximum depths $z_{\text{min}}$ and $z_{\text{max}}$. Adapted from Malinverno (2002).

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**Figure 1.** 1-D model parametrization with $k$ layers, each of which is assigned a conductivity value and, optionally, magnetic permeability and electric permittivity values. The $k$–1 layer interfaces are between user-specified minimum and maximum depths $z_{\text{min}}$ and $z_{\text{max}}$. Adapted from Malinverno 2002.

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### Forward model

Given a layered earth model, the forward EM response is calculated using the equations for vertical and horizontal magnetic dipole source and receiver coils provided by Ward & Hohmann (1987). Expressions for the total (primary plus secondary) magnetic field for commonly used coil combinations are

$$H_{zz} = \frac{m}{4\pi} \int_{0}^{\infty} \left[ e^{-\omega z (k_{0} + k_{1})} + r_{\text{TE}} e^{\omega z (k_{0} - k_{1})} \right] \frac{\lambda^{2}}{\mu_{0}} J_{0}(\lambda r) \, d\lambda \quad (3)$$

for horizontal transmitter and receiver coils (vertical magnetic dipole source), and

$$H_{ss} = -\frac{m}{4\pi} \left( \frac{1}{r} - \frac{2x^{2}}{r^{3}} \right) \int_{0}^{\infty} \left[ e^{-\omega z (k_{0} + k_{1})} - r_{\text{TE}} e^{\omega z (k_{0} - k_{1})} \right] \lambda J_{1}(\lambda r) \, d\lambda$$

$$- \frac{m}{4\pi} \frac{x^{2}}{r^{3}} \int_{0}^{\infty} \left[ e^{-\omega z (k_{0} + k_{1})} - r_{\text{TE}} e^{\omega z (k_{0} - k_{1})} \right] \lambda^{2} J_{0}(\lambda r) \, d\lambda \quad (4)$$

for vertical transmitter and receiver coils with axes oriented in the $x$-direction (horizontal magnetic dipole). Eq. (4) can also be used for $y$-oriented coils by transposing the $x$ and $y$ coordinates of the coils. In practice, transmitter and receiver coils often have the same orientation and elevation, resulting in one of the three geometries shown at the top of Fig. 1: horizontal coplanar (HCP), vertical coplanar (VCX) or vertical coplanar (VCP).

In eqs (3) and (4), $m$ is the transmitter moment; $r = (x^{2} + y^{2})^{1/2}$ is the transmitter–receiver coil separation; $h_{m}$ is the transmitter coil elevation above the ground surface; $\lambda = (k_{0}^{2} + k_{1}^{2})^{1/2}$, where $k_{0}$ and $k_{1}$ are the horizontal wavenumbers; $u_{i} = (\lambda^{2} - k_{i}^{2})^{1/2}$ where $k_{i} = (\omega^{2} \mu_{i} \sigma_{i} - j \omega \mu_{i} \sigma_{i})^{1/2}$ is the wavenumber of the $i$th layer, $\omega$ is the angular frequency, $\mu_{i}$ is the magnetic permeability of the $i$th layer, $\sigma_{i}$ is the dielectric permittivity of the $i$th layer, $\epsilon_{i}$ is the conductivity of the $i$th layer and $j = \sqrt{-1}$; $J_{0}$ and $J_{1}$ are the zeroth- and first-order Bessel functions of the first kind; and $r_{\text{TE}}$ is a reflection coefficient that, for layered media, is calculated recursively using expressions from Ward & Hohmann (1987) that are provided in the Supporting Information. The Hankel transforms in eqs (3) and (4) are computed using the digital linear filter equations provided by Guptaarma & Singh (1997).

FDEM data are typically reported in parts-per-million (ppm) of the primary field for a number of different transmitter frequencies,

$$d(\omega) = \frac{H(\omega) - H_{0}(\omega)}{H_{0}(\omega)} \times 10^{6}, \quad (5)$$

where $H$ is the total magnetic field in eqs (3) and (4) and $H_{0}$ is the free-space magnetic field. Computational efficiency in the forward problem is an important part of this algorithm because the MCMC approach requires calculating the forward response to many trial models.

### Bayesian formulation

The Bayesian formulation for the posterior probability density function (pdf) of a model ($m$) given data ($d$) and prior information ($I$) is given by

$$p(m | d, I) = \frac{p(m | I) p(d | m, I)}{p(d | I)} \quad (6)$$

The denominator in eq. (6) is a normalizing constant, also called the evidence, where

$$p(d | I) = \int p(m | I) p(d | m, I) \, dm \quad (7)$$

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This integral over the entire model space is difficult to calculate directly, particularly for high-dimensional problems, which necessitates the use of the MCMC sampling approach discussed in the next section. Analysis of the evidence, however, provides valuable insight into the naturally parsimonious aspect of the trans-dimensional algorithm that favours models with fewer layers (Malinverno 2002; Sambridge et al. 2006).

The posterior distribution is therefore proportional to the product of the prior distribution \( p(m | l) \) and the likelihood function \( p(d | m, l) \). Following the work of Malinverno (2002), this can be expanded as

\[
p(m | d, l) \propto p(k | l) p(z | k, l) p(I | k, z, l) p(d | k, z, \sigma, h^i, l).
\]

(8)

The first four terms in eq. (8) describe the prior distributions for the number of layers in the model, the interface depths, layer conductivities and transmitter elevation. The last term in eq. (8) is the likelihood function, which is a measure of data fit.

No explicit assumption is made about the number of layers in the model; therefore, the prior pdf for the number of layers is defined as a uniform distribution.

\[
p(k | l) = \begin{cases} 
1/(k_{\max} - 1) & 1 \leq k \leq k_{\max} \\
0 & \text{otherwise}
\end{cases}.
\]

(9)

The maximum number of layers, \( k_{\max} \), is generally much greater than the number of layers needed to fit the data, and is used to define the minimum layer thickness according to eq. (2). The minimum number of layers is one, which corresponds to a half-space model.

Malinverno (2002) provides the appropriate form for the prior pdf on layer interface depth given a model with \( k \) layers, which comes from the pdf of order statistics.

\[
p(z | k, l) = \frac{(k - 1)!}{\prod_{i=0}^{k-1} \Delta z(i)}.
\]

(10)

The numerator in eq. (10) is the number of ways that \((k - 1)\) interfaces can be ordered, and \( \Delta z(i) = (z_{\text{max}} - z_{\text{min}}) - 2i h_{\text{min}} \) describes the depth interval that is available to place a layer when there are already \( i \) interfaces in the model.

A multivariate normal distribution is used to describe the joint prior pdf for log-conductivity values in all layers,

\[
p(\sigma | k, I) = \left[ (2\pi)^{k/2} |C_{\sigma} \right]^{-1/2} \exp\left[ -\frac{1}{2}(\sigma - \sigma_0)^T C_{\sigma}^{-1} (\sigma - \sigma_0) \right].
\]

(11)

Layer conductivities are constrained to a reference log-conductivity model, \( \sigma_0 \), with prior covariance \( C_{\sigma_0} \). The reference log-conductivity model and prior covariance can be any function that varies with depth based on prior knowledge. In this study, \( \sigma_0 \) is chosen to be the best fitting half-space model. Strictly speaking, this violates the rule that a prior distribution should be entirely independent of the data (Scales & Snieder 1997) since the data are used to estimate the best half-space model. The prior covariance for log-conductivity values, \( C_{\sigma} \), is assigned as a diagonal matrix with elements \( \log(1 + f_{\text{ac}}c)^2 \), where \( f_{\text{ac}} \) represents the factor within which conductivity is expected to vary (one standard deviation). Note that the term \((2\pi)^{-k/2}\) in eq. (11) implicitly favours models that have fewer layers.

An alternative to constraining estimated models to a prior reference model is to constrain the vertical smoothness of the model, which is a common strategy in traditional least-squares algorithms (e.g. Constable et al. 1987; Farquharson et al. 2003). The physical basis for this type of prior pdf is that strong oscillations in the Earth properties are unlikely over short distances. In this case, the vertical gradient of the model is constrained to have a mean of zero and a variance that limits the magnitude of conductivity gradients,

\[
p(\sigma | k, I) = \left[ (2\pi)^{k/2} |C_{\sigma} \right]^{-1/2} \exp\left[ -\frac{1}{2}(\sigma - \sigma_0)^T C_{\sigma}^{-1} (\sigma - \sigma_0) \right].
\]

(12)

The conductivity gradient at the \( i \)th interface \((i = 1:k-1)\) is defined as

\[
\nabla_i^\sigma = \frac{\sigma_{i+1} - \sigma_i}{h_i - h_{i-1}}.
\]

(13)

where \( \sigma_i \) and \( \sigma_{i+1} \) are the log-conductivities on either side of an interface, \( h_i \) is the log-thicknesses of the \( i \)th layer, and \( h_{\text{min}} \) is the minimum log thickness defined in eq. (2). Eq. (13) ensures that as the thickness of a layer approaches the minimum thickness, the log-conductivity contrast at the layer interface approaches zero. This formulation still allows large contrasts at layer interfaces, but requires that they be accompanied by appropriately large layer thicknesses. Hence, this is an effective way to penalize \( a \) \( \text{prior} \) models that oscillate strongly, and also is a more appropriate prior distribution because it is independent of the data.

A uniform distribution is used for the prior pdf for transmitter elevation,

\[
p(h^i | l) = \begin{cases} 
\frac{1}{h^i_{\max} - h^i_{\min}} & h^i_{\min} \leq h^i \leq h^i_{\max} \\
0 & \text{otherwise}
\end{cases}.
\]

(14)

where \( h^i_{\min} \) and \( h^i_{\max} \) provide limits on the transmitter elevation. For an airborne system, these limits can be calculated based on reasonable deviations expected from typical helicopter maneuvers, bird swing or pitch and vegetation cover. For ground-based systems, reasonable limits can be designed based on the stability of the platform that carries the EM instrument. Because of the non-unique relationship between transmitter elevation and inferred near-surface resistivity, it is important to limit the range of values to the smallest reasonable region. When auxiliary data are available to constrain the actual instrument elevation (Davis et al. 2009), this information could be used to help reduce the uncertainty in near-surface resistivity.

The likelihood function in eq. (8) is an expression of data fit, and also is a normal distribution

\[
p(d | k, z, \sigma, h^i, l) = \left[ (2\pi)^{m/2} |C_{d} \right]^{-1/2} \exp\left[ -\frac{1}{2}(d - \hat{d})^T C_{d}^{-1} (d - \hat{d}) \right],
\]

(15)

where \( d_{\text{obs}} \) are the observed data, and \( \hat{d} \) is the forward response for a given model calculated using eqs (3)–(5). \( C_{d} \) is the data covariance matrix which, in this work, consists of a diagonal matrix with entries equal to the estimated error variance \((\sum^2)\) for each frequency. When data errors are expected to be non-Gaussian and contaminated by outliers, an alternative choice for the likelihood function is the Laplace distribution, which is broader tailed than the normal distribution. The use of this distribution, which contains a measure of the absolute error rather than squared errors, is akin to L1-norm minimization methods that have been successful in least-squares algorithms (Claerbout & Muir 1973; Farquharson & Oldenburg 1998).

Trans-dimensional MCMC algorithm

The application of MCMC algorithms to Bayesian inference problems has been widely used in the scientific literature (e.g. Mosegaard & Tarantola 1995; Gilks et al. 1996). Specifically, MCMC algorithms are used to draw models from the posterior of eq (6), without
explicitly evaluating this function. The Markov chain follows a random walk through the model space, where each new model in the chain depends on the previous sample.

This work is based on the two-step Metropolis–Hastings sampling algorithm (Metropolis et al. 1953; Hastings 1970). First, a new model \((m')\) is proposed from a proposal distribution, \(q(m'|m)\), which is a function of the current model \(m\) in the Markov chain and is described later. The proposed model is then either accepted or rejected based on an acceptance probability that is also described later.

Green (1995) extended the Metropolis–Hastings algorithm to include the case where the dimension of \(m\) (i.e. the number of parameters) is allowed to vary throughout the Markov chain, which is often referred to as reversible-jump or trans-dimensional MCMC, and has been recently incorporated in several geophysical applications (Malinverno 2002; Malinverno & Leaney 2005; Hopcroft et al. 2007; Bodin & Sambridge 2009; Agostinetti & Malinverno 2010). The form of trans-dimensional MCMC implemented here is ‘birth-death’ MCMC, whereby the model that is proposed to be added to the Markov chain may have the same number of layers, one more layer or one less layer than the current model has. The following sections provide a general outline of the trans-dimensional MCMC algorithm, along with specific details relevant to each step.

**Initialization**

Parameters that define the prior distributions in eqs (9)–(14) are fixed during the initialization stage. This includes placing reasonable limits on the model geometry \((k_{max}, z_{min}, z_{max}, h_{min})\) and the allowed transmitter elevation range \((h_{max}^{\theta}, h_{min}^{\theta})\), assigning errors in the data covariance matrix \(C_d\), defining the prior mean log-conductivity model \(\sigma_0\), and defining the model covariance matrix \(C_s\). In this work, a fine-search is performed to determine the best fitting half-space model, which is used as the prior log-conductivity model.

The first model in the Markov chain is given two layers \((k = 2)\), but with both layer log-conductivity values equal to \(\sigma_0\). The layer interface is placed midway between \(z_{max}\) and \(z_{min}\). The initial transmitter elevation can be either a nominal value for the survey or a measured value (e.g. the reported laser altimeter reading from an airborne system).

**Model proposal**

A new model, defined separately for each component of \(m\), is proposed from a proposal distribution that is a function of the current model in the Markov chain

\[
q(m'|m) = q(k'|k)q(z'|k')q(\sigma'|k', z')q(h'|k, z').
\]

In the birth-death MCMC algorithm used here, which follows the work of Green (1995) and Malinverno (2002), one of four options with probability \((p)\) described below is chosen for the proposed model as follows.

1. Birth \((p = 1/6)\): A layer is added at a random depth between \(z_{max}\) and \(z_{min}\), ensuring that no layers thinner than \(h_{min}\) are created. \(k' = k + 1\).
2. Death \((p = 1/6)\): An interface chosen at random is deleted from the model. \(k' = k - 1\).
3. Perturbation of a single interface \((p = 1/6)\): The depth of a randomly selected interface is shifted by a value drawn from a uniform distribution on \((-h_{min}, h_{min})\). \(k' = k\).
4. No layer change \((p = 1/2)\): No change is made to the number of layers or interface depths. \(k' = k\).

The relevant proposal distribution for the number of layers is therefore

\[
q(k'|k) = \begin{cases} 
1/6 & k' = k + 1 \text{ (birth)} \\
1/6 & k' = k - 1 \text{ (death)} \\
2/3 & k' = k \text{ (perturbation, no change)}
\end{cases}
\]

and

\[
q(z'|k, z) = \begin{cases} 
1/\Delta z(k) & \text{birth} \\
1/k & \text{death} \\
1/(2h_{min}) & \text{perturbation} \\
1 & \text{no change}
\end{cases}
\]

for the interface depths.

At every step in the Markov chain, a new conductivity model is proposed based on a normal distribution that has the current log-conductivity model as its mean

\[
q(\sigma'|k', z', \sigma) = \left[2\pi \sigma_{k', z'}^{\sigma} \right]^{-1/2} \exp \left[ -\frac{1}{2} (\sigma - \sigma_{k', z}'^{\sigma})^T C_{\sigma_{k', z}^{-1}} (\sigma - \sigma_{k', z}'^{\sigma}) \right].
\]

The mean log-conductivity model is written as \(\sigma_{k', z}'^{\sigma}\) because its values are taken from the current log-conductivity model (\(k\)), but the mean model must have dimension \(k'\). In the case of a proposed birth step, the new interface is added to the mean log-conductivity model and the layers on either side of the interface are assigned the same log-conductivity as the layer that was split. In the case of a death step, one interface is deleted and the log-conductivity for the two layers on either side of the interface is averaged to form a single layer.

Efficiency of the MCMC algorithm is strongly influenced by the choice of the proposal distribution. While a poor proposal distribution will still allow the chain to sample the posterior distribution, it may take an unreasonable amount of time if proposed models are either too exploratory (many proposals are rejected because they fall in low-probability regions) or not exploratory enough (many proposals are accepted, but they do not stray far from high-probability regions). The covariance term, \(C_{\sigma_{k', z}^{-1}}\) in eq. (19) must be carefully chosen so that the posterior distribution is effectively sampled.

Generally speaking, near-surface and more conductive layers are usually better constrained by FDEM data than deeper or more resistive layers due to the sensitivity of the instrument to the subsurface. Consequently, the proposal distribution should incorporate a different search range for parameters with different sensitivities. A proposal covariance that is small will be effective for shallow layers, but will not effectively search the range of acceptable conductivity values at depth. A large proposal covariance will be effective in sampling values at depth, but will result in many shallow conductivity values that result in poor data likelihood and will therefore be rejected.

Malinverno (2002) suggested an effective way to define the proposal covariance term based on a linearized estimate of the posterior model covariance (e.g. Aster et al. 2005),

\[
C_{\sigma_{k', z}^{-1}} \approx [J^T C_{\sigma_{k}^{-1}} J + C_{\sigma_{k}^{-1}}]^{-1},
\]

which is adopted in this study. \(J\) is the linearized sensitivity about \(\sigma_{k}^{\sigma}\), that is, \(J = \partial \sigma_{k}^{\sigma} / \partial \sigma_{k}^{\sigma}\), which is derived in the Supporting
Information, and \( C_y \) and \( C_{eq} \) are the data error covariance and prior conductivity covariance matrices, respectively. This definition for the proposal covariance provides a smaller search range for parameters with high sensitivity and a wide search range for those with low sensitivity. Computing \( I \) requires approximately three quarters of the total execution time of the algorithm, but without this term the Markov chain does not effectively sample the model space.

Finally, the proposal distribution for transmitter elevation is defined as a univariate normal distribution,

\[
q \left( h^{\text{tx}} | h^{\text{tr}} \right) = (2\pi C_{h^{\text{tx}}})^{-1/2} \exp \left( -\frac{ \left( h^{\text{tx}} - h^{\text{tr}} \right)^2 }{2 C_{h^{\text{tx}}}} \right),
\]

where \( C_{h^{\text{tx}}} \) defines the proximity of a proposed transmitter elevation to the current elevation in the chain. This value should be large enough that the range of reasonable values can be sampled, but not so large that it requires a simultaneous large change in near-surface conductivity to still fit the data.

**Model acceptance criterion**

The second step of the Metropolis–Hastings algorithm involves deciding whether to accept the proposed model, which occurs with probability \( \alpha \),

\[
\alpha = \min \left[ \frac{ p \left( m | d, I \right) q \left( m' | m \right) }{ p \left( m | d, I \right) q \left( m' | m \right) } \right].
\]

In the general form of trans-dimensional MCMC, there is an additional Jacobian term that multiplies the acceptance probability ratio in eq (22) to account for the potential jump in dimensions between models (Green 1995). However, Agostinetti & Malinverno (2010) show that this term is equal to one for the types of dimension changes allowed here, and the Jacobian term is therefore not included.

The acceptance probability is meant to bias samples in the Markov chain towards higher probability regions of the model. The first term in the ratio compares the posterior probability for the proposed model to that of the current model. If the proposed model has a higher probability, it has a greater chance of being accepted. The second term in the ratio is a correction factor for the case where the proposal distribution is not symmetric. If the combined ratio on the right-hand side of eq (22) is greater than one, the proposed model is always accepted and it is added to the Markov chain. If it is less than one, the proposed model is accepted with probability \( \alpha \), otherwise the current model is duplicated and repeated in the chain.

Substituting eq (8) into eq (22), it is clear that the acceptance probability is equal to the product of the prior probability ratio,

\[
\frac{ p \left( m' | I \right) }{ p \left( m | I \right) } = \frac{ p \left( k' | I \right) p \left( \sigma' | k', z, I \right) p \left( h^{\text{tx}} | I \right) }{ p \left( k | I \right) p \left( \sigma | k, z, I \right) p \left( h^{\text{tx}} | I \right) },
\]

times the likelihood ratio,

\[
\frac{ p \left( d | m', I \right) }{ p \left( d | m, I \right) } = \frac{ p \left( d | k', \sigma', h^{\text{tx}}, I \right) }{ p \left( d | k, \sigma, h^{\text{tx}}, I \right) },
\]

times the proposal ratio,

\[
\frac{ q \left( m' \right) }{ q \left( m \right) } = \frac{ q \left( k' | k, m' \right) q \left( \sigma' | k, z, m' \right) q \left( h^{\text{tx}} | h^{\text{tx}} \right) }{ q \left( k | k, m \right) q \left( \sigma | k, z, m \right) q \left( h^{\text{tx}} | h^{\text{tx}} \right) },
\]

(25)

calculated for the proposed and current models using eqs (9)–(21).

A number of simplifications can be made to these ratios. First, Malinverno (2002) shows that both the prior and proposal ratios for \( k \) and \( z \) can be removed from the acceptance probability in eq (22). This is because when \( k' = k \), both the prior and proposal ratios for \( k \) and \( z \) equal one. When \( k' \neq k \) the prior ratio for \( k \) and \( z \) is the inverse of the proposal ratio for these parameters so that

\[
\frac{ p \left( k', z' | I \right) q \left( k, z | m' \right) }{ p \left( k, z | I \right) q \left( k', z' | m \right) } = 1.
\]

(26)

Additionally, the proposal distribution for the transmitter elevation as expressed in eq (21) is symmetric, so that the proposal ratio for this term equals one. Eq (22) is therefore simplified to

\[
\alpha = \min \left[ \frac{ p \left( \sigma' | k', z, I \right) p \left( d | k', \sigma', z, h^{\text{tx}} | I \right) }{ p \left( \sigma | k, z, I \right) p \left( d | k, \sigma, z, h^{\text{tx}} | I \right) } \right].
\]

(27)

Once the decision is made to accept or reject the model, the algorithm is repeated from the model proposal step described earlier.

**Output and stopping criteria**

Generally, there is a burn-in period at the beginning of the Markov chain before the generated samples are representative of the posterior distribution. Because the half-space model used to initialize the chain may be in a very low-probability region of the model space, a number of low-probability (but steadily improving) models must be accepted before the chain begins sampling the posterior. In this work, the burn-in period is specified to last until a model in the Markov chain fits the data within an expected error tolerance. This typically occurs within several hundred model proposals, but can take longer if the assumed data errors are very small or if the initial model is in a very low posterior probability region.

For the assumption of normally distributed data residuals in eq. (15), the L2 measure of data misfit is given by

\[
\phi_d = \left( C_{d}^{-1/2} \left( d^{\text{obs}} - d \left( m \right) \right) \right)^2.
\]

(28)

If the estimated data error variances in \( C_{d} \) are representative of the true errors, then the expected value of \( \phi_d \) is equal to the number of data, \( N \) (e.g. Aster et al. 2005). In practice, a target value for the data misfit can be scaled to account for incorrect assumptions about the errors, that is, \( \phi_d^{\text{tar,L2}} = \chi^2 \), where \( \chi^2 \) is a scaling factor (Farquharson & Oldenburg 1998). If a Laplace distribution is used for the likelihood function, then a more appropriate representation of data fit is the L1 measure,

\[
\phi_d = \left( C_{d}^{-1/2} \left( d^{\text{obs}} - d \left( m \right) \right) \right)_1.
\]

(29)

with \( \phi_d^{\text{tar,L1}} = \chi \sqrt{2/\pi} N \) (Parker & McNutt 1980; Farquharson & Oldenburg 1998).

Assigning a stopping criterion to determine when the Markov chain has become stationary is a subject of ongoing research, and can be particularly difficult to quantify for trans-dimensional MCMC algorithms (Sisson 2005). Diagnostic tools for assessing the stationarity of fixed-dimension chains include tracking the change in the distribution of certain parameters both within a single chain and across multiple chains run in parallel (Gelman & Rubin 1992; Gilks et al. 1996). In this work, Markov chains are run for several hundred thousand steps, by which time the inferred distribution of models does not appear to change appreciably. Future work will involve incorporating a more formal assessment of how stopping criteria should be implemented.
Once the MCMC algorithm is completed, all of the models from the burn-in point onwards are output. Numerous inferences can be made about parameter values, uncertainty, non-uniqueness and correlation from this ensemble of models. The following synthetic and field data examples illustrate the type of information that can be gained from this sampling algorithm.

**EXAMPLES**

**Synthetic airborne data set**

The first example uses a simple three-layer resistivity model (Fig. 2A). In all of the following examples, models are displayed as resistivity ($\rho$) versus depth profiles even though the MCMC algorithm works in the logarithm of conductivity. The forward response to this model is calculated using eqs (3) and (4) and characteristics typical of the Fugro RESOLVE$^1$ airborne FDEM system provided in Table 1 (Fig. 2B).

Several variations on the MCMC algorithm described earlier are run for the purposes of illustrating how different types of prior information effect the resulting distribution of models. For each of the three cases outlined later, which use different prior assumptions, two scenarios are run. In the first, the transmitter elevation is assumed to be known exactly, and is fixed at 30 m. In the second case, the transmitter elevation is allowed to vary with a uniform prior pdf from 0 to 50 m.

1 Any use of trade, product or firm names is for descriptive purposes only and does not imply endorsement by the US Government.

### Table 1. System characteristics used to model the forward response for the synthetic airborne FDEM example.

<table>
<thead>
<tr>
<th>Frequency (Hz)</th>
<th>Orientation</th>
<th>Elevation, $h^0$ (m)</th>
<th>Coil separation, $r$ (m)</th>
<th>Nominal error (ppm, ±1σ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>395</td>
<td>HCP</td>
<td>30</td>
<td>7.9</td>
<td>10</td>
</tr>
<tr>
<td>1822</td>
<td>HCP</td>
<td>30</td>
<td>7.9</td>
<td>10</td>
</tr>
<tr>
<td>3262</td>
<td>VCX</td>
<td>30</td>
<td>9.0</td>
<td>10</td>
</tr>
<tr>
<td>8199</td>
<td>HCP</td>
<td>30</td>
<td>7.9</td>
<td>20</td>
</tr>
<tr>
<td>38 760</td>
<td>HCP</td>
<td>30</td>
<td>7.9</td>
<td>40</td>
</tr>
<tr>
<td>128 755</td>
<td>HCP</td>
<td>30</td>
<td>7.9</td>
<td>50</td>
</tr>
</tbody>
</table>

Additionally, a prior constraint is added that restricts the minimum and maximum resistivity for any model to fall between 0.04 Ωm and 71,000 Ωm [which represents three standard deviations from the best half-space model in scenario (1) above]. That is, a model with any layer resistivity outside these bounds is given a prior probability of zero. This latter constraint is not strictly necessary, but helps to limit the model space that must be searched when the data provide no constraint on the parameter values.

(3) In addition to the prior on the conductivity values in scenario (1), an explicit prior on the number of layers is added. This component of the prior is defined by an exponential distribution that explicitly favours models with fewer layers.

In each example, the MCMC algorithm is run for 300,000 models after the burn-in period is reached. A summary of the output from the first three simulations with fixed transmitter elevation is illustrated in Fig. 3. The shaded background in Figs 3(A)–(C) shows the composite distribution of all models in the MCMC ensemble; regions with darker shading indicate that a greater number of models in the ensemble have a given resistivity-depth value. Superimposed on these images are the bounds that contain 95 per cent of the MCMC models at a given depth (magenta), the prior mean resistivity value plus and minus two standard deviations (brown) used in the first and third examples, the model with the maximum posterior probability (blue), the true model (red) and the model recovered using the least-squares algorithm EM1DFM (Farquharson et al. 2003) (green).

Fig. 4 illustrates a typical distribution of predicted data for the ensemble of models captured in Figs 3(A)–(C), showing that all of the output models fit the data within the expected errors. Note that predicted data are only computed at the measured frequencies in Table 1; therefore, predicted values at intermediate frequencies are

1 Any use of trade, product or firm names is for descriptive purposes only and does not imply endorsement by the US Government.
Bayesian MCMC algorithm for model assessment

Figure 3. Summary of MCMC simulations for the synthetic airborne data set using a fixed conductivity prior (A, D, G), a prior on the vertical conductivity gradient (B, E, H) and an explicit prior on the number of layers in addition to the fixed conductivity prior (C, F, I). Left column (A–C) shows the composite MCMC model distribution, along with prior and posterior resistivity ranges, the model with maximum posterior probability, the true model and the model recovered using a least-squares algorithm (EM1DFM). Centre column (D–F) shows the distribution of all interface depths in the MCMC models, with red lines indicating the true interface depths. In all three cases, this posterior distribution of interface depths indicates that interfaces near 15 and 50 m depth are likely, where the width of the peaks provides a measure of uncertainty on the interface depth. For the example with the prior on the mean conductivity (Fig. 3D), the peaks at 15 and 50 m are much less sharp than those in Figs 3(E) and (F), which indicates less certainty on the interface depths due to the prior on the mean conductivity value.

Figs 3(G)–(I) show histograms of the number of layers in the MCMC distribution of models. In Figs 3(G) and (H), models with fewer layers occur more frequently compared with the uniform prior shown as a dashed line, which is due to the naturally parsimonious aspect of the trans-dimensional sampling algorithm. Note, however, that models with five–eight layers are more common than the true model with three layers, which is similar to observations made by Malinverno (2002). In Fig. 3(H), the prior on vertical smoothness has biased the results towards fewer layer models compared with Fig. 3(G) due to the penalty on oscillatory models with many layers. Finally, in Fig. 3(H), the explicitly defined exponential prior on the number of layers is clearly manifested in the posterior distribution.

There is a significant amount of information regarding parameter uncertainty, non-uniqueness and correlation that can be obtained from the distribution of MCMC models. The information in Fig. 3 illustrates the general trend of increasing uncertainty in resistivity values with depth. Eventually, the 95 per cent region of output models covers such a wide range that it indicates little-to-no sensitivity to the data, which is related to other metrics for the depth.

Figure 4. Typical data fit for composite of 300 000 MCMC models. Regions with darker shading indicate a high occurrence of the predicted data amplitude for a given frequency. Predicted data are only calculated at the six survey frequencies, and intermediate values are interpolated for display purposes.

Interpolated for display purposes only and should not be considered accurate.

Figs 3(D)–(F) show histograms of the layer interface depths from all 300 000 models in each scenario, with red lines indicating the true interface depths. In all three cases, this posterior distribution of interface depths indicates that interfaces near 15 and 50 m depth are likely, where the width of the peaks provides a measure of uncertainty on the interface depth. For the example with the prior on the mean conductivity (Fig. 3D), the peaks at 15 and 50 m are much less sharp than those in Figs 3(E) and (F), which indicates less certainty on the interface depths due to the prior on the mean conductivity value.

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of investigation (DOI) of geophysical data (Oldenburg & Li 1999).

Additionally, it is clear that while there is reasonable sensitivity to
the interface between the second and third layers, the upper limit on
the resistivity value within the second layer is poorly constrained
due to the well-known difficulty in imaging resistive targets with
inductive methods.

In general, the results for the prior pdf on the mean conductivity
value (Figs 3A, D and G) are the poorest, with increased uncertainty
on resistivity values at a given depth and in the estimated interface
depths. This increased uncertainty results from the use of a very
uninformative prior that allows for a wide range of model values.
Mathematically, this accurately reflects the parameter uncertainty
given little influence from the prior, that is, it is controlled almost
entirely from constraints provided by the data. Geologically, how-
ever, this uninformative prior allows for extremely unlikely models
that oscillate strongly over small depth intervals. By using the prior
on the vertical gradient (case 2), this class of strongly oscillating
models is effectively removed, resulting in reduced and more realistic uncertainties. A similar improvement is found by placing an
explicit prior on the number of layers in addition to the prior on the
mean conductivity (case 3) because this penalizes oscillating mod-
els that require additional layers. Because the prior on the vertical
gradient is geologically meaningful, this is the preferred approach,
though some care must be taken to ensure that the constraint is
neither over- nor underrestrictive. This result highlights the im-
portance of understanding how the choice of a certain prior distribution
effects the posterior distribution of models (Scales & Snieder 1997).

Fig. 5 provides another view of the uncertainty that can be
attributed to resistivity values at depth for the three cases in
Figs 3(A)–(C). In this figure, slices of the posterior distribution

![Figure 5](image-url)

**Figure 5.** Slices through the posterior distribution of models at depths of 10, 35 and 80 m show how different prior constraints impact the ability to resolve resistivity values. Results are shown for the cases where the prior is defined for (A) the mean resistivity value, (B) the vertical gradient of the resistivity and (C) the number of layers and the mean resistivity value, which correspond to Figs 3(A)–(C).
Bayesian MCMC algorithm for model assessment

for resistivity are shown at depths of 10, 35 and 80 m, along with the true values (red lines) at these depths. For the 10-m depths (black curves), all of the scenarios are peaked and centred on the true value of 50 $\Omega$ m, indicating good resolution at shallow depths. Deeper in the model, the peaks become significantly more diffuse, indicating a loss of resolution with depth and increased model uncertainty. In all three scenarios, the second layer is the most poorly defined due to its higher resistivity. Additionally, the distributions in all three cases are biased to resistivities below the true value for the second layer due to non-uniqueness. At a certain point, increasing the resistivity in the second layer does not improve the data fit and, because this increase requires models with reduced prior probability, the true solution leads to a lower posterior probability. Finally, note that the resistivity distribution, particularly in the second layer, is not symmetric. This indicates a better constraint on the lower resistivity bound, while the upper bound is poorly constrained. Asymmetric estimates of parameter uncertainty are generally not obtainable using traditional least-squares algorithms that use the linearized posterior covariance matrix to estimate uncertainty.

Fig. 6 further illustrates information about parameter uncertainty, as well as parameter correlations. The information in this figure is extracted from 10 060 (~3 per cent of the total) models that have three layers ($k = 3$) in the example that uses a prior pdf on the vertical gradient (Fig. 3B). The histograms along the diagonals show the distribution of parameter values (log resistivities for the three layers and two interface depths) for these models, with the true values indicated in red. The off-diagonals are cross-plots for all combinations of the five parameters for these models. Linear relationships are evident between the log-resistivity of the first layer and depth to the top of the second layer, as well as the log-resistivity of the half-space and the depth to the top of the half-space. For the second layer, however, there is clearly a non-linear relationship between the log-resistivity of this layer and the depth to the top of the layer. Additionally, a relatively sharp lower bound for the resistivity of the second layer is evident, and the resistivity distribution for this layer is not log-normal as the other layers appear to be. As expected, the resistivity in the first layer is uncorrelated with the resistivity of the third layer and the depth of the second interface.

Next, the same three prior scenarios are run, but the system elevation is allowed to vary between 10 and 50 m according to the uniform prior distribution in eq (14). Fig. 7 summarizes the results of these simulations in the same format as Fig. 3. In all three cases, the resistivity of the upper layer is poorly constrained (Figs 7A–C) and the interface depth histograms (Figs 7D–F) no longer show a well-defined interface at 15 m depth, though the interface at 50 m is still observed. Instead, because of the non-unique relationship between near-surface parameters and system elevation, there is a wider range of resistivities and thicknesses that can be used to fit the data.

Fig. 8 shows the posterior distribution of transmitter elevations for each scenario (which all had a uniform prior probability equal to 0.025), along with the true value (red), the value for the MCMC

![Figure 6. Parameter cross-plot for all three-layer models ($k = 3$) extracted from the ensemble of models in Fig. 3(B) (prior pdf on vertical conductivity gradient). Diagonals show histograms for the values of each parameter along with the true model values (red lines). Off-diagonals show cross-plots for all parameter combinations, along with true values (red crosses). Note that the illustration is symmetric about the diagonal.](image-url)
Figure 7. Summary of MCMC simulations for the synthetic airborne data set as in Fig. 3, but with transmitter elevation as a free parameter. Results are shown for a fixed resistivity prior (A, D, G), a prior on the vertical resistivity gradient (B, E, H), and an explicit prior on the number of layers in addition to the fixed resistivity prior (C, F, I). Left column (A–C) shows the composite MCMC model distribution, along with prior and posterior resistivity ranges, the model with maximum posterior probability, the true model and the model recovered using a least-squares algorithm (EM1DFM). Centre column (D–F) shows the distribution of all interface depths in the MCMC models, along with the true values. Right column (G–I) shows a histogram of the number of layers in the ensemble of MCMC models.

model with the maximum posterior probability (blue) and the mean value over all of the MCMC models. In all three cases, the posterior distribution is smoothly distributed in a much narrower range than the prior. The mean and most probable estimates are close to the true value of 30 m.

Another view of the relationship between system elevation and the estimated near-surface parameters is provided in Fig. 9. This figure shows a cross-plot of the transmitter elevation against the conductivity-thickness product of the first layer in all of the accepted MCMC models for the case that uses the prior constraint on the vertical conductivity gradient (Fig. 7B). The cross-plots are coloured by the resistivity of the first layer (Fig. 9A), the thickness of the first layer (Fig. 9B) and the posterior probability for each model (Fig. 9C) as defined by eq (8). Overall, Fig. 9 shows that there is a strong non-linear relationship between system elevation and first layer conductivity–thickness product. Fig. 9(A) shows that there is a strong correlation, however, between the system elevation and resistivity of the first layer, which generally increases with decreasing system elevation. There is a slight bias towards thinner layers at lower system elevations (Fig. 9B), though this observation is complicated by the fact that information about deeper layers is not included. Fig. 9(C) shows a broad region of high-probability models, centred on the true values, which exhibit a positive correlation between system elevation and conductivity–thickness product, and represents the bulk of the histogram in Fig. 8(B). Interestingly, there is also a region of high-probability models at low system elevations (∼27–29 m) that have a thin, but resistive, first layer. This thin, resistive upper layer has little impact on the data as long as the resistivity of the second layer is close to the true value for the upper layer, resulting in this branch of models with reasonably high probability.

Synthetic ground-based example and survey design considerations

Next, a ground-based example is considered using the characteristics of the GEM-2 system (Huang & Won 2003), which is a multifrequency fixed-coil system that can be hand carried or towed in HCP or VCP modes, and has been utilized primarily for mapping shallow (less than approximately 10 m) features. The MCMC algorithm is utilized in this ground-based example to illustrate how parameter uncertainties change as a function of the acquisition parameters such as: frequency bandwidth, coil orientation, survey elevation or various combinations of these. This exercise is a valuable survey design tool that can help provide insights into what survey parameters should be used to achieve a desired level of model uncertainty, or to determine how well a specific model can be resolved.

Fig. 10(A) shows the simple three-layer model used for this example, which has a 10 Ω m layer embedded in a 100 Ω m host. The 10 Ω m layer is 5 m thick, with interfaces at 1 and 6 m. Fig. 10(B)
Bayesian MCMC algorithm for model assessment

Figure 8. Histograms of the posterior distribution of transmitter elevations for the three different prior scenarios in Fig. 7. The true transmitter elevation, elevation for the model with the highest posterior probability and mean elevations are superimposed on each figure.

shows the simulated data for this model using a default HCP survey orientation and elevation of 1 m, which is a typical height when the system is hand carried. The scenarios summarized in Table 2 all use 10 frequencies to keep the number of data consistent, and compare parameter and uncertainty estimates using different survey configurations. Data errors, unless stated otherwise, are assigned at 50 ppm for all frequencies and the true instrument elevation is assumed to be known. Scenario 1 represents the ‘nominal’ configuration; scenario 2 uses a limited band of frequencies; scenario 3 uses twice the nominal data errors; scenario 4 uses half the nominal survey elevation; scenario 5 uses the VCP configuration; scenario 6 uses only the quadrature part of the data; scenario 7 combines both HCP and VCP orientations, alternating orientation every other frequency; and scenario 8 combines both low and high survey elevations, alternating elevation every other frequency.

Fig. 11 illustrates the distribution of accepted MCMC models (Figs 11A, C, E, G, I, K, M and O) and histogram of interface depths (Figs 11B, D, F, H, J, L, N and P). These figures help to convey differences in the ability to resolve various parameters as a function of survey configuration. Additionally, Table 2 provides a summary of the estimated parameter errors for the MCMC most probable model. These errors are reported as individual parameter errors for the log-conductivities and log-depths for each layer, as well as the total parameter error norm. Because log-parameter values are used, the reported errors represent the logarithm of the ratio of the most probable model to the true model; values close to zero indicate that the estimated parameter is close to the true parameter.

The results can be loosely categorized into three groups. (1) The nominal configuration (scenario 1), which has an intermediate total error (0.61) and does a reasonable job of estimating the true model, but with moderate uncertainty regarding the upper layer depth and resistivity. (2) The single configuration perturbations to the nominal scenario (scenarios 2–6), which have larger total errors (>1.0) and are deficient in estimating at least one aspect of the true
model. For example, the low-survey elevation scenario (scenario 4) does a good job estimating the shallow interface (Fig. 11H), but is relatively insensitive to parameters at greater depth. (3) The third category consists of the examples that combine multiple configurations (scenarios 7–8). These configurations have significantly reduced total error (<0.25), are best able to capture the shallow interface (Figs 11N and P), and have reduced regions of uncertainty at depth.

This example has significant implications for survey design. By quantifying the expected uncertainty for different survey parameters, one can make informed decisions regarding the survey settings or data quality that is necessary to image a target of interest. For example, the benefit of reduced uncertainty attained in scenarios 7–8 needs to be weighed against the additional survey time required to collect the multiple configuration data. In a broader context, this approach could also be used as a tool to compare the relative merits of different survey methods (e.g. inductive EM vs. dc resistivity) for their ability to image a specific target.

**Field airborne data set**

The final example considers an airborne FDEM field data set acquired in 2009 in western Nebraska using the Fugro Resolve system (Smith et al. 2010). The primary purpose for acquiring these data was to provide information that could be used in conjunction with hydrogeological measurements to better constrain groundwater models. One of the primary objectives was to use the geophysical data to infer the topography, geometry and interconnectedness of the primary aquifer system in the survey area, as these have a significant impact on groundwater flow simulations.

The airborne survey covered a total of 937 line-km in several different areas of western Nebraska, of which 253 line-km were flown.
Bayesian MCMC algorithm for model assessment

Figure 10. (A) Three-layer synthetic resistivity model. (B) Forward response with nominal errors for the synthetic model using the characteristics of the GEM-2 system in HCP mode at 1-m survey elevation.

Table 2. Summary of simulated configurations and model errors for the ground-based parameter estimation example.

| Scenario | Orientation | Elevation (m) | Frequency range (kHz) | Other settings | Parameter error ($m^l - m^{true}$) | Total model error $||m - m^{true}||^2$ |
|----------|-------------|---------------|-----------------------|----------------|-----------------------------------|-------------------------------------|
| 1        | HCP         | 1.0           | 1–100                 | -              | 0.66 0.13 0.18 0.32 −0.11 −0.61  
| 2        | HCP         | 1.0           | 10–50                 | -              | 0.96 0.15 −0.86 0.52 −0.02 1.95  
| 3        | HCP         | 1.0           | 1–100                 | Data errors doubled (100 ppm) | 0.69 0.26 0.82 0.42 −0.30 1.48  
| 4        | HCP         | 0.5           | 1–100                 | -              | 0.24 0.56 0.95 0.40 −0.60 1.80  
| 5        | VCP         | 1.0           | 1–100                 | -              | 0.84 0.37 0.68 0.59 −0.29 1.72  
| 6        | HCP         | 1.0           | 1–100                 | Quadrature only | 0.89 0.10 −0.41 0.42 −0.01 1.13  
| 7        | HCP & VCP  | 1.0           | 1–100                 | Orientation alternates every other frequency | 0.13 0.02 −0.13 0.06 0.03 0.04  
| 8        | HCP         | 0.5 & 1.0     | 1–100                 | Elevation alternates every other frequency | 0.39 0.04 0.26 0.13 −0.05 0.24  

along ten 400 m-spaced lines near the town of Morrill (Fig. 12). In this area of the North Platte River system, the aquifer consists primarily of Quaternary alluvium ranging in thickness from zero to greater than 100 m on top of Tertiary White River Group siltstone, which acts as an aquitard (Weeks et al. 1988; Steele et al. 1998). The alluvial aquifer material consists of coarse materials that are electrically resistive, whereas the underlying siltstone formation is more conductive. This roughly binary system with the resistive alluvium underlain by more conductive material provides a good target for airborne FDEM systems.

Characteristics of the airborne system are the same as outlined in Table 1, with five HCP coil pairs and one VCX pair spanning a frequency range of approximately 0.4–128 kHz. The nominal survey elevation was 30 m, though the actual elevation varies during flight, and was recorded using a laser altimeter mounted on the system. Initial analysis of this block of over 74 000 individual soundings involved using the least-squares inversion algorithm EM1DFM (Farquharson et al. 2003) to estimate the distribution of resistivity with depth for each sounding (Smith et al. 2010). This inversion solved for the resistivity value in each of 25 model layers that have fixed thicknesses, where thicknesses increase with depth to account for the loss of resolution at depth. To solve this over-parametrized problem, regularization is used to recover the solution that minimizes a combined measure of data fit, vertical smoothness and proximity to a fixed reference model.

Fig. 13 shows an example of the estimated resistivity model along the easternmost survey line shown in Fig. 12. Note that there is significant vertical exaggeration (~30:1) in the inverted cross-section image given the approximately 25 km line length compared with only 100 m depth. Additionally, the estimated model is shaded by applying transparency to the image that is proportional to the DOI metric described by Oldenburg & Li (1999). The DOI metric provides a measure of regions within the model that are strongly influenced by the data, as compared with regions that are mainly influenced by the model regularization. By making transparent those regions with high DOI (which are controlled by regularization), the image conveys information about model values that are reliably inferred from the data, reducing the likelihood that features controlled by regularization will be misinterpreted. The DOI truncates the model at depths of about 75–100 m, which is typical for the...
Resolving the system. There are also shallow, resistive features that are partly transparent, indicating the decreasing resolution of resistive features with this system.

The resistive alluvium overlying the more conductive siltstone formation is clearly imaged in Fig. 13, which also illustrates the significant variability in the topography and thickness of the alluvial aquifer material. This cross-section is consistent with known features, such as the present-day North Platte River system that appears as a broad and deep resistive channel near 4645 km N. Presently, the topography of the base of the aquifer is estimated by choosing a resistivity value that represents the transition between alluvium and the underlying siltstone. In conjunction with sparsely distributed lithology and resistivity logs, this provides a good first estimate of the aquifer geometry for use in a groundwater model. A quantitative measure of parameter uncertainty, both in terms of resistivity values and the depths at which layer interfaces occur, is not conveyed in this estimated cross-section. Information about uncertainty can be used in the groundwater modelling study to infer uncertainty in flow distributions, or to assess what parameters are well defined when calibrating a groundwater model.

Data are extracted from four different locations that are characteristic of different regions of the model in Fig. 13, and are analysed with the MCMC algorithm. Location I represents an area where there does not appear to be resistive alluvial material at shallow depths. Location II is from the deepest portion of the resistive channel defined by the present-day North Platte River system, where it is unclear whether the data can determine the depth to the base of the resistive aquifer material. Location III is more clearly defined, with the transition from alluvial sediments to conductive material at a shallower depth that appears well resolved. Location IV is within one of the most resistive domains in the cross-section where there is some question regarding the depth to which the data are sensitive. This location is also coincident with a 119-m-deep borehole that has lithology and resistivity logs. Because of the computational expense involved with the MCMC method, it is not presently feasible to process entire lines of data with thousands of soundings. Instead, the MCMC algorithm is used in conjunction with the conventional inversion as a tool to estimate uncertainty in different regions of the model.

The panels on the top row of Fig. 14 show the MCMC models for each of the four locations shown in Fig. 13. Superimposed on these images are the most probable MCMC model (blue) as measured by eq (8), the model recovered using the least-squares algorithm EM1DFM (green), and the bounds that contain 95 per cent of the MCMC models (magenta). The prior pdf in eq (12) is used to constrain the vertical gradient of the conductivity at each location. The lower row of panels shows the observed data with error bars, along with the distribution of predicted responses that corresponds to the models in the upper panels. Again, the predicted responses are only calculated at the six survey frequencies, and are interpolated in between. At all of the locations, the most probable MCMC model has two layers, though the layer interface depth is variable. Table 3 summarizes the parameters for the most probable model at each location. Additionally, the MCMC models agree well with the EM1DFM inversion results.
Figure 12. Map of a portion of the airborne FDEM survey lines flown in 2009 in western Nebraska.

Figure 13. Resistivity model along the eastern-most survey line in Fig. 12 recovered using the least-squares inversion algorithm EM1DFM. Vertical dashed lines indicate locations that are extracted for analysis with the MCMC algorithm.

Fig. 15 provides a summary of the posterior distribution of parameters for the models in Figs 14(A), (C), (E) and (G). The top row of histograms (Figs 15A, D, G and J) shows the distribution of layer interface depths extracted from the ensemble of MCMC models. Peaks in these histograms correspond with the interface depths in Table 3, though the widths of the peaks vary with depth to the interface and resistivity values. The interface depths at locations II and IV are not as well defined as those at locations I and III because of the depth of the interface (II) and high resistivity (IV).

Also superimposed on each figure is a curve that is meant to be a proxy for the DOI discussed earlier. This curve is defined by the width of the 95 per cent credible region shown in Fig. 14, normalized by the width at the maximum depth of 150. Values are then scaled to the horizontal-axis of the underlying histogram such that the value at 150 m represents a metric of one. Small values of...
Figure 14. Distribution of MCMC models (A, C, E and G) for each of the locations shown in Fig. 13 along with the most probable model, the model obtained using EM1DFM, and the 95 per cent model credible region. (B, D, F and H) Measured data with error bars for each sounding, along with the distribution of predicted data for the various models above each panel.

Table 3. Summary of MCMC most probable model values for the locations shown in Fig. 13.

<table>
<thead>
<tr>
<th></th>
<th>I (4640N)</th>
<th>II (4645N)</th>
<th>III (4650N)</th>
<th>IV (4657.5N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer 1 resistivity (Ω m)</td>
<td>12.5</td>
<td>63.4</td>
<td>92.8</td>
<td>306.3</td>
</tr>
<tr>
<td>Layer 2 resistivity (Ω m)</td>
<td>6.6</td>
<td>11.4</td>
<td>7.8</td>
<td>82.6</td>
</tr>
<tr>
<td>Interface depth (m)</td>
<td>10.6</td>
<td>54.8</td>
<td>22.6</td>
<td>7</td>
</tr>
<tr>
<td>$h'<em>\text{MCMC} - h'</em>\text{obs}$ (m)</td>
<td>-1.3</td>
<td>-3.8</td>
<td>-1.2</td>
<td>+4.1</td>
</tr>
</tbody>
</table>

The DOI-metric represent areas where the resistivity is well defined within a relatively narrow range of values. Conversely, large values represent depths where a wide range of resistivity values can be present and still are consistent with the measured data. There is generally a rapid increase in the DOI metric at depths greater than approximately 60 m, indicating a gradually decreasing ability to resolve layers. This loss of depth-resolution occurs at shallower depths for resistive layers compared with conductive layers due to the reduced sensitivity of the FDEM method to resistive features. Evidence for this asymmetric loss in depth-resolution is evident in Fig. 14, where the upper limit of the 95 per cent credible region increases more rapidly than the lower limit.

The middle row of histograms (Figs 15B, E, H and K) shows the distribution of the number of layers in the ensemble of MCMC models, all of which are biased towards few-layer models. The bottom row of histograms (Figs 15C, F, I and L) shows the distribution of transmitter elevation for the various models. At locations I and III, which have shallow interfaces and relatively low resistivities, the distribution of transmitter elevations that are consistent with the data is relatively narrow, and the most probable value is close to the measured value. At location IV, the resistive near-surface layer results in a much broader distribution of allowable transmitter elevations, which would extend to greater elevations was it not for the uniform prior distribution that constrains values to fall within 5 m of the measured height.

Finally Fig. 16 compares the results from location IV (Fig. 14G) with data from a borehole drilled approximately 20 m away from the sounding. Short- and long-normal resistivity logs are superimposed in yellow, and are generally consistent with both the MCMC and EM1DFM results. The right-hand side of this figure shows the general lithology, along with the formation factor (the ratio of the bulk resistivity to the fluid resistivity) computed from the electric log data. The upper silt layer observed in this borehole (approximately 25 m depth) is not found in other wells in the area, which typically indicate a single transition from alluvium to the siltstone aquitard at depth. This thin silt layer is not interpreted as the base of aquifer, though it likely complicates the hydrogeology in this portion of the model. As discussed later, the low resistivity of this layer limits the ability to accurately constrain the resistivity of the sand and gravel unit beneath it.

Although the resistivity-log data are consistent with the MCMC models, the logs indicate a transition to lower resistivity associated with the first silt and clay layer at approximately 25 m, whereas the MCMC most probable model indicates a transition at approximately 20 m. This discrepancy could be attributed to differences in the sensitivity volume for the resistivity log compared with the airborne footprint and/or a lack of vertical resolution in the airborne data. The increase in resistivity indicated by the log data from approximately 40 to 70 m depth is not a pronounced feature in the MCMC distribution due to the limited sensitivity to resistive targets at depth, but the distribution of models is somewhat biased towards greater resistivity values in this depth range. At approximately 70 m depth, the resistivity logs capture a sharp transition to low resistivity associated with the silt and clay layers that form the impermeable base of the aquifer. While the sensitivity of the airborne data is significantly limited at this depth, the distribution of MCMC...
Figure 15. Posterior distribution of various parameters extracted from the models in Fig. 14. (A, D, G and J) Distributions of layer interface depths for all locations are generally consistent with two-layer models, though with varying interface depth. The superimposed line on these panels represents the width of the 95 per cent credible region at each depth, normalized by the value at 150 m, and represents an estimate of the depth of investigation. (B, E, H, and K) Histograms show the number of layers in the ensemble of MCMC models, which is biased towards few-layer models. (C, F, I and L) Distributions of the transmitter elevations \( h^T \) for the models in Fig. 14 along with the most probable value and the value measured from the laser altimeter.

models indicates a trend towards lower resistivity values, but with little constraint on the interface depth or resistivity value.

This example clearly indicates the value in estimating the space of plausible models given the available data, rather than providing just a single ‘best model’. In fact, there are a number of four-layer models in the MCMC ensemble that closely match the characteristics of the resistivity logs. While these models do not have a particularly large posterior probability, they are nonetheless acceptable models that are consistent with the measured data and should be considered in the interpretation.

**DISCUSSION**

Uncertainty is intrinsic to geophysical surveys due to the non-unique nature of geophysical measurements and limited prior information about true model parameters. The nature of this uncertainty depends on many factors such as the geophysical method that is used, instrumentation and survey parameters, data errors, prior assumptions and model errors. Presenting a single ‘best-fit’ model, even with traditional linear estimates of uncertainty, often does not fully capture the ambiguity in geophysical models, and can result in a misleading or inaccurate interpretation. A comprehensive assessment of model uncertainty and non-uniqueness is a valuable tool when interpreting geophysical data sets. By presenting results in a probabilistic framework, the interpreter has greater insight into which aspects of the model are well defined, and which are not, allowing them to make informed decisions based on the geophysical data.

This work has attempted to highlight the uncertainty associated with airborne and ground-based FDEM data sets. The trans-dimensional Bayesian MCMC approach provides significant flexibility in model parametrization, and helps to reveal information about parameter estimates and uncertainty, such as

1. identification of asymmetric bounds on parameter uncertainty, where lower bounds on resistivity values are generally better defined than upper bounds, particularly for high-resistivity layers;
2. assessment of the depth to interfaces, with probabilistic information about how well or poorly constrained interfaces are;
3. assessment of uncertainty in the system elevation, and how this is linked to uncertainty in near-surface resistivity values;
4. identification of non-linear correlations between different model parameters in the parameter estimation problem, and
5. assessment of the impact of changes in system configuration on parameter uncertainty, which can be used as a survey-design tool to test the system parameters that are required to achieve a desired level of resolution or reduction in uncertainty.

Due to the significant computational expense associated with the MCMC sampling approach, this technique is presently best utilized in conjunction with fast least-squares algorithms. Images of ‘best-fit’ parameter estimates over large survey areas can be generated using traditional least-squares methods, and the MCMC algorithm can be used to assess uncertainty in several distinct regions of the model. Future efforts will focus on implementing the Bayesian MCMC approach over larger areas in two or three dimensions, which will require the use of a different parametrization strategy as well as parallel computing resources.

**CONCLUSIONS**

A trans-dimensional Bayesian MCMC algorithm has been introduced for the purpose of improving model assessment and uncertainty analysis of FDEM data, and the efficacy of the algorithm has been demonstrated with both synthetic and field-data examples. This approach is flexible in that it can be applied to various
airborne or ground-based systems, providing estimates of subsurface resistivity distributions while allowing for uncertainty in the system elevation. Allowing the number of layers to be an unknown parameter that is estimated from the data provides a significant degree of flexibility that avoids biases that are due to the choice of parametrization. Important inferences can be made about parameter values, uncertainty, non-uniqueness, sensitivity and correlation by exploring the posterior distribution of MCMC models which, in turn, leads to a much more robust interpretation of the measured data and allows end-users of these data to make better informed decisions.

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REFERENCES


**Supporting Information**

Additional Supporting Information may be found in the online version of this article:

**Supplement.** Forward response and sensitivity calculations.

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