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Transdimensional Electrical Resistivity Tomography

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Key Points:

- Voronoi cells provide a more flexible inversion parameterisation compared to previous research
- Including full non-linearity allows us to image deeper into the solid Earth with the same data
- Uncertainty loop topologies are observed in multiple types of physics

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Abstract

This paper shows that imaging the interior of solid bodies with fully non-linear physics can be highly beneficial compared to imaging with the equivalent linearised tomographic methods, and that this is true for a variety of different types of physics. Including full non-linearity provides interpretable uncertainties, and far greater depth of image penetration into unknown targets such as the Earth’s subsurface. We use an adaptively parameterised Monte Carlo method to invert electrical resistivity data for the conductivity structure of the Earth, and demonstrate the method on two field datasets. Key results include the observation of directly interpretable uncertainty loops which define possible geometrical variations in the edges of isolated anomalies, hence quantifying the spatial resolution of these boundaries. These topologies of uncertainties are similar to those observed when performing fully non-linear seismic travel time tomography. This shows that loop-like uncertainty topologies are expected in the solutions to a wide variety of tomographic problems, using a variety of data types and hence laws of physics (here the Laplace equation; in previous work the Eikonal or ray equations). We also show that the depth to which we can construct a tomographic image using electrical data is extended by up to a factor of 8 using non-linear methods compared to linearised inversion using common standard linearised programs. These advantages come at the cost of significantly increased computation. All of these results are illustrated on both synthetic and real data examples.

1 Introduction

Geophysical imaging methods are routinely employed in both industry and academia to obtain information about the composition of the Earth’s subsurface and its changes over time. While in some cases one might be satisfied by finding the single model which best explains the recorded data, it may often be the case that a single best-fitting model is of little value to decision makers since a comprehensive assessment of risk may only be carried out by assessing the full range of possible models that fit our observations (i.e., the post-experiment or *posterior* distribution of models given the available data). This set of models and statistics of their distribution are commonly referred to as the model *uncertainty*. For instance, when geophysical methods are employed to evaluate the size of a subsurface plume of leaked fluids or to monitor its changes over time, an accurate evaluation of model uncertainty, the range of subsurface models that may be permissible, is necessary in order to assess the risk related to the volumes and rates of escaping fluids.

In a typical imaging scenario, geophysical data are acquired at the Earth’s surface or within boreholes. Depending on the type of data acquired, inversion might be required in order to recover the subsurface properties of interest from the recorded quantities. Mathematically speaking, this involves inferring a set of model parameters \mathbf{m} from a set of observed data \mathbf{d}^{obs} , and is achieved by solving an expression such as $\mathbf{d}^{obs} = \mathbf{d}^{true} + \epsilon = \mathbf{g}(\mathbf{m}) + \epsilon$ for \mathbf{m} , where \mathbf{d}^{true} represents the data that would be recorded in the absence of sources of error, ϵ is an error term, and \mathbf{g} is a function that describes the physics relating \mathbf{m} to \mathbf{d}^{true} . In this framework, ϵ represents the effects on recorded data of any elements of the physics relating \mathbf{d}^{obs} to \mathbf{m} that are not represented within function \mathbf{g} . The distribution of possible values of ϵ therefore represents the uncertainties in the observed data when compared to $\mathbf{d}^{true} = \mathbf{g}(\mathbf{m})$. However note that in practical applications, $\mathbf{g}(\mathbf{m})$ is normally evaluated using numerical methods which involve a number of approximations in function \mathbf{g} , and which result in further sources of error.

In electrical resistivity tomography (ERT), electrical currents are actively injected into the ground from pairs of electrodes, and the resulting electrical potential is measured as the potential difference between other pairs of electrodes located on or below the Earth’s surface. These measurements constitute a set of observations \mathbf{d}^{obs} , and are used to estimate the resistivity structure of the subsurface parameterised by vector \mathbf{m} . In ERT, the *forward problem* consists of finding a set of potential differences \mathbf{d}^{pred} through resistivity model \mathbf{m} , which

61 can be calculated computationally by simulating the potential field induced within model
 62 \mathbf{m} by the electric currents [Dey and Morrison, 1979a,b; Pridmore et al., 1981]. The *inverse*
 63 *problem* involves inferring the set of models \mathbf{m} such that $\mathbf{g}(\mathbf{m})$ matches the observed poten-
 64 tial differences \mathbf{d}^{obs} to within their observational uncertainties (since all such models in that
 65 set represent possible subsurface structures).

66 However, solving an inverse problem in geophysics poses challenges which go beyond
 67 merely finding a solution that mathematically fits observed data. It is almost always the case
 68 that more than one model \mathbf{m} may adequately fit the observations \mathbf{d}^{obs} to within their uncer-
 69 tainties. Inverse problems may be solved by using optimisation or stochastic (often Bayesian)
 70 methods. In an optimisation framework (e.g., Parker [1994]), the combination of param-
 71 eters that minimises an objective function (involving data misfit and regularisation terms) is
 72 generally regarded as the model solution. This makes sense in cases where it does not par-
 73 ticularly matter which solution is found out of the set of possible solutions (for example,
 74 when optimising the model parameterisation to best represent measured information [Cur-
 75 tis and Snieder, 2002]), designing an optimal experiment or survey to constrain parameters
 76 [Curtis, 1999a,b; Maurer et al., 2000], finding parameters that smoothly interpolate through
 77 data [Sambridge et al., 1995], or where the problem is so large that it is computationally in-
 78 tractable to find more than one solution from the set [Simmons et al., 2012]). By contrast,
 79 stochastic inversion schemes do not limit the solution to a single model but produce a large
 80 ensemble of valid models. Typically such methods are associated with Bayesian inversion
 81 where the desired set of models are distributed according to a so-called *posterior* probability
 82 density function (PDF), so that each model parameter has a distribution of possible values
 83 rather than a single value [Mosegaard and Tarantola, 1995; Tarantola, 2005]. Obviously,
 84 regardless of the inversion scheme employed, the solution to a geophysical inverse problem
 85 must also make sense physically.

86 Within the context of ERT, a number of authors have employed stochastic methods in
 87 order to overcome the problem of non-uniqueness and include prior information in the so-
 88 lution (e.g., Kaipio et al. [2000], Ramirez et al. [2005]). In addition, a number of studies
 89 have employed stochastic methods to invert direct current (DC) resistivity datasets jointly
 90 with other types of data. For instance, JafarGandomi and Binley [2013] use multiple types of
 91 geophysical datasets in a joint transdimensional MCMC inversion algorithm combining data
 92 from DC resistivity, electromagnetic induction and ground penetrating radar (GPR); Linde
 93 et al. [2006] invert DC resistivity and GPR traveltimes data with a regularised least-squares
 94 algorithm, but use stochastic regularization operators based on geostatistical models to con-
 95 strain the solution; Irving and Singha [2010] use MCMC to jointly invert DC resistivity and
 96 borehole tracer concentration data to obtain posterior information on hydraulic conductivity;
 97 Jardani et al. [2013] perform a fully-coupled inversion of hydrogeochemical and geoelectrical
 98 data by combining DC resistivity, self-potential, and salinity measurements.

99 Data uncertainties play a fundamental role in geophysical inverse problems as they
 100 determine how accurately the model should fit observed data. Sources of uncertainty in geo-
 101 physical inversion are diverse and normally include contributions from both data measure-
 102 ment and modelling errors. In the context of ERT, measurement errors might for instance be
 103 caused by inaccuracy of the voltmeter and/or ammeter and electrode charge-up effects, while
 104 modelling errors are typically due to approximations in the physics of the forward problem
 105 represented by function \mathbf{g} or in the numerical methods used to evaluate $\mathbf{g}(\mathbf{m})$ for any \mathbf{m} , and
 106 to the mislocation of electrodes in the acquisition array leading to geometrical errors. Given
 107 the presence of contaminating noise during acquisition and the limitations in instrumental
 108 sensitivity, resolution, and computational power, such errors are unavoidable and must be
 109 accounted for correctly when evaluating the uncertainty associated with the set of solutions
 110 to the inverse problem. For instance, in cases where ERT is used to evaluate the size of a
 111 leakage plume or to monitor its changes over time, the solution must include an estimate of
 112 uncertainty in order to correctly assess the spatial resolution of the plume through inversion
 113 or whether leakage is still ongoing. Hence, in situations where assessing the veracity of a

particular potential event or hypothesis is paramount, the use of stochastic, rather than optimisation, inversion methods is particularly beneficial since an estimate of model uncertainty can be evaluated directly from the posterior PDF of each model parameter.

However, the benefits of stochastic tomography methods are often accompanied by increases in the computational time and resources required to perform the inversion. In the case of ERT, such increases are mainly due to the repeated computation of the forward problem which must be solved tens or hundreds of thousands of times. A number of authors have attempted to mitigate the computational expense of stochastic ERT by reducing the size of the space of plausible solutions. For instance, *Ramirez et al.* [2005] use prior information to parameterise subsurface contaminant plumes as a set of simple volumes embedded in a homogeneous medium, and combine Markov chain Monte Carlo (MCMC) with 3D ERT to monitor changes in the shape and size of the plumes with time; *Rosas-Carbajal et al.* [2014] employ a smoothing constraint in joint ERT and RMT inversion to favour models showing smooth spatial transitions, hence decreasing the size of the model space to those satisfying this constraint; and *Andersen et al.* [2003] define the model in terms of a set of vertices which can be joined to create polygons whose number and size is determined by a set of user-defined tuning parameters.

Within this paper we present a stochastic inversion method for resistivity tomography which uses Bayesian theory [*Bayes and Price*, 1763], the reversible-jump Markov chain Monte Carlo algorithm (rj-MCMC – *Green* [1995, 2003]), and model parameterisation with Voronoi cells [*Bodin et al.*, 2009; *Bodin and Sambridge*, 2009] to solve the inverse problem of ERT and to produce an ensemble of valid solutions which are distributed according to the Bayesian posterior PDF. This method can be referred to as ‘transdimensional’ in that the dimensionality of the model space (the number of model parameters) is allowed to vary between different models. Transdimensional inversion is a relatively new concept in electrical resistivity tomography, but has previously shown great potential in tackling a number of diverse inverse problems such as regression [*Gallagher et al.*, 2011], inversion of frequency-domain [*Minsley*, 2011] and controlled source [*Ray et al.*, 2014] electromagnetic data, geoaoustic inversion of seabed reflection coefficients [*Dettmer et al.*, 2010], inversion of surface-wave phase and group velocities [*Young et al.*, 2013] and traveltimes [*Bodin and Sambridge*, 2009; *Galetti et al.*, 2015], joint inversion of surface-wave dispersion and receiver function data [*Bodin et al.*, 2012a], inversion of DC resistivity sounding curves [*Malinverno*, 2002], and full waveform inversion of marine seismic data [*Ray et al.*, 2016]. In addition, *Hawkins and Sambridge* [2015] recently developed a new class of transdimensional solvers that sample over tree structures, and this sampling approach has successfully been applied in 2D to the time-domain electromagnetic inverse problem [*Hawkins et al.*, 2017] and to seismic low-frequency full waveform inversion *Ray et al.* [2018].

One advantage of a transdimensional approach lies in the fact that, by allowing the model parameters (in our case the number of Voronoi cells used to discretise the Earth’s subsurface resistivity structure) to vary in number, shape and size, the space of possible a priori parameterisations is broadened, ensuring a more comprehensive estimation of the a posteriori uncertainty since this becomes independent of any particular choice of model parameterisation. In addition, thanks to the ‘natural parsimony’ of Bayesian inference, posterior models are only as complex as is required by the data or by prior information: among similar models that provide equal fit to the observations, simpler ones (those having fewer Voronoi cells) are assigned a higher probability since larger prior volumes are penalised. A mathematical proof of this concept is given by *Ray et al.* [2016, 2018], who describe ‘natural parsimony’ as the result of a trade-off between Occam Factor (i.e., the ratio of posterior accessible volume to prior accessible volume [*MacKay*, 2003]) and high likelihood (low misfit), and how this trade-off automatically provides a solution similar to regularisation but largely dependent on the data. Finally, by reducing the model space dimensionality to only what is required to explain the data, one avoids over-parameterising the space of solutions. The computational demands of stochastically exploring higher-dimensional spaces explodes exponentially

(called the *curse of dimensionality* – *Scales and Snieder* [1997], *Curtis and Lomax* [2001]), so the natural parsimony also enormously reduces the computation required to find the solution set by limiting its number of dimensions. In turn, this makes uncertainty estimation tractable.

In the next section, we provide an overview of the forward problem in electrical resistivity tomography and present the transdimensional electrical resistivity tomography (TERT) method, showing how it can be used to perform a fully non-linear inversion of potential difference measurements. In Section 3, we present results of two synthetic experiments in which TERT was used to perform the inversion, and compare the results to those obtained using a more traditional, iterative-linearised inversion method. In Section 4, we apply TERT to a real dataset acquired at an archaeological site in Scotland, and we present a further observational example using a dataset acquired at an archaeological site in Slovakia in the online Supporting Information. We then discuss the main advantages and disadvantages of this method, and outline directions for future work before concluding.

2 Method

2.1 The forward problem

In electrical resistivity imaging, pairs of ‘current electrodes’, located either on the Earth’s surface or within boreholes, are used to inject electrical currents into the ground, while the resulting electric potentials are measured by pairs of many ‘potential electrodes’ along an array. The forward problem therefore consists of solving the following equation for the electrical potential $\Phi(\mathbf{x})$ at each potential electrode location, and calculating potential differences between many pairs of electrodes:

$$\nabla \cdot \left[\frac{1}{\rho(\mathbf{x})} \nabla \Phi(\mathbf{x}) \right] = -I (\delta(\mathbf{x} - \mathbf{x}_+) - \delta(\mathbf{x} - \mathbf{x}_-)) \quad (1)$$

where $\rho(\mathbf{x})$ denotes resistivity at location \mathbf{x} , and \mathbf{x}_+ and \mathbf{x}_- represent the location of a positive and negative current electrode, respectively (for completeness, the simpler case of current injection from a single electrode is described in Appendix A:).

Analytical solutions to equation 1 can be found for simple cases such as a buried sphere in a homogeneous medium or a vertical boundary separating two media of different resistivity (see examples in *Telford et al.* [1991]). However, more sophisticated numerical techniques are needed when the resistivity structure of the subsurface is more complex. Such techniques include the linear filter method in 1D (e.g., *Koefoed* [1979]), and finite-difference and finite-element methods in 2D and 3D (e.g., *Dey and Morrison* [1979a,b]; *Pridmore et al.* [1981]).

Many authors have developed linearised numerical techniques and programs to solve equation 1 for complex resistivity geometries $\rho(\mathbf{x})$ in 2D and 3D [*Dey and Morrison*, 1979a,b; *Pridmore et al.*, 1981; *Lowry et al.*, 1989; *Loke*, 1994; *Li and Spitzer*, 2002; *Rücker et al.*, 2006; *Pidlisecky and Knight*, 2008; *Binley*, 2013a,b]. Within our inversion algorithm, we solve the forward problem using a finite-difference scheme adapted from the MATLAB modelling code *FW2_5D* by *Pidlisecky and Knight* [2008]. Besides being completely open source and easily understood, *FW2_5D* is a highly efficient and customizable code, and we easily optimised and integrated it into our own inversion program. The forward modelling routines in *FW2_5D* are based on the 2.5D modelling algorithm of *Dey and Morrison* [1979a] in which subsurface structures are described in 2D (i.e., they are assumed to be constant along the y direction) but the current flow is modelled in all three dimensions using a Fourier-cosine transform. Hence, the 3D physics of current flow is accounted for without the need for far more expensive three dimensional modelling. Nevertheless, since the inversion algorithm is entirely separate from the forward calculations, the forward modeller could easily be replaced by alternative routines.

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2.2 Inversion with the rj-McMC algorithm

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The rj-McMC algorithm by *Green* [1995] was first applied to geophysical tomography problems by *Bodin and Sambridge* [2009], who implemented this method within a linearised, iterative seismic traveltime inversion scheme. In each iteration they used the rj-McMC algorithm to produce an ensemble of velocity models which fit the observed travel-time data, but with fixed ray paths (thus linearising the problem). The forward problem of calculating source-receiver traveltimes was then solved using the average velocity structure obtained from the ensemble of models to fix seismic ray paths for the next iteration. In doing so, *Bodin and Sambridge* [2009] partly accounted for the non-linearity of the tomographic problem since raypaths and traveltimes were updated at the end of each Markov chain loop. Later, *Galetti et al.* [2015] modified their algorithm to make it fully nonlinear: in the approach of *Galetti et al.* [2015], the forward problem was solved for every individual model in the ensemble, thus no linearisation-related forward modelling approximations and biases were introduced into the solution.

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Within this study, we adapted the approach of *Galetti et al.* [2015] to the inverse problem of ERT in order to produce a fully nonlinear inversion method. Similarly to *Bodin and Sambridge* [2009] and *Galetti et al.* [2015], this method uses an irregular Voronoi cell tessellation to parameterise the model and allows uncertainty in the solution to be estimated correctly. In this section, we review the rj-McMC tomography framework of *Bodin and Sambridge* [2009] by providing an overview of the model parameterisation employed and describing the Bayesian approach used by the algorithm. Further details on the mathematical theory behind the algorithm can be found in Appendix B: .

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2.2.1 Bayes' theorem

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Within a Bayesian framework, information is represented by probability density functions. Bayesian inference makes use of Bayes' theorem [*Bayes and Price*, 1763] to estimate the *a posteriori* PDF (also known as 'posterior distribution') $p(\mathbf{m}|\mathbf{d}^{obs})$, which can be defined as the probability density of model \mathbf{m} given observed data \mathbf{d}^{obs} . Bayes' theorem states that $p(\mathbf{m}|\mathbf{d}^{obs})$ can be estimated by combining information from observations with *a priori* information about the model according to

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$$p(\mathbf{m}|\mathbf{d}^{obs}) \propto p(\mathbf{d}^{obs}|\mathbf{m})p(\mathbf{m}) \quad (2)$$

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Here, $p(\mathbf{d}^{obs}|\mathbf{m})$ is called the likelihood function, which expresses the probability of observing dataset \mathbf{d}^{obs} given model \mathbf{m} , and prior information about model \mathbf{m} (i.e., everything we knew about the model before performing the inversion) is represented by the *prior* probability density $p(\mathbf{m})$. Equation 2 therefore represents how prior information about the model is updated by new data to give the posterior state of information described by $p(\mathbf{m}|\mathbf{d}^{obs})$.

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2.2.2 Model parameterisation with Voronoi cells

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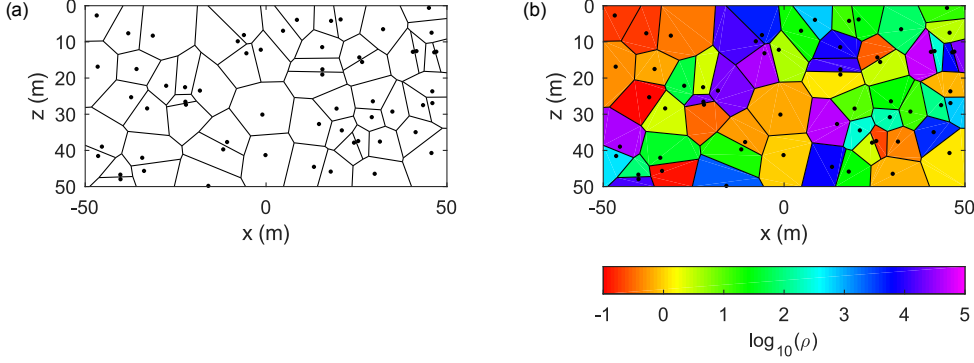
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Our implementation of the rj-McMC algorithm in ERT uses Voronoi cells to parameterise the resistivity model. A Voronoi tessellation of a 2D xz plane of resistivity values is achieved by defining a set of n nuclei (the black dots in Figure 1) which are identified by their xz coordinates, and a value of $\log_{10}(\text{resistivity})$ for each nucleus. For simplicity, from here onwards we drop the subscript in \log_{10} and simply denote the logarithm in base 10 as \log . The 2D plane is then divided into n non-overlapping regions (Voronoi cells) of different resistivity such that each region contains the portion of the plane which is closest to its nucleus. Note that Voronoi nuclei are not necessarily located at the centre of their corresponding cells, but rather cell boundaries are defined by the perpendicular bisectors of pairs of neighbouring nuclei. A resistivity model can therefore be defined as $\mathbf{m} = [n, \mathbf{c}, \boldsymbol{\mu}]$, where \mathbf{c} and $\boldsymbol{\mu} = \log(\boldsymbol{\rho})$ are n -row arrays of nuclei xz coordinates and $\log(\text{resistivity})$ values, respectively. In our implementation resistivity is constant within each Voronoi cell so the dimension of model \mathbf{m} is $3n + 1$.



264 **Figure 1.** Example of Voronoi tessellation of a 2D plane. (a) Each Voronoi cell is identified by the location
 265 of its nucleus (black dots), and cell boundaries are defined purely by the perpendicular bisectors of pairs of
 266 neighbouring nuclei (black lines). (b) The Voronoi tessellation is turned into a resistivity model by assigning
 267 a value of $\log(\text{resistivity})$ to each cell.

268 During the inversion, the location and number of Voronoi nuclei in the model is al-
 269 lowed to vary, making the number of Voronoi cells in the model one of the inversion param-
 270 eters. Since Voronoi cells change shape and size throughout the inversion, the model param-
 271 eterisation dynamically adapts to the spatial distribution of both information and subsurface
 272 structure.

273 2.2.3 Data noise parameterisation

274 Within a transdimensional inversion framework, the magnitude of data uncertainties
 275 influences the level of complexity (here, the number of Voronoi cells) in the final solution.
 276 In a similar framework for seismic traveltime tomography, *Bodin et al.* [2012b] proposed
 277 a method to parameterise uncertainty which allows data noise to be varied and estimated
 278 during the inversion. As the use of accurate uncertainties prevents data over- or under-fitting,
 279 so doing allows the observations to be fit up to the appropriate uncertainty level, and makes
 280 the rj-McMC method almost entirely data-driven.

281 If data uncertainty estimates are available, then those *a priori* uncertainties σ^{prior}
 282 (scaled arbitrarily in absolute terms) may be up- or down-scaled by a factor λ which can be
 283 estimated during inversion. Hence, for datum k with *a priori* uncertainty σ_k^{prior} , the *a poste-*
 284 *riori* uncertainty σ_k^{post} is given by

$$285 \sigma_k^{post} = \lambda \times \sigma_k^{prior} \quad (3)$$

286 Since λ is an additional parameter to be determined during the inversion, this makes the di-
 287 mension of the model equal to $3n + 2$. If multiple independent datasets with potentially dif-
 288 ferent data noise levels are combined such that a λ value is determined for each dataset, the
 289 model dimension becomes $3n + n_{ds} + 1$, where n_{ds} is the number of datasets.

290 If no information on data uncertainties is available, data noise must be estimated dur-
 291 ing inversion since evaluating the data fit of any model requires that the uncertainty of each
 292 datum be taken into account. Although a single uncertainty value could be assigned to all
 293 measurements, in real acquisition scenarios it is likely that each measured potential differ-
 294 ence will be affected by a different amount of noise. For instance, *Binley et al.* [1995] sug-
 295 gest a type of data noise parameterisation in which data variance (the square of data standard
 296 deviation) increases linearly with the square of the measured resistance R (the measured po-
 297 tential difference divided by the injected current) as in

$$298 (\sigma_k^{post})^2 = a^2 \times R^2 + b^2 \quad (4)$$

where a and b represent hyperparameters that could be estimated during the inversion. This type of data noise parameterisation makes the model dimension equal to $3n + 3$ if a single a and b are estimated for the entire dataset, and $3n + 2 \times n_{ds} + 1$ if n_{ds} datasets with different a and b parameters are combined.

When data noise is parameterised and estimated during the inversion, the model is defined by the combined set $\mathbf{m} = [n, \mathbf{c}, \boldsymbol{\mu}, \mathbf{h}]$, where \mathbf{h} is the array of vector hyperparameters ($\mathbf{h} = [\lambda_1, \lambda_2, \dots]$ or $\mathbf{h} = [a_1, b_1, a_2, b_2, \dots]$), and where n , \mathbf{c} and $\boldsymbol{\mu}$ are defined in Section 2.2.2.

However, note that data uncertainty estimation in ERT is an ongoing topic of research, hence a more sophisticated type of parameterisation for data uncertainties may be developed in future. For instance, *Tso et al.* [2017] recently highlighted how ERT measurement errors may not be uncorrelated as is often assumed, and developed an error model that includes the effect of the combination of electrodes used for each measurement as well as the linear relationship between measurement error and transfer resistance (equation 4). In addition, note that the term ‘noise’ in this paper refers to *both* measurement and modelling errors, hence the posterior uncertainty σ_k^{post} in equations 3–4 encapsulates any effect by which the model cannot explain the observed data.

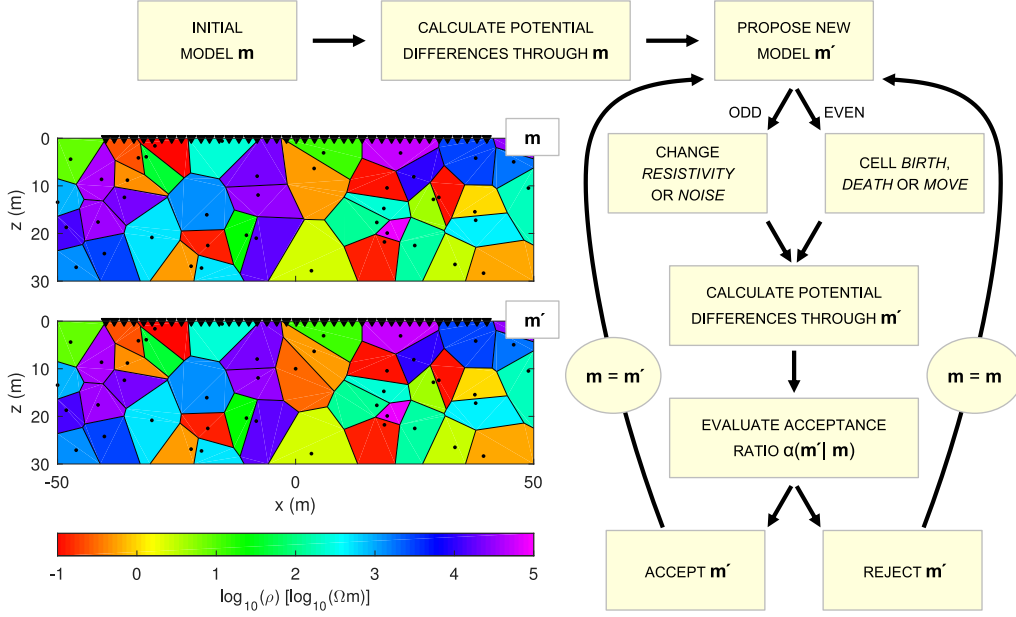
2.2.4 A transdimensional Bayesian approach to tomography

As shown in equation 2, Bayesian inference is a valuable method to characterise the posterior PDF $p(\mathbf{m}|\mathbf{d}^{obs})$ by combining prior information with measured data. However, since the posterior PDF cannot normally be expressed in analytic form, it must be evaluated numerically at different positions in the model parameter space which involves solving the forward problem at each position. If the inverse problem has many dimensions as is usually the case in geophysics, the number of forward functions that need to be solved to explore the full parameter space becomes huge, making uniform sampling of the posterior computationally infeasible (e.g., *Curtis and Lomax* [2001]) and the use of alternative sampling methods a necessity.

Markov chain Monte Carlo (MCMC) provides an iterative stochastic framework which generates samples from the Bayesian posterior PDF as expressed in equation 2. Using an MCMC sampler such as the Metropolis-Hastings (MH) algorithm [*Metropolis et al.*, 1953; *Hastings*, 1970], samples are generated in sequence along a chain, each sample being a random perturbation of the one that precedes it. The initial model of the chain is selected randomly from the prior distribution described in the previous section, and often a randomly-selected model parameter or combination of parameters is perturbed at each step of the chain. However, compared to traditional MCMC, the reversible jump Markov chain Monte Carlo (rj-MCMC) algorithm [*Green*, 1995] does not fix the dimensionality of the model, hence ‘jumps’ in model dimensionality can also be made by adding or deleting model parameters (in our case Voronoi cells).

Our algorithm essentially consists of the following seven steps, which are displayed in the workflow diagram in Figure 2:

1. An initial resistivity model \mathbf{m} is drawn from a Uniform distribution of Voronoi-tessellated models and data noise parameters.
2. Potential differences for all required configurations of current and potential electrodes are calculated through \mathbf{m} (see Section 2.2.6 for implementation details in a Voronoi-cell model).
3. A new model \mathbf{m}' is proposed by randomly perturbing the current model \mathbf{m} using one of the following types of perturbation: *birth* to add a cell; *death* to delete a cell; *move* to change the location of a cell; *resistivity* to change the resistivity of a cell; *noise* to change a data noise parameter (see Appendix B.3 for more details on each perturbation type).



336 **Figure 2.** Workflow of the transdimensional electrical resistivity tomography (TERT) method. This sam-
 337 ples the posterior PDF by producing an ensemble of Voronoi-tessellated models of subsurface resistivity using
 338 the rj-MCMC algorithm. Each Voronoi cell is defined by the location of its nucleus (the black dots in \mathbf{m} and
 339 \mathbf{m}') and a value of $\log(\text{resistivity})$ ($\log(\rho)$). In this example, the geometry of model \mathbf{m} is perturbed in a *birth*
 340 step by adding a Voronoi nucleus at [0 10] m.

- 353 4. Potential differences for all required configurations of current and potential electrodes
 354 are calculated through \mathbf{m}' (note that no forward computations are needed for a *noise*
 355 step).
 356 5. The acceptance ratio $\alpha(\mathbf{m}'|\mathbf{m})$ is calculated according to the following equation [Bodin
 357 and Sambridge, 2009]:

$$358 \quad \alpha(\mathbf{m}'|\mathbf{m}) = \min \left[1, \frac{p(\mathbf{m}')}{p(\mathbf{m})} \times \frac{p(\mathbf{d}^{obs}|\mathbf{m}')}{p(\mathbf{d}^{obs}|\mathbf{m})} \times \frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})} \times |\mathbf{J}| \right] \quad (5)$$

359 where the second term in the square bracket involves the product of the prior, likeli-
 360 hood and proposal ratios for \mathbf{m} and \mathbf{m}' , and the Jacobian of the transformation from \mathbf{m}
 361 to \mathbf{m}' (see Appendix B.4 for a more detailed description of equation 5).

- 362 6. Depending on the value of $\alpha(\mathbf{m}'|\mathbf{m})$, the chain goes back to step 3 after either accept-
 363 ing or rejecting the proposed model \mathbf{m}' . If $\alpha \geq r$ where r is a random deviate from a
 364 Uniform distribution between 0 and 1, the change is accepted, and \mathbf{m}' replaces \mathbf{m} as
 365 the new current model. If $\alpha < r$, the change is rejected, \mathbf{m}' is discarded, and model \mathbf{m}
 366 is retained as the sample from this iteration.
 367 7. Iterate from step 3 until sufficient samples have been generated.

368 Multiple chains are normally run independently of one another in parallel, ensuring
 369 that a larger volume of the model space is explored by starting the chains from different ini-
 370 tial conditions. In addition, by solving the forward problem at each Markov chain iteration,
 371 we ensure that the non-linearity of the forward and inverse problems are fully accounted for
 372 and that no modelling-related approximations and biases are introduced into the solution.

373 At the end of the inversion, an ensemble of representative posterior samples is obtained
 374 by discarding the first few hundred thousand iterations from each Markov chain as ‘burn-in’
 375 (samples that might still be biased by the initial randomly-chosen sample), and by retain-

ing only one model every few tens or hundreds of iterations thereafter to ensure that each sample in the ensemble is approximately independent of others (since consecutive samples in Markov chains can be strongly correlated). In practice, there are no hard and fast rules for choosing a burn-in period and a thinning interval, and some studies even suggest that thinning may not always be necessary [Link and Eaton, 2011]. However, a number of studies provide diagnostics that can be used to select and tune these parameters. For instance, Markov chain convergence may be assessed by comparing between-chain and within-chain variances for each model parameter [Gelman and Rubin, 1992; Brooks and Gelman, 1998], and the autocorrelation of posterior model parameters may be used to obtain an estimate of an appropriate thinning interval (e.g., Aster *et al.* [2013]). Within our study, we selected the burn-in period for each example by visually analysing plots displaying the change in misfit and number of cells with sample number across all Markov chains, discarding an initial window of samples for which these quantities had not yet stabilised. In terms of thinning, our choices were mainly dictated by a compromise between allowing enough separation between samples and having a large enough ensemble of samples within a reasonable computation time. Further details on Markov chain convergence are given in Section 5.2.

The posterior PDF on log(resistivity) at different locations in the subsurface can then be calculated from the ensemble by defining a regular grid of discrete points $[\bar{x}_i \ \bar{z}_i]$, extracting log(resistivity) at each grid point in each sample in the ensemble, and binning all of the posterior log(resistivity) values extracted at each point into a histogram. Maps showing different statistical properties of the subsurface resistivity field can also be obtained from the ensemble by calculating a number of statistical moments at each of these discrete points over the M samples in the ensemble, and merging these points together in order to create 2D maps of these statistical moments (see Appendix B.5 for details). However, it is important to emphasize that none of these statistics alone provides comprehensive information about the solution to the inverse problem; each should be considered within the context of a fully probabilistic solution.

Alternatively, the posterior probability distribution may be visualised in terms of marginal histograms of resistivity with depth (i.e., across all z locations for a particular horizontal position x) or with horizontal position (i.e., across all x locations for a particular depth z). While we do not present such plots herein, the reader is referred to Bodin *et al.* [2012a] and Ray *et al.* [2018] for examples of such plots in 1D and 2D, respectively.

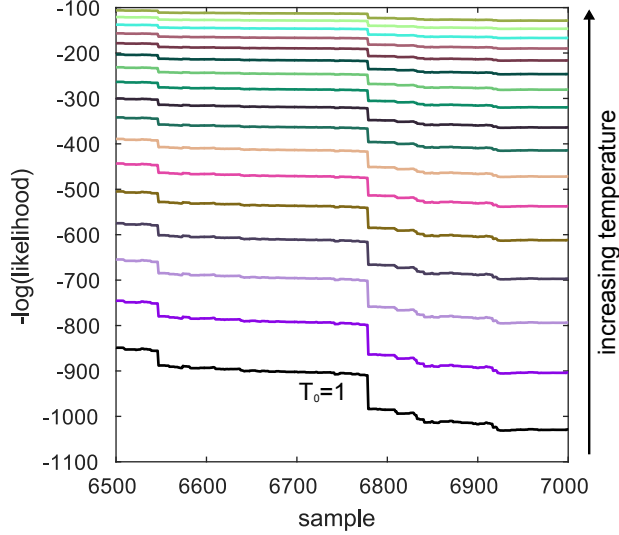
2.2.5 Parallel tempering

As in any MCMC scheme, convergence in rj-MCMC inversion may be substantially hampered if Markov chains effectively become trapped while exploring local likelihood maxima. This normally occurs when the maximum being explored is surrounded by relatively low-likelihood models; the Markov chain tends to reject steps that would move from high to low likelihood due to the proposal ratio term in equation 5, so the chain only progresses from one maximum to another with very low probability, hence usually only after many attempts or steps.

This issue is normally overcome by running multiple independent Markov chains in parallel, ensuring that different parts of model space can be explored at the same time by following different random walks. In addition, the likelihood function may be ‘tempered’ by assigning a different temperature T_l to each of the L parallel chains [Swendsen and Wang, 1987; Earl and Deem, 2005; Sambridge, 2014]. By doing so, the likelihood becomes a function of model \mathbf{m}_l and temperature T_l :

$$\mathcal{L}(\mathbf{m}_l, T_l) = p(\mathbf{d}^{obs} | \mathbf{m}_l)^{1/T_l} \quad (6)$$

where we drop the dependence of \mathcal{L} on data \mathbf{d}^{obs} for notational convenience since \mathbf{d}^{obs} is measured and hence fixed. When $T_0 = 1$, the tempered likelihood $\mathcal{L}(\mathbf{m}_0, 1)$ is the same as that from equation 2, and the chain at $T_0 = 1$ is referred to as the *target* chain. When



433 **Figure 3.** An example of tempered likelihood, calculated from equation 6 at increasingly higher tempera-
 434 tures (equally spaced on a logarithmic scale) from the target temperature $T_0 = 1$ (black line) to the highest
 435 temperature $T_l = 8$. The likelihood at the target temperature was calculated by running a Markov chain
 436 at $T_0 = 1$ using the synthetic dataset from Section 3.1. The other chains use the same samples but with
 437 recalculated tempered likelihoods according to equation 6.

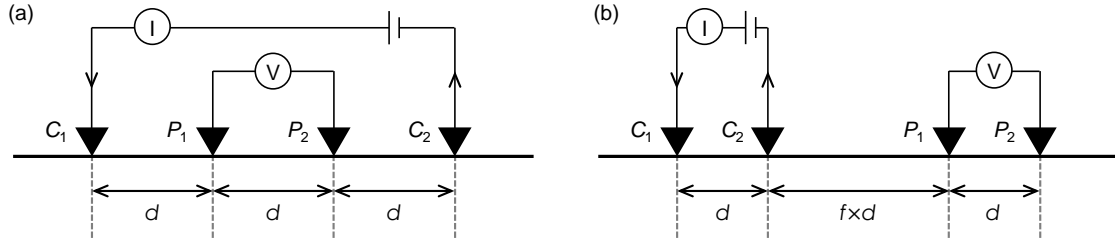
426 $T_l > 1$, the likelihood function $\mathcal{L}(\mathbf{m}_l, T_l)$ is a smoother version of the untempered likeli-
 427 hood $p(\mathbf{d}^{obs} | \mathbf{m}_0)$ (i.e., it has lower ‘relief’ with flatter peaks and valleys), and it is therefore
 428 easier for a chain to explore since regions of high probability can be escaped more readily.
 429 As an example, Figure 3 shows the likelihood calculated along the same Markov chain run
 430 for the synthetic example described in Section 3.1 at the target temperature $T_0 = 1$ (black)
 431 and recalculated using equation 6, at 16 increasingly higher temperatures equally spaced in
 432 $\log(T)$, up to $T_l = 8$.

438 At each Markov chain iteration, any two randomly-chosen chains at different tempera-
 439 tures are allowed to exchange states (models) using the following Metropolis-Hastings accep-
 440 tance criterion:

$$441 \alpha_{swap} = \min \left[1, \frac{\mathcal{L}(\mathbf{m}_{hot}, T_{cold})}{\mathcal{L}(\mathbf{m}_{hot}, T_{hot})} \times \frac{\mathcal{L}(\mathbf{m}_{cold}, T_{hot})}{\mathcal{L}(\mathbf{m}_{cold}, T_{cold})} \right] \quad (7)$$

442 where $T_{hot} > T_{cold}$, and \mathbf{m}_{hot} and \mathbf{m}_{cold} are the current models on the ‘hot’ and ‘cold’
 443 chain, respectively. Hence, the expression $\mathcal{L}(\mathbf{m}_{hot}, T_{cold})$ corresponds to evaluating equa-
 444 tion 6 using the model on the ‘hot’ chain \mathbf{m}_{hot} and the ‘cold’ temperature T_{cold} . The swap
 445 is accepted if $\alpha_{swap} \geq r$, where r is a random deviate from a Uniform distribution between
 446 0 and 1, and rejected otherwise. Note that, as suggested by *Sambridge* [2014], the exchange
 447 swaps are not restricted to neighbouring temperature levels, but are allowed between any pair
 448 of randomly-chosen levels.

449 Swapping models between chains at different temperatures promotes inter-chain mix-
 450 ing and allows local likelihood maxima to be escaped, ultimately speeding up convergence
 451 to the posterior PDF. This is particularly beneficial in cases where forward modelling cal-
 452 culations are computationally expensive so that considerable computing time may be spent
 453 on a single Markov chain iteration. Examples of applications of parallel tempering to geo-
 454 physical inverse problems include the inversion of controlled-source electromagnetic data
 455 [Ray et al., 2013], finite-fault [Dettmer et al., 2014] and direct-seismogram [Dettmer et al.,
 456 2015] inversion, the inversion of surface wave dispersion and receiver function data [Roy and
 457 Romanowicz, 2017], seismic body-wave [Bottero et al., 2016] and ambient-noise [Valentová



485 **Figure 4.** Electrode geometries used for the experiments described in this paper. Current electrodes are lo-
 486 cated at C_1 and C_2 , and potential electrodes are located at P_1 and P_2 . (a) In a Wenner-alpha array, electrodes
 487 are equally spaced with separation d . (b) In a dipole-dipole array, current and potential electrodes have the
 488 same spacing d , and the two dipoles C_1 – C_2 and P_1 – P_2 are separated by distance $f \times d$ (where f is generally
 489 an integer value).

488 *et al.*, 2017] tomography, inversion of airborne electromagnetic data *Hawkins et al.* [2017],
 489 and full-waveform inversion of marine seismic data [*Ray et al.*, 2018].

489
 490 In all of the examples presented in this paper, we performed TERT by running 32
 491 Markov chains in parallel, and setting 16 chains at temperature $T_0 = 1$ (the *target* tem-
 492 perature) and 16 chains at log-uniformly spaced increasing temperatures up to $T_l = 8$ (the
 493 ‘hottest’ temperature). Posterior inferences were made only from samples in the chains at the
 494 *target* temperature (but these are influenced by the other chains through equation 7). Alterna-
 495 tively, samples at higher temperatures could be re-weighted to $T_0 = 1$ using an appropriate
 496 weighting function [*Brooks and Neil Frazer*, 2005; *Dosso et al.*, 2012], and added to the pos-
 497 terior ensemble.

498 2.2.6 Implementation details

499
 500 Since the finite-difference forward modeller that we employed requires the resistivity
 501 structure to be defined on a regular grid of points, at each Markov chain iteration we sampled
 502 the Voronoi-tessellated resistivity model over a regular grid and solved the forward problem
 503 using this grid. In addition, given that resistivity values can span several orders of magnitude
 504 in Earth science scenarios, our inversion routine was set up to invert for $\mu = \log(\rho)$ rather
 505 than absolute resistivity values.

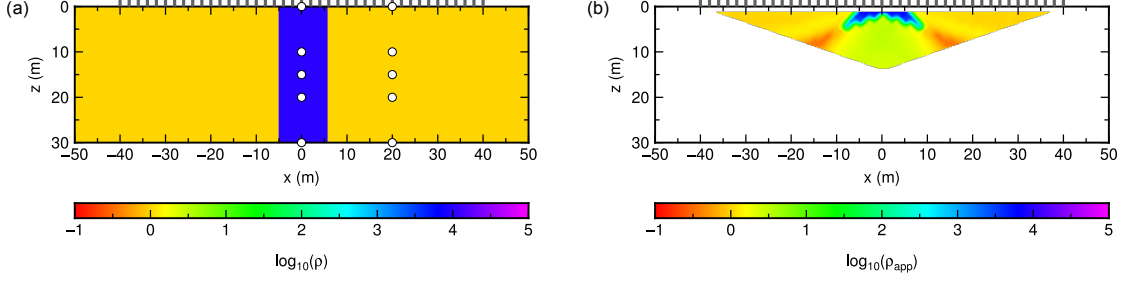
506
 507 Finally, in its current implementation, our inversion code does not allow for topography
 508 to be taken into account. However, given that the forward modelling routine is completely
 509 separate from the inversion algorithm, the forward modeller could easily be swapped with
 510 one in which topography is considered, and where the z -coordinate of the Voronoi nuclei
 511 represents the depth of the nucleus below the Earth’s surface.

512 3 Synthetic experiments

513
 514 In order to test the effectiveness of the TERT method, we performed a number of syn-
 515 thetic tests using different resistivity models and acquisition geometries (Figure 4). We bench-
 516 marked our results against those obtained from a well known iterated-linearised inversion
 517 code (*R2* by *Binley* [2013b]). These experiments are presented below.

518 3.1 Example 1

519
 520 In this first experiment we created a synthetic dataset for the simple resistivity model
 521 shown in Figure 5(a) using the forward modelling functions in *FW2_5D*. Using a Wenner-



506 **Figure 5.** Synthetic resistivity model for the example application described in Section 3.1. (a) True resistivity section. (b) Resistivity pseudosection acquired using a Wenner-alpha configuration for 41 electrodes
 507 located between -40 and 40 m, with a minimum and a maximum spacing of $d = 2$ and $d = 26$ m in the
 508 geometry shown in Figure 4(a). A resistivity pseudosection is a contour plot where each datum (i.e., apparent
 509 resistivity calculated using equation 8 for a Wenner-alpha configuration) is plotted horizontally at the mid-
 510 point of the set of 4 electrodes used for the measurement, and vertically at the median depth of investigation
 511 [Edwards, 1977] of the electrode array used. In panel (a), the white circles denote the location of the points at
 512 which the posterior PDFs on $\log(\rho)$ in Figure 6 were calculated. In both panels, the grey ticks at $z = 0$
 513 m denote electrode locations.
 514

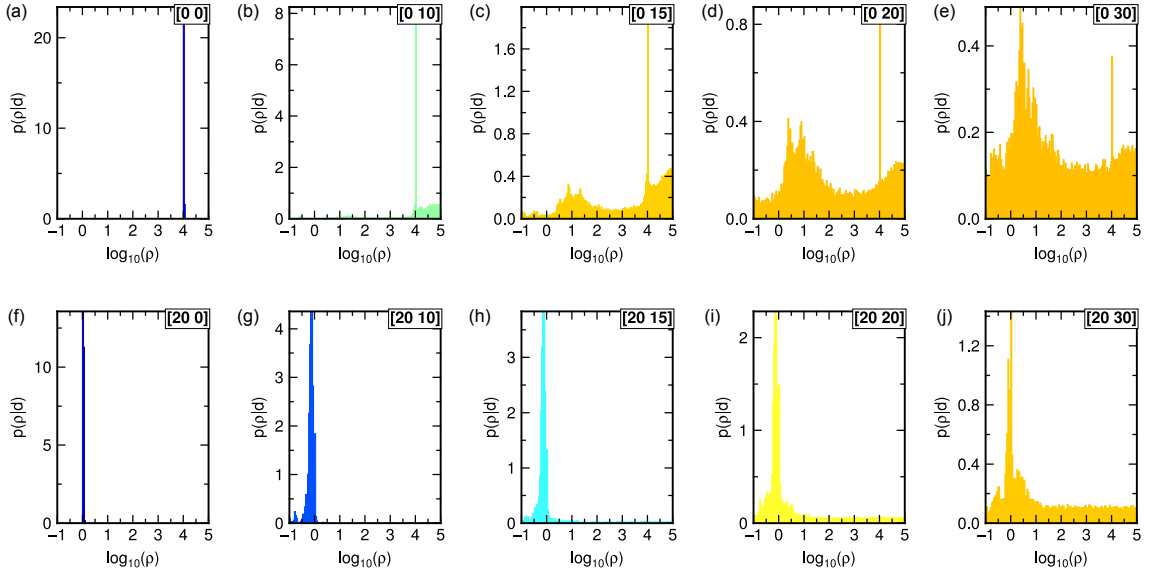
493 alpha configuration (Figure 4(a)) with 41 electrodes located at regular intervals of 2 m, we
 494 modelled 260 potential differences for different combinations of current and potential elec-
 495 trodes with a minimum and maximum d spacing of 2 and 26 m, respectively. In order to emu-
 496 late real scenarios where measurements are contaminated by noise, each computed potential
 497 difference k was perturbed by random Gaussian noise with standard deviation σ_k^{prior} equal
 498 to 3% of the measurement, which was then considered as the *prior* data noise level during in-
 499 version. The apparent resistivity pseudosection is shown in Figure 5(b). In order to generate
 500 this image, each modelled potential difference ΔV_k was first converted to apparent resistivity
 501 according to

$$502 \quad \rho_{appk} = 2\pi d \frac{\Delta V_k}{I_k} \quad (8)$$

503 where I_k denotes the injected current, and then plotted in a contour plot where each datum is
 504 located horizontally at the mid-point of the set of 4 electrodes used for the measurement, and
 505 vertically at the median depth of investigation [Edwards, 1977] of the electrode array used.

515 In order to account for measurement and modelling errors, data noise was assumed to
 516 be proportional to prior data uncertainties σ_k^{prior} , and noise parameter λ (equation 3) was
 517 determined during the inversion. Uniform priors were given on the number of Voronoi cells
 518 as $[3, 4, \dots, 100]$, on $\mu = \log(\rho)$ as $[-1, 5]$, on the x and z coordinates of model boundaries as
 519 $[-50, 50]$ and $[0, 30]$, respectively, and on noise parameter λ as $[0.01, 10]$. We ran 32 tem-
 520 pered Markov chains (of which 16 were at the target temperature $T_0 = 1$) in parallel for
 521 6×10^5 iterations, allowing two randomly-chosen chains to swap models at each iteration
 522 provided the condition stated in equation 7 was satisfied. Every 100th sample at the target
 523 temperature after a burn-in period of 2×10^5 iterations was considered as a representative
 524 model from the posterior PDF. This gave a solution to the inverse problem consisting of an
 525 ensemble of 64×10^3 samples $\mathbf{m} = [n, \mathbf{c}, \boldsymbol{\mu}, \mathbf{h}]$, where each parameter in \mathbf{m} is distributed
 526 according to its posterior marginal PDF.

537 Information about the resistivity distribution in the subsurface may be visualised using
 538 histograms showing the marginal PDFs at a number of points in the xz plane (e.g., Figure
 539 6) or by evaluating various statistics from the full PDF as described in Section 2.2.4. Some
 540 of these statistics are shown in Figure 7. Information on the resistivity of different subsur-
 541 face structures can be obtained from the arithmetic mean, the median, the mode and the root-

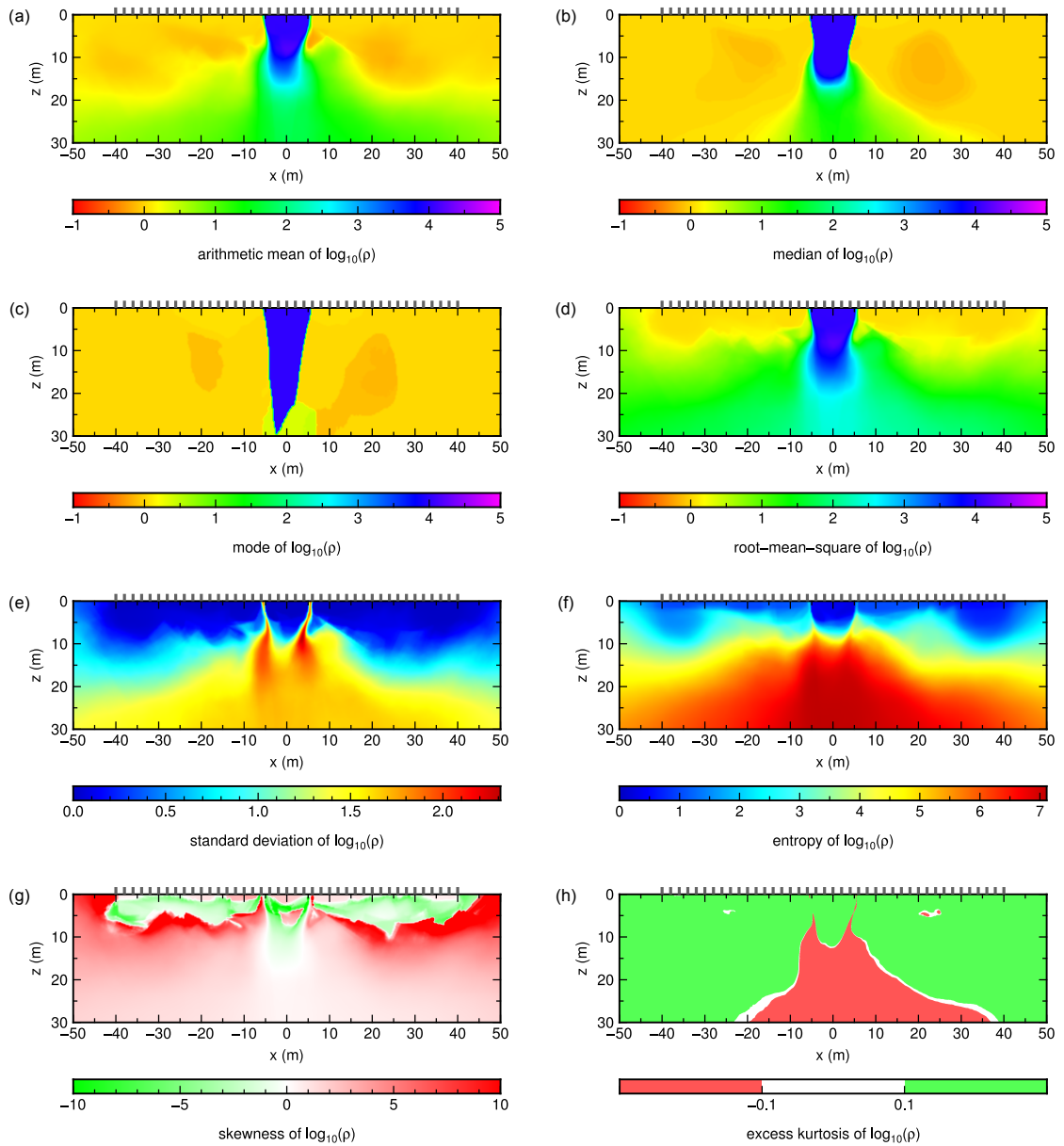


527 **Figure 6.** Posterior PDFs of $\log(\rho)$ at locations shown in Figure 5(a) estimated using the TERT algorithm.
 528 Posteriors in the top row are calculated at $x = 0$ m and (a) $z = 0$ m, (b) $z = 10$ m, (c) $z = 15$ m, (d) $z = 20$
 529 m, (e) $z = 30$ m. Posteriors in the bottom row are calculated at $x = 20$ m and (f) $z = 0$ m, (g) $z = 10$ m, (h)
 530 $z = 15$ m, (i) $z = 20$ m, (j) $z = 30$ m. Histograms are colour-coded according to the standard deviation at their
 531 corresponding locations from Figure 7(e).

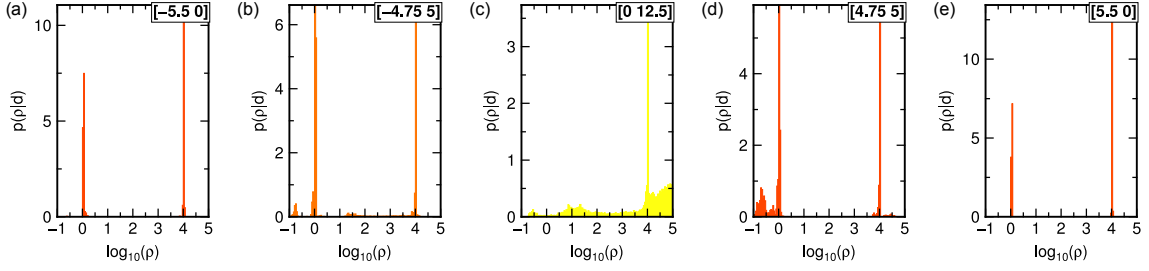
542 mean-square maps. While each single Voronoi model in the ensemble is discontinuous and
 543 unrealistic, each of these statistical measures provides a smoother representation of the true
 544 resistivity field and highlights specific features of the PDF across the imaged area. In addition,
 545 an impression of the *uncertainty* in our state of knowledge about the subsurface resistivity
 546 field may be obtained from the standard deviation and entropy maps, while skewness
 547 and excess kurtosis highlight information related to the *shape* of the PDF at each location in
 548 the xz plane. As previously noted in Section 2.2.4, none of these statistics can ever represent
 549 the complete solution to the inverse problem on their own, but should instead be interpreted
 550 together as part of a fully probabilistic solution.

551 As can be observed in Figures 7(a)–(d), the high-resistivity vertical structure in the
 552 centre of the model is resolved to varying degrees of accuracy to depths of between 10 m
 553 (arithmetic mean) and >20 m (mode, i.e., the maximum-a-posteriori value of every individual
 554 binned posterior resistivity pixel), while the background resistivity is generally resolved
 555 to larger depths (with the exception of the root-mean-square model). The standard deviation
 556 map in Figure 7(e) shows an increase in uncertainty vertically with increasing depth, and horizontally
 557 as the distance from the centre of the model increases. In fact, the increase in uncertainty
 558 with depth can also be observed on marginal PDFs along vertical profiles at $x = 0$
 559 and $x = 20$ m (Figure 6): as depth increases, peaks in the PDF become less defined and the
 560 distribution approaches the Uniform prior (although still with peaks around the two values of
 561 $\log(\text{resistivity})$ that appear in the true model in Figure 5). Similarly, excess kurtosis (Figure
 562 7(f)) is positive in areas of low standard deviation indicating a more ‘peaked’ distribution,
 563 while it is negative in areas of high standard deviation when the posterior PDF approaches
 564 the Uniform prior.

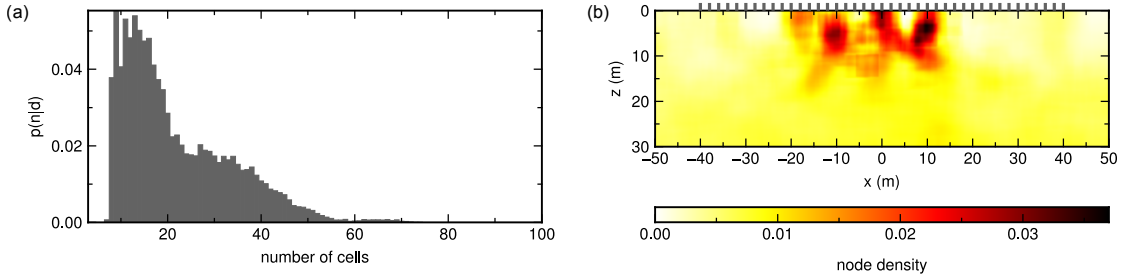
569 In addition, the standard deviation plot in Figure 7(e) displays an increase in uncertainty
 570 along the vertical edge of the high-resistivity structure, showing that the exact shape and
 571 size of this body cannot be reconstructed. Indeed this high-uncertainty feature defines



532 **Figure 7.** Inversion results for the synthetic model in Figure 5(a) found using the TERT algorithm. (a)
 533 Arithmetic mean. (b) Median. (c) Mode (i.e., maximum-a-posteriori). (d) Root-mean-square. (e) Standard
 534 deviation. (f) Entropy. (g) Skewness. (h) Excess kurtosis. Note that the excess kurtosis map is simplified to
 535 only 3 distinct groups of values due to the many orders of magnitude spanned by this statistical moment. In all
 536 panels, the grey ticks at $z = 0$ m denote electrode locations.



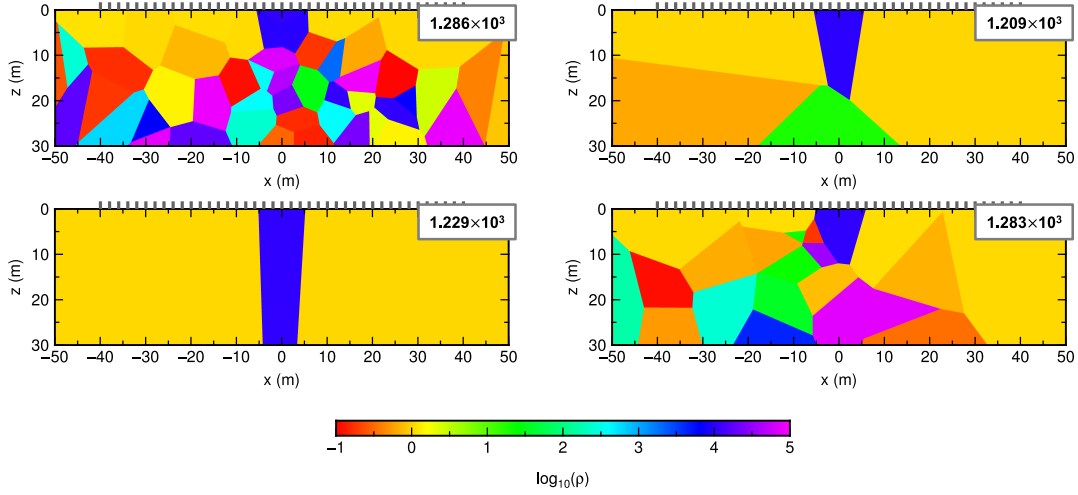
565 **Figure 8.** Posterior PDFs on $\log(\rho)$ for the synthetic model in Figure 5(a) found using the TERT algorithm.
 566 Posteriors are calculated at (a) $x = -5.5$ m and $z = 0$ m, (b) $x = -4.75$ m and $z = 5$ m, (c) $x = 0$ m and
 567 $z = 12.5$ m, (d) $x = 4.75$ m and $z = 5$ m, (e) $x = 5.5$ m and $z = 0$ m. Histograms are colour-coded according
 568 to the standard deviation at their corresponding locations from Figure 7(e).



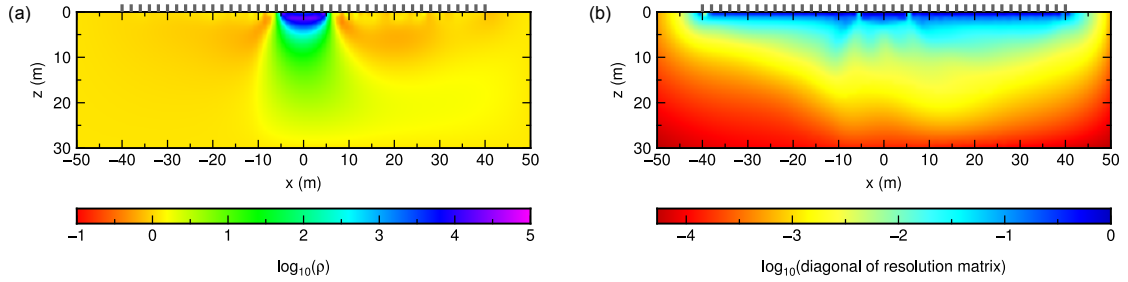
593 **Figure 9.** Information on the number of cells n in the posterior distribution and their locations found using
 594 the TERT algorithm. (a) Posterior PDF on the number of Voronoi cells ($p(n|\mathbf{d}^{obs})$). (b) Density of Voronoi
 595 nuclei across the ensemble of models in the PDF. At each pixel, density is measured within a $5\text{ m} \times 5\text{ m}$
 596 square sector centred on the pixel and is plotted as the average number of Voronoi nuclei per m^2 per sample.
 597 The grey ticks at $z = 0$ m in panel (b) denote electrode locations.

572 precisely the spatial resolution of this boundary, and its presence is independent of the elec-
 573 trode geometry employed since it occurs as a consequence of the true resistivity structure
 574 of the subsurface. Similar topologies have been observed in seismic traveltime tomography.
 575 Defined as ‘uncertainty loops’ by *Galetti et al.* [2015], they surround high- and low-velocity
 576 anomalies and characterise the uncertainty in the location of their boundaries. *Galetti et al.*
 577 [2015] conjectured that uncertainty loops should be observed in almost all tomographic sys-
 578 tems provided that the full nonlinearity in the forward physics is embodied within the inver-
 579 sion, and that they may (erroneously) disappear in the solution of linearised systems. Loops
 580 have not previously been recognised in electrical resistivity tomography to the best of our
 581 knowledge, which may be because most publications employ inversion schemes involving
 582 linearised physics, or because those publications that do employ non-linearised, stochastic
 583 inversion methods fail to report uncertainty maps.

584 The origin of the loops is confirmed by the posterior PDFs on $\log(\rho)$ at points located
 585 near the edge of the high-resistivity anomaly (Figure 8): since these points may fall either
 586 inside or outside of the anomaly in the ensemble of accepted models, depending on exactly
 587 where the boundary of the anomaly is located in each model, their posterior PDFs are mul-
 588 timodal, and present two distinct peaks: one peak corresponds to the $\log(\text{resistivity})$ of the
 589 anomaly while the other corresponds to the background $\log(\text{resistivity})$. Excess kurtosis
 590 along the edges of the anomaly is also negative as a consequence of the distribution being
 591 bi-modal. The loops therefore appear because of our uncertainty in the geometrical location
 592 of the boundary of the anomaly, as embodied in the set of models in the ensemble.



614 **Figure 10.** Example of 4 Voronoi models from the ensemble obtained from the TERT algorithm. The
 615 log-likelihood of each model is shown in the top-right corner of each plot. In all panels, the grey ticks at $z = 0$
 616 m denote electrode locations.



617 **Figure 11.** Inversion results for the synthetic model in Figure 5 found using the iterated-linearised code
 618 *R2* by Binley [2013b]. (a) Best-fit resistivity map obtained after 4 iterations. (b) Resolution map showing the
 619 logarithm of the diagonal elements of the resolution matrix (log values near 0 indicate better resolution). In
 620 both panels, the grey ticks at $z = 0$ m denote electrode locations.

598 In this transdimensional approach the number of model parameters n is itself a param-
 599 eter. A posterior PDF is therefore also obtained on the number of Voronoi cells needed to
 600 constrain the data. The posterior $p(n|\mathbf{d}^{obs})$ is shown in Figure 9(a), while Figure 9(b) shows
 601 the density of Voronoi nuclei (given as average number of nuclei per m^2 per sample) in $5 \text{ m} \times 5 \text{ m}$
 602 square sectors centred on each pixel. As expected, the highest density of Voronoi nuclei
 603 is found near to the edges of the resistivity anomaly since this is the area in which the
 604 data is sufficient to resolve strongly heterogeneous structure which must be represented in
 605 almost any model in order to have a high enough likelihood to be included in the ensemble.
 606 However, although the structure of the true model is relatively simple and could easily
 607 be described by only 3 Voronoi cells (if the cell nuclei are located at specific positions),
 608 the posterior on the number of cells peaks around 14. This is likely to be due to the fact that
 609 this acquisition array has very low sensitivity to structure below 10 m depth, hence Voronoi
 610 cells may be added or deleted from the model below this depth without significantly affecting
 611 the likelihood. For instance, this is illustrated in Figure 10 which shows 4 different Voronoi
 612 models from the ensemble that, despite the different number of cells, have very similar likeli-
 613 hoods.

621 In order to benchmark the TERT algorithm against a standard optimisation-based
 622 inversion scheme, we inverted the same dataset using the iterative linearised code *R2* by *Binley*
 623 [2013b]. This code first uses a uniform resistivity model to estimate the data, and then iter-
 624 atively adjusts the model until a target misfit value between observed and predicted data is
 625 reached. The resulting best-fit resistivity model obtained after 4 iterations is shown in Fig-
 626 ure 11(a): although the background resistivity is correctly resolved across the model area, the
 627 high-resistivity structure in the middle of the model is only resolved down to ~ 5 m, approxi-
 628 mately half the depth to which it was observed in the arithmetic mean resistivity section from
 629 TERT (Figure 7(a)) and less than a quarter of that observed using the mode (Figure 7(c)).
 630 However, since a single best-fitting model is produced by the algorithm, it is not possible
 631 to evaluate the distance of the solution from the true model when that model is not known.
 632 The reliability of the solution in this optimisation inversion scheme must be assessed indi-
 633 rectly, for instance by analysing the resolution matrix \mathbf{R} (e.g., see equation (5.18) in *Binley*
 634 *and Kemna* [2005]) computed using physics that is linearised around the model found in the
 635 final iteration. When \mathbf{R} equals the identity matrix \mathbf{I} , all parameters are correctly resolved
 636 and uniquely determined; when \mathbf{R} does not resemble the identity matrix, then each param-
 637 eter is given by a weighted average of the true model parameters. The diagonal elements of
 638 the resolution matrix corresponding to the target misfit model in Figure 11(a) are shown in
 639 Figure 11(b). As expected from the acquisition geometry, resolution is higher (diagonal ele-
 640 ments are closer to 1) near the surface and drops towards the bottom and lateral edges of the
 641 model. However, unlike the standard deviation map in Figure 7(e), the resolution matrix does
 642 not provide a range on the expected resistivities at any point in the model, hence it cannot be
 643 used as a direct measure of the uncertainty on the structures observed in Figure 11(a).

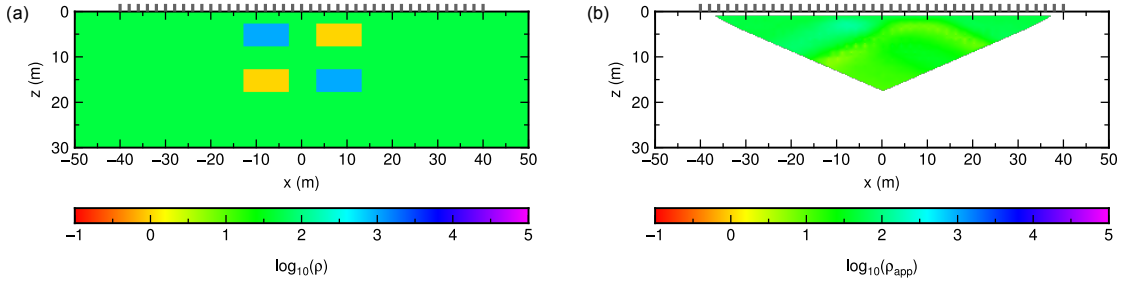
644 3.2 Example 2

645 In this second experiment, we created a synthetic dataset for the more complex resis-
 646 tivity model shown in Figure 12(a) using the forward modelling functions in *FW2_5D* and a
 647 dipole-dipole acquisition geometry (Figure 4(a)) with 41 electrodes located at regular inter-
 648 vals of 2 m. By letting the electrode spacing d vary between 2 and 26 m, and the dipole sep-
 649 aration factor f vary between 1 and 6, we modelled 903 potential differences and perturbed
 650 each measurement k using random Gaussian noise with a standard deviation σ_k^{prior} of 3% of
 651 the observed value. The apparent resistivity pseudosection is shown in Figure 12(b). In this
 652 case, for a dipole-dipole electrode configuration, apparent resistivity is related to the mea-
 653 sured potential difference ΔV_k by:

$$654 \rho_{appk} = \pi d f (f + 1)(f + 2) \frac{\Delta V_k}{I_k} \quad (9)$$

663 We assume Uniform priors on the number of Voronoi cells as $[3, 4, \dots, 100]$, on $\mu =$
 664 $\log(\rho)$ as $[-1, 5]$, on the x and z coordinates of model boundaries as $[-50, 50]$ and $[0, 30]$,
 665 respectively, and on noise parameter λ as $[0.01, 10]$, and ran 32 tempered Markov chains (of
 666 which 16 were at the target temperature $T_0 = 1$) in parallel for 1.2×10^6 iterations allowing
 667 two randomly-chosen chains to swap models at each iteration according to equation 7. Every
 668 100th sample at the target temperature after a burn-in period of 4×10^5 iterations was consid-
 669 ered as a representative model from the posterior PDF, giving an ensemble of 128×10^3 valid
 670 samples.

676 Figures 13(a)–(d) map information retrieved by TERT about the distribution of resis-
 677 tivity in the subsurface in terms of different statistical moments. The background resistivity
 678 is relatively well resolved across the model, while the four rectangular anomalies are resolved
 679 to a different extent by the different statistics. The top two anomalies are resolved by all sta-
 680 tistical moments in panels (a)–(d), while among the bottom two anomalies only the high-
 681 resistivity one on the right is resolved by all moments. The bottom low-resistivity anomaly
 682 is only visible as an area of slightly lower resistivity than the background in the median and
 683 mode maps, while it is not visible in the average and root-mean-square sections. This is not
 684 surprising given the higher sensitivity to larger values of these two statistical moments.

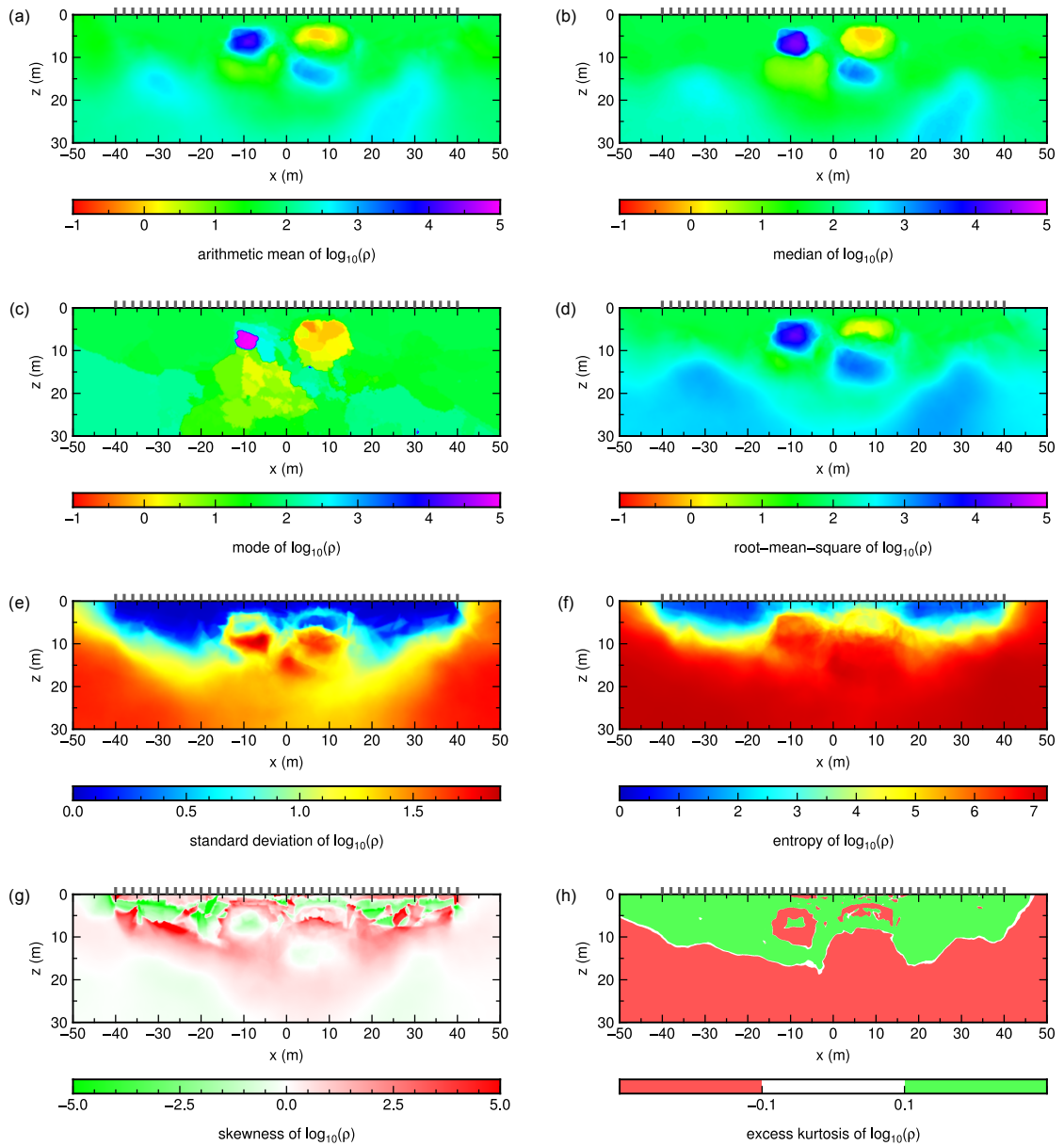


655 **Figure 12.** Synthetic resistivity model for the example application described in Section 3.2. (a) True re-
 656 sistivity section. (b) Resistivity pseudosection acquired using a dipole-dipole configuration for 41 electrodes
 657 located between -40 and 40 m, with electrode spacing d between 2 and 26 m and dipole separation factor f
 658 between 1 and 6 in the geometry shown in Figure 4(b). A resistivity pseudosection is a contour plot where
 659 each datum (i.e., apparent resistivity calculated using equation 9 for a dipole-dipole configuration) is plotted
 660 horizontally at the mid-point of the set of 4 electrodes used for the measurement, and vertically at the median
 661 depth of investigation [Edwards, 1977] of the electrode array used. In both panels, the grey ticks at $z = 0$ m
 662 denote electrode locations.

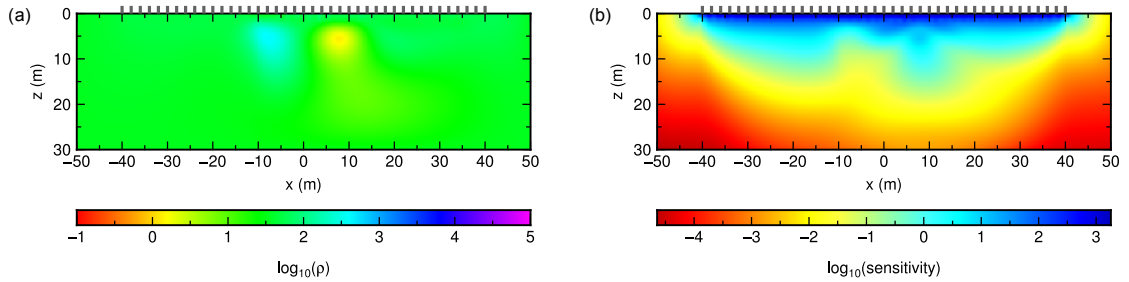
685 The uncertainty on the solution can be visualised on the standard deviation and en-
 686 tropy maps in panels (e)–(f). Similarly to the previous example, loops of higher standard
 687 deviation define the edges of the top two anomalies, and large values of standard deviation
 688 are also found vertically between the two sets of anomalies (around 10 m depth). Compari-
 689 son of these high uncertainty features with the actual location of the anomalies’ edges shows
 690 that the true edges fall within the high standard deviation loops, supporting our previous sug-
 691 gestion that these uncertainty topologies define the spatial resolution of boundaries between
 692 different bodies.

693 The skewness map shows areas of negative skewness corresponding to the two high
 694 resistivity anomalies, indicating that the tail of the PDF at these locations is longer on the
 695 low-resistivity side. On the other hand, the top low resistivity anomaly seems to correspond
 696 to an area of positive skewness, indicating that the PDF in this sector has a longer tail to-
 697 ward high resistivity values. This seems to agree with the fact that the background resistivity
 698 falls in between the resistivities of the low and high anomalies. The kurtosis map shows re-
 699 markable similarity to the entropy map, with areas of high entropy corresponding to areas of
 700 negative kurtosis. This is intuitively correct since negative kurtosis indicates flatter distribu-
 701 tions, which in turn correspond to a greater degree of disorder or uncertainty as identified by
 702 entropy. In addition, a loop of negative kurtosis marks the edges of the top-left anomaly as
 703 a consequence of the posterior PDF being bi-modal in this region. However, it is important
 704 to note that both skewness and kurtosis maps may also be affected by the size of the prior,
 705 hence their interpretation should be treated with caution.

706 The least-misfit solution obtained using the linearised code *R2* is shown in Figure
 707 14(a). In this case, only the top two anomalies are resolved, while the bottom two are not vis-
 708 ible. In terms of assessing uncertainty, calculation of the resolution matrix \mathbf{R} (which involves
 709 the inversion of a large matrix with rank equal to the number of model parameters, in this
 710 case 4032) was not possible computationally using *R2*. As a less computationally-intensive
 711 alternative, we calculated the sensitivity map \mathbf{s} (see equation (5.20) in Binley and Kemna
 712 [2005]), which may be used instead of \mathbf{R} as a less expensive image appraisal measure. Sen-
 713 sitivity is high in areas where the data is more strongly influenced by the model, while it is
 714 low in areas where the model has little effect on the data and hence may be mainly affected
 715 by the regularisation. However, note that using the sensitivity map to estimate uncertainty



671 **Figure 13.** Inversion results for the synthetic model in Figure 12 found using the TERT algorithm. (a)
 672 Arithmetic mean. (b) Median. (c) Mode (i.e., maximum-a-posteriori). (d) Root-mean-square. (e) Standard
 673 deviation. (f) Entropy. (g) Skewness. (h) Excess kurtosis. Note that the excess kurtosis map is simplified to
 674 only 3 distinct groups of values due to the many orders of magnitude spanned by this statistical moment. In all
 675 panels, the grey ticks at $z = 0$ m denote electrode locations.



718 **Figure 14.** Inversion results for the synthetic model in Figure 12 found using the iterated-linearised code *R2*
 719 by *Binley* [2013b]. (a) Best-fit resistivity map obtained after 3 iterations. (b) Sensitivity map. In both panels,
 720 the grey ticks at $z = 0$ m denote electrode locations.

716 may be misleading in this case, since relatively high sensitivity is found at the location of the
 717 bottom-right, high-resistivity anomaly which is not resolved by the best-fit model.

721 4 Observational data experiments

722 In order to test the efficiency and reliability of the TERT method on observational data,
 723 we applied the method to two observational datasets acquired at archaeological sites in Scot-
 724 land and Slovakia. The results from the Scotland dataset are presented below, while those
 725 from the Slovakia dataset are presented in the online Supporting Information.

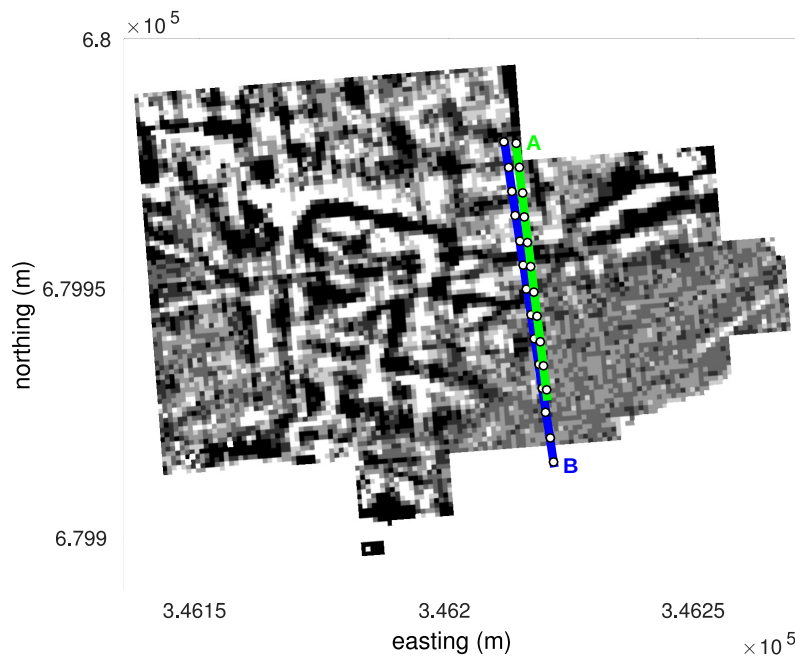
726 4.1 Scotland dataset

727 In this experiment, we inverted two observational datasets recorded at an archaeologi-
 728 cal site at Glebe Field in Aberlady (Scotland). Glebe Field is listed as an officially Scheduled
 729 (protected) monument, and in recent years has yielded a number of Anglo-Saxon finds in-
 730 cluding small artefacts and coins. The site was also surveyed using magnetics [*Neighbour*
 731 *et al.*, 1995] and electrical resistance mapping [*Neighbour et al.*, 1998; *Blackwell*, 2008],
 732 revealing the presence of a number of linear features which were interpreted as building
 733 foundations. A resistance map (i.e., a standard archaeological twin-array output) obtained
 734 by *Blackwell* [2008] in the south-western corner of the field is shown in Figure 15.

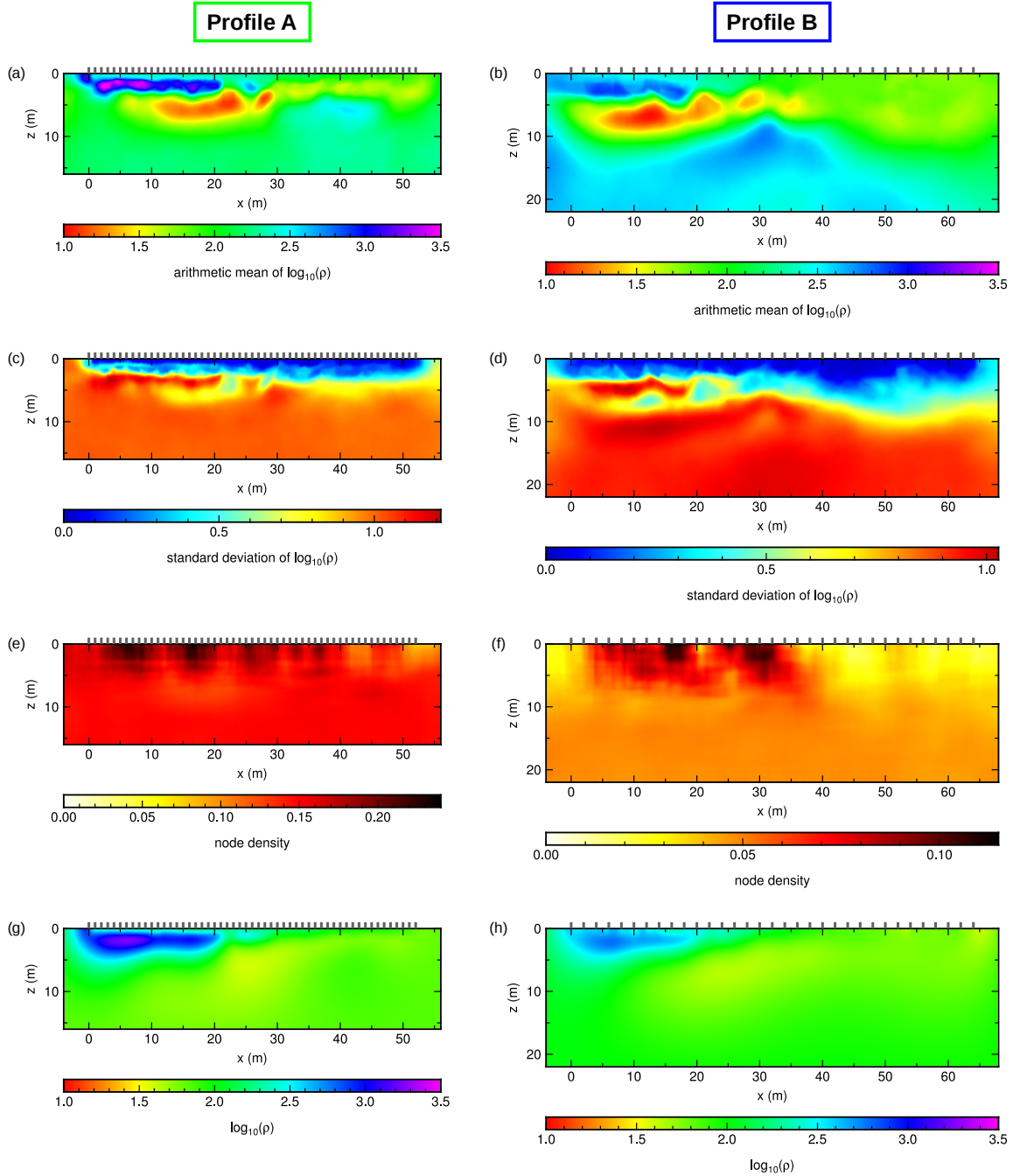
740 We inverted two datasets recorded using a Wenner-alpha configuration along the two
 741 profiles shown in Figure 15: profile *A* (the green line in Figure 15) was acquired using 53
 742 electrodes at 1 m spacing; profile *B* (the blue line in Figure 15) was acquired using 33 elec-
 743 trodes at 2 m spacing. Following an initial data quality check, the two profiles included 295
 744 and 150 measured potential differences, respectively. We assumed data noise to be unknown,
 745 hence also inverted for parameters a and b in equation 4 in both cases.

746 We assumed Uniform priors on the number of Voronoi cells as $[5, 6, \dots, 200]$, on $\mu =$
 747 $\log(\rho)$ as $[0.5, 4]$, and on noise parameters a as $[0.0001, 0.2001]$ and b as $[0.1, 1.1]$, respec-
 748 tively. Uniform priors on the x and z coordinates of model boundaries were assumed as
 749 $[-4, 56]$ and $[0, 16]$ for profile *A*, and as $[-4, 68]$ and $[0, 22]$ for profile *B*. We ran 32 tem-
 750 pered Markov chains (of which 16 were at the target temperature $T_0 = 1$) in parallel for
 751 1×10^6 iterations allowing two randomly-chosen chains to swap models at each iteration
 752 according to equation 7. Every 100th sample at the target temperature after a burn-in period
 753 of 2×10^5 iterations was considered as a representative model from the posterior PDF, giving
 754 an ensemble of 128×10^3 valid samples.

761 The results from the inversion using the TERT algorithm are shown in Figure 16(a)–
 762 (f), while panels (g) and (h) in Figure 16 show the inversion results obtained using the lin-



735 **Figure 15.** Resistance map of the south-west corner of Glebe Field, Aberlady (Scotland) by *Blackwell*
 736 [2008]. The two profiles for which imaging results are presented in Section 4.1 are denoted by the green (pro-
 737 file *A*) and blue (profile *B*) lines, where distance along the profile is measured from the northern end of the
 738 lines. The white circles on the two lines are for reference and denote 5-meter segments. Note that the location
 739 of the resistance map is approximate due to the original survey by *Blackwell* [2008] not being georeferenced.



755 **Figure 16.** Inversion results for the observational datasets described in Section 4.1 found using (a)–(f) the
 756 TERT algorithm, and (g)–(h) the iterated-linearised code *R2* by *Binley* [2013b]. The left column shows results
 757 for profile A in Figure 15, the right column for profile B. (a)–(b) Arithmetic mean. (c)–(d) Standard deviation.
 758 (e)–(f) Node density (measured within a 5 m × 5 m square sector centred on each pixel). (g)–(h) Best-fit
 759 resistivity map from *R2*. Note that the colour scale in (a)–(b) and (g)–(h) is clipped between 1 and 3.5 to aid
 760 visualisation. In all panels, the grey ticks at $z = 0$ m denote electrode locations.

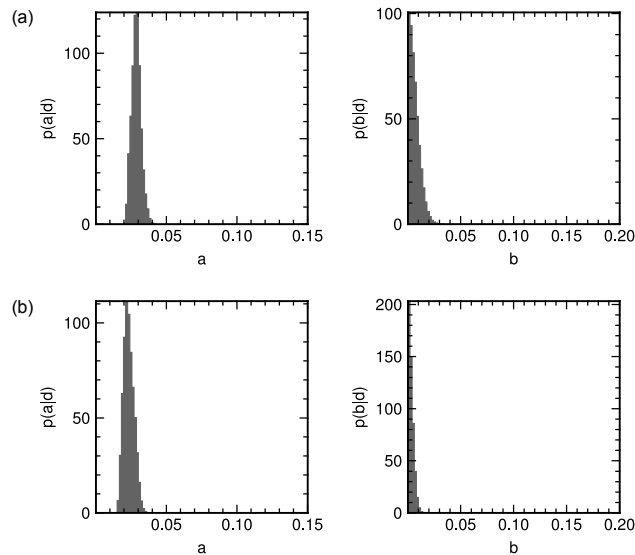


Figure 17. Posterior PDF on noise hyperparameters a and b for the observational dataset described in Section 4.1 obtained from TERT. (a) Profile A. (b) Profile B.

earised code $R2$. The posterior on noise hyperparameters a and b are shown in Figure 17. When inverting the data using $R2$ the noise was assumed to be proportional to the measured resistances according to equation 4, and a and b were set to 0.02 and 0.001, respectively.

In both profiles A and B, a high-resistivity structure is resolved near 2 m depth at the northern end of the lines, and it is likely to correspond to buried paving from a building or walkway. This feature appears to be thinner and better resolved in the average maps from TERT compared to the linearised results from $R2$, probably as a result of smoothing in the linearised solution.

In addition, the average maps from TERT reveal the presence of a high-resistivity structure at depth (visible near $x = 40$ m and $z = 6$ m on profile A, and below $z = 10$ m on profile B) which is not resolved at all in the linearised solution. This feature is located in a region of high uncertainty and poor resolution as suggested by the standard deviation maps. However, as shown by the synthetic example in Section 3.2, meaningful structure may still be resolved by TERT in areas of high uncertainty (see the bottom-right anomaly in Figure 13), hence it is not possible to tell whether this high-resistivity feature represents real structure or an artefact from the inversion. Nevertheless, the fact that it is visible on both profiles A and B seems to indicate that it is a robust feature which may represent resistive bedrock or some other archaeological structure.

In terms of Voronoi cell density across the ensemble of valid models, similarly to the previous example the highest density of Voronoi nuclei is found near the surface where resolution is higher.

5 Discussion

5.1 Uninformative vs. informative priors

In all of the examples presented in this study we employed uninformative Uniform priors on all model parameters. This choice was mainly dictated by the fact that we wished to assume little to no prior knowledge about the medium, and it prevented the emergence of

791 uncertainty loops and the increased depth resolution from being in any sense confounded
792 between the information contained in the priors and in the data.

793 However, were more detailed prior information available in the form of alternative sur-
794 veys or boreholes, such information could be included within the inversion in terms of infor-
795 mative priors. The use of Voronoi cells to represent the model creates a very flexible type
796 of model parameterisation, and such cells could easily provide approximate representations
797 of both such prior information and the resulting posteriors: if prior information were both
798 strong (permitting only tightly constrained, geologically-realistic structures) and detailed,
799 then the number of cells may increase to reflect that level of detail; in contrast, in the absence
800 of strong priors, Voronoi cells would provide a lower-dimensional, more approximate repre-
801 sentation of the geology – to the extent that the geology would be reflected in the ERT data
802 alone during inversion.

803 Alternatively, linearised inversion starting from different initial models might be used
804 to produce a set of solutions which may then be used as starting points for non-linear inver-
805 sion using TERT (with each Markov chain or a set of Markov chains using a different lin-
806 earised solution as an initial model). If the linearised solutions are significantly different, this
807 ‘hybrid’ method might allow convergence to be reached more quickly.

808 While we have not implemented either of the two approaches suggested above, we be-
809 lieve they would provide an interesting topic for further research.

810 5.2 Convergence

811 In any MCMC inversion scheme it is important to collect a sufficient number of sam-
812 ples so that the ensemble of sampled models will be reasonably representative of the poste-
813 rior PDF. If a Markov chain could be run for an infinite amount of time, it would explore the
814 full model space and reach convergence in the region of highest probability. However, since
815 computational limitations impose a practical limit on the running time of the inversion, con-
816 vergence may not be reached by the end of the chain if it gets trapped in a local likelihood
817 maximum. A practical solution to this problem is to run a series of Markov chains in parallel
818 by starting from different initial conditions. This ensures that different regions of the model
819 space can be explored simultaneously, and that anomalous Markov chains that are stuck in a
820 local likelihood maximum can easily be identified.

821 Although few tools are currently available for assessing convergence in a transdimen-
822 sional framework, information on Markov chain convergence may be obtained by plotting the
823 variation of a model parameter as a function of iteration. However, as opposed to traditional
824 MCMC methods where model parameterisation is fixed, in a rj-MCMC tomography scheme
825 the use of cell position and $\log(\text{resistivity})$ values (\mathbf{c} , μ) to assess convergence is pointless
826 since the dimensionality of the geometry of the model may change at each step of the chain.
827 Instead, useful convergence diagnostics may be obtained from plots of number of cells, noise
828 hyperparameters, or $\log(\text{resistivity})$ at a certain location versus iteration number. Conver-
829 gence of one of these parameters may be said to have been reached when its value becomes
830 relatively stationary and no drifts are present as the parameter is plotted as a function of sam-
831 ple number.

832 One of the main factors affecting the speed at which convergence is reached is the
833 choice of the perturbation step sizes (see Appendix B.3 for a detailed description of these
834 terms). In order to promote convergence and prevent biases in the evaluated posterior PDF,
835 the shape of the proposal distribution from which each proposed model is drawn should be
836 as similar as possible to that of the posterior PDF. However, this is problematic given that
837 the shape of the posterior is not known *a priori*. Hence, as expressed in equation B.12, the
838 proposal distribution for \mathbf{m}' is chosen to be conditionally dependent on the current model
839 \mathbf{m} , so that the proposed model is simply a perturbation of \mathbf{m} whose magnitude is determined
840 by the step size. Suitable step sizes are normally chosen through trial and error by analysing

841 the acceptance rates (i.e., number of accepted samples over number of proposed samples) for
 842 the various types of perturbation, and a number of authors have suggested acceptance rates
 843 of around 1/4 for optimal sampling [Gelman *et al.*, 1996; Sherlock and Roberts, 2009]. If a
 844 certain acceptance rate is too low, the step size of the perturbation is likely to be too large as
 845 the proposed models fall either in regions of lower probability or outside of the prior bounds.
 846 If the acceptance rate is too high, then the proposed models are likely to be too close to the
 847 current models, causing the algorithm to explore only a small portion of the model space and
 848 slowing down convergence.

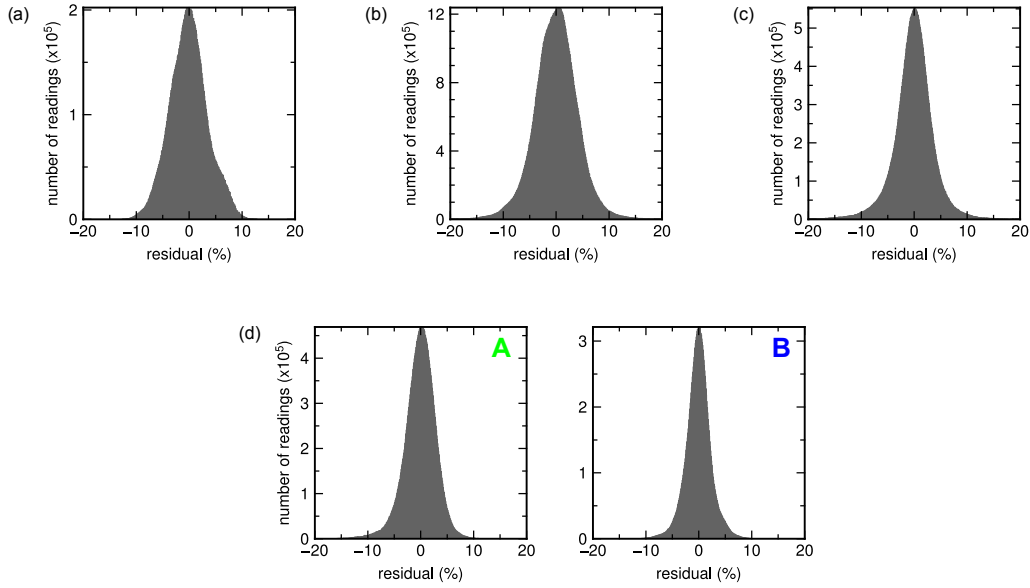
849 However, monitoring acceptance rates and manually tuning step sizes during a number
 850 of test runs may be cumbersome and computationally prohibitive due to the large computa-
 851 tional cost of the inversion (see Section 5.3). Similarly to Bodin and Sambridge [2009], we
 852 overcome this issue for non-transdimensional steps by implementing the ‘delayed rejection’
 853 scheme of Tierney and Mira [1999], which allows a second proposal on the value or posi-
 854 tion of Voronoi nuclei to be made by using a smaller step size if the first proposal is rejected.
 855 While this appears to improve the acceptance of *resistivity* and *move* steps, we find that the
 856 acceptance rates of transdimensional steps (birth and death) are normally very low ($< 10\%$).
 857 Hence, a natural extension of this study might include attempting to improve the accep-
 858 tance rates of transdimensional steps by implementing a ‘transdimensional delayed rejec-
 859 tion’ scheme as developed by Green and Mira [2001], and/or by sampling the $\log(\text{resistivity})$
 860 value for newly-generated Voronoi cells from the prior rather than using a Gaussian perturba-
 861 tion (equation B.16) as suggested by Dosso *et al.* [2014].

862 The choice of the prior also plays a role on Markov chain convergence, with wider pri-
 863 ors normally causing convergence to be slower. This is intuitive since, for the same Markov
 864 chain length, wider prior boundaries imply that a larger portion of model space must be ex-
 865 plored. Hence, although the use of a wider prior ensures that fewer prior-related biases are
 866 introduced into the solution, it also means that Markov chains need to be run for a longer
 867 time in order to reach convergence. A compromise between prior width and practicality must
 868 therefore sometimes be made given the limitations on the available computing time (even
 869 though this violates a strictly Bayesian approach where the prior should be independent of
 870 the current data and inversion algorithm).

871 The fit to the observed data may be estimated by calculating the residuals obtained
 872 from each Voronoi model within the ensemble, which for the examples considered in this pa-
 873 per are shown in Figure 18 as a percentage of the observed potential differences. In all cases,
 874 the distribution of the residuals resembles a Gaussian distribution and is centered around 0.

878 5.3 Computational cost

879 We initially implemented the TERT algorithm in MATLAB since it allowed for rapid
 880 testing, modification and debugging. In addition, given that the resistivity modelling code
 881 *FW2_5D* by Pidlisecky and Knight [2008] which we employed is freely available as a suite
 882 of MATLAB functions, implementation in MATLAB allowed us to make use of a thoroughly
 883 tested and, to the best of our knowledge, error-free forward modeller. However, despite the
 884 use of the Parallel Computing MATLAB Toolbox, executing inversions in MATLAB re-
 885 quired a substantial amount of computation time, hence we re-wrote our program entirely
 886 in Fortran after the initial testing stage. This gave us a considerable gain in computation
 887 time (around 1/3 time required for an inversion) and allowed us to leverage the resources of a
 888 computing cluster by using parallel computing tools such as MPI in the inversion algorithm.
 889 As an example, in its current Fortran implementation the running time of the code for the
 890 electrode geometries discussed in Section 3 is on average 4 hours for 10^4 iterations, using
 891 32 cores for 32 parallel Markov chains on the cluster at the University of Edinburgh. Fur-
 892 ther reductions in computation time could be made in future by also parallelising the forward
 893 modelling routines.



875 **Figure 18.** Residuals as percentage of the measured data evaluated for each Voronoi model in the en-
 876 sibles obtained for the examples described in (a) Section 3.1, (b) Section 3.2, (c) Section 1 of the Supporting
 877 Information, (d) Section 4.1 (profile *A* on the left, profile *B* on the right).

894 In terms of its applications, while TERT is computationally expensive in its current
 895 implementation, it is nevertheless applicable to the monitoring of higher-value targets where
 896 larger cost is acceptable. Examples include the detection and monitoring of leaks from nu-
 897 clear waste storage sites, or monitoring CO₂ plumes which might escape from subsurface
 898 storage reservoirs through chimney structures.

899 5.4 A note on natural parsimony

900 As described earlier, the rj-MCMC algorithm provides a naturally parsimonious way
 901 of performing tomography in that among models giving similar data fit, simpler ones (i.e.,
 902 those with fewer Voronoi cells) are assigned higher probability. This becomes obvious when
 903 Bayes' theorem (equation 2) is analysed together with the prior function in equation B.11,
 904 which decreases exponentially as the number of cells n increases (Figure B.1).

905 However, the concept of natural parsimony is not as straightforward to grasp when we
 906 consider the Metropolis-Hastings algorithm (which we employ to draw samples from the
 907 posterior PDF) since the number of cells n does not explicitly appear in any of the expres-
 908 sions for the acceptance parameter $\alpha(\mathbf{m}'|\mathbf{m})$ when a change in model dimension is involved
 909 (equations B.26 and B.27). In order to gain more intuition on the concept of natural parsim-
 910 ony, let us analyse equations B.26 and B.27 in more detail.

911 As described in Section 2.2.4, a proposed model \mathbf{m}' is accepted if $\alpha(\mathbf{m}'|\mathbf{m}) \geq r$, where
 912 r is a random deviate from a Uniform distribution between 0 and 1, while it is randomly ac-
 913 cepted or rejected if $\alpha(\mathbf{m}'|\mathbf{m}) < r$. This selection criterion ensures that all samples that im-
 914 prove the data fit are accepted, while also allowing lower-probability regions in the model
 915 space to be explored.

916 In the case of perturbation types of *fixed* dimensionality (i.e., changing resistivity or
 917 noise, or moving a Voronoi nucleus), the acceptance parameter $\alpha(\mathbf{m}'|\mathbf{m})$ only depends on the
 918 likelihoods of the current and proposed models (equation B.25), and the proposed model \mathbf{m}'

919 is always accepted if its likelihood is greater than that of the current model \mathbf{m} . In the case
 920 of birth and death steps, however, the acceptance parameter $\alpha(\mathbf{m}'|\mathbf{m})$ depends not only on
 921 the likelihoods of \mathbf{m} and \mathbf{m}' , but also on a number of other parameters such as the standard
 922 deviation of the step size σ_{bd} , the prior probability of $\log(\text{resistivity})$ $\Delta\mu$, and the difference
 923 in $\log(\text{resistivity})$ between the current and proposed model at the location where a Voronoi
 924 nucleus is added or removed (equations B.26–B.27). As a result, in order for a birth/death
 925 step to be definitely accepted, the term in the square brackets of equation B.26/B.27 must
 926 be greater than or equal to 1 (or, equivalently, its logarithm must be greater than or equal
 927 to 0). By taking the natural logarithm of this term, setting it equal to or greater than 0, and
 928 rearranging the terms, we obtain

$$929 \quad \psi(\mathbf{m}) - \psi(\mathbf{m}') \geq -2 \times \left[\ln \left(\frac{\sigma_{bd} \sqrt{2\pi}}{\Delta\mu} \right) + \frac{(\mu'_{n+1} - \mu_i)^2}{2\sigma_{bd}^2} \right] \quad (10)$$

930 in case of a birth step, and

$$931 \quad \psi(\mathbf{m}) - \psi(\mathbf{m}') \geq -2 \times \left[\ln \left(\frac{\Delta\mu}{\sigma_{bd} \sqrt{2\pi}} \right) - \frac{(\mu'_j - \mu_i)^2}{2\sigma_{bd}^2} \right] \quad (11)$$

932 in case of a death step, where $\mu = \log(\rho)$, $\psi(\mathbf{m})$ and $\psi(\mathbf{m}')$ denote the data misfit (defined in
 933 equation B.2) of the present and proposed model, σ_{bd} is the proposal step size for birth and
 934 death steps, \ln denotes the logarithm in base e, and for simplicity we have assumed data noise
 935 to be constant between model \mathbf{m} and \mathbf{m}' (i.e., $\sigma_k = \sigma'_k$ in equations B.26–B.27).

936 Equations 10 and 11 illustrate how, for a birth or death step to be definitely accepted,
 937 the difference in misfit between the current and the proposed model ($\psi(\mathbf{m}) - \psi(\mathbf{m}')$) must
 938 be greater than or equal to the quantity on the right-hand-side of each equation, while the
 939 model is randomly accepted or rejected if the difference in misfit is less than this quantity
 940 (see Section 2.2.4). The right-hand-side of equations 10 and 11 is displayed in Figure 19
 941 as a function of the change in $\log(\text{resistivity})$, $\delta\mu$, between the proposed and current model
 942 (where $\delta\mu = |\mu'_{n+1} - \mu_i|$ in a birth step, and $\delta\mu = |\mu'_j - \mu_i|$ in a death step), using the same
 943 prior and step size as in the synthetic examples from Section 3. The two curves in Figure 19
 944 cross at

$$945 \quad \delta\mu_0 = \sigma_{bd} \sqrt{2 \times \ln \left(\frac{\Delta\mu}{\sigma_{bd} \sqrt{2\pi}} \right)} \quad (12)$$

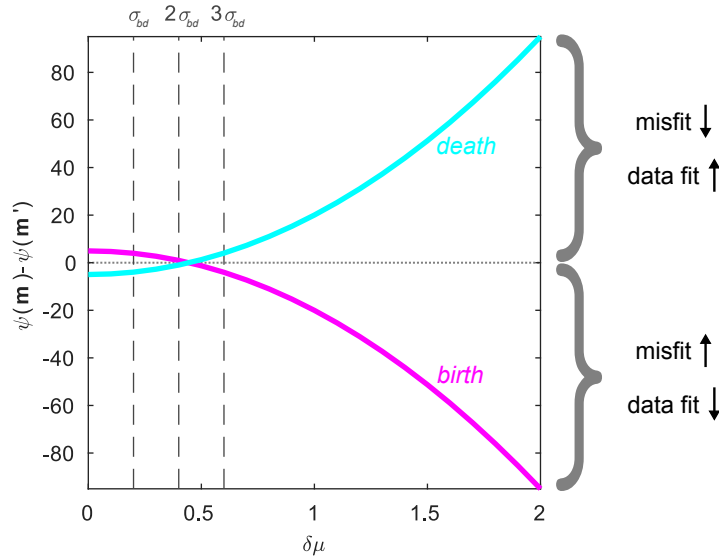
946 This value is important as it separates the values of $\delta\mu$ for which there are expected to be
 947 more death steps than birth steps (to the left of this value) from those for which the reverse is
 948 true (to the right). This value varies with the proposal step size σ_{bd} and peaks at

$$949 \quad \sigma_{bd}^{max} = \frac{\Delta\mu}{\sqrt{2\pi}} e^{-1/2} \quad (13)$$

950 For simplicity, let us refer to the area of the plot in Figure 19 located to the left of $\delta\mu_0$ as
 951 the region where the change in the model is small, and the region to the right of $\delta\mu_0$ as the
 952 region where the change in the model is large.

960 When the change in the model is small, all death steps which decrease the misfit (even
 961 by a very small amount) are accepted, while birth steps are only definitely accepted if model
 962 \mathbf{m}' yields a significantly lower misfit than the current model. This ensures that an increase
 963 in model dimensions is justified by a substantial decrease in misfit from \mathbf{m} to \mathbf{m}' if the two
 964 models are similar, and that the number of model dimensions always decreases if accompa-
 965 nied by an improvement in data fit – according to the principles of natural parsimony. How-
 966 ever, note that, in practical applications, the acceptance rate of birth steps is normally found
 967 to be low when the step size σ_{bd} is very small, since it is unlikely that the decrease in misfit
 968 will be large enough for small model perturbations.

969 When the change in the model is large, birth steps are always accepted if they improve
 970 the data fit, while death steps must yield a substantial improvement in fit in order to be defi-
 971 nitely accepted. Although this appears to be against the principles of natural parsimony, note

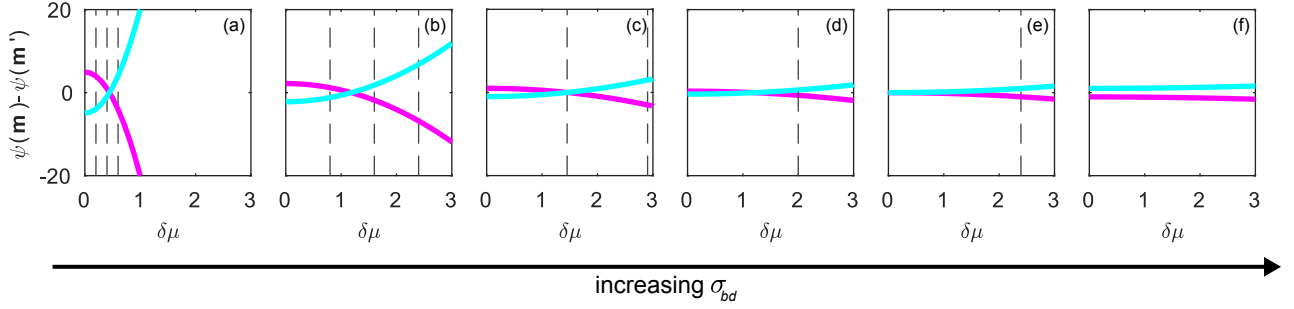


953 **Figure 19.** Difference in misfit between current model \mathbf{m} and proposed model \mathbf{m}' as a function of change
 954 in $\log(\text{resistivity})$, $\delta\mu$ (where $\delta\mu = |\mu'_{n+1} - \mu_i|$ in a birth step, and $\delta\mu = |\mu'_j - \mu_i|$ in a death step), calculated
 955 using equations 10 (birth, purple line) and 11 (death, light blue line), and the prior parameters from the syn-
 956 thetic examples in Section 3. Model \mathbf{m}' is always accepted if the difference in misfit $\psi(\mathbf{m}) - \psi(\mathbf{m}')$ lies above
 957 the purple line for a birth step and above the light blue line for a death step, and randomly accepted or rejected
 958 otherwise. The vertical dashed lines indicate the values below which $\delta\mu$ is likely to fall with probability
 959 68.27% (at σ_{bd}), 95.45% (at $2\sigma_{bd}$) and 99.73% (at $3\sigma_{bd}$).

972 that the majority of the time the change in $\log(\text{resistivity})$, $\delta\mu$, will be less than σ_{bd} , which
 973 is assumed to be significantly less than the prior range of $\log(\text{resistivity})$, $\Delta\mu$. In fact, be-
 974 cause the proposal distributions for birth and death steps are Gaussian, $\delta\mu$ has a probability
 975 of around 68%, 95% and 99.7% of falling respectively within one, two and three standard
 976 deviations σ_{bd} from μ_i , as displayed by the vertical dashed lines in Figure 19.

977 Similarly to Figure 19, the right-hand-side of equations 10 and 11 for different values
 978 of σ_{bd} is displayed in Figure 20. As σ_{bd} increases, the crossing point $\delta\mu_0$ moves to the right
 979 (panels (a)–(c)) (extending the region of naturally parsimonious proposals to the right) up to
 980 $\sigma_{bd} = \sigma_{bd}^{max}$ in panel (c). The crossing point $\delta\mu_0$ moves back to the left for $\sigma_{bd} > \sigma_{bd}^{max}$
 981 (panels (d)–(e)), and the two curves cross at $\delta\mu_0 = 0$ when $\sigma_{bd} = \Delta\mu/\sqrt{2\pi}$ (panel (e)).
 982 Beyond this value all birth steps that improve the data fit are accepted, while only death steps
 983 that provide a substantial decrease in misfit are always accepted (panel (f)).

990 Clearly the latter case is not parsimonious as birth steps are likely to exceed death steps
 991 (and $\delta\mu$ would be so large that either μ'_{n+1} would fall outside the prior support or model \mathbf{m}'
 992 could not be considered ‘similar’ to model \mathbf{m} as required by natural parsimony), and hence
 993 this places a bound on reasonable values of σ_{bd} . Plots such as those shown in Figure 20 may
 994 therefore be used to choose an appropriate value for σ_{bd} , such that the crossing point of the
 995 two curves is greater than 1 or 2 standard deviations from μ_i , ensuring that natural parsimony
 996 will be achieved on average. Alternatively, the resistivity of a newly-generated cell in a birth
 997 step may be sampled from the prior as suggested by *Dosso et al.* [2014], which obviates the
 998 need for such tuning when prior ranges are narrow.



984 **Figure 20.** Difference in misfit between current model \mathbf{m} and proposed model \mathbf{m}' as a function of change in
 985 log(resistivity) $\delta\mu$ (where $\delta\mu = |\mu'_{n+1} - \mu_i|$ in a birth step, and $\delta\mu = |\mu'_j - \mu_i|$ in a death step), calculated using
 986 equations 10 (birth, purple line) and 11 (death, light blue line), the prior on log(resistivity) from the synthetic
 987 examples in Section 3, and different proposal sizes σ_{bd} : (a) 0.2, (b) 0.8, (c) 1.4518 (i.e., σ_{bd}^{max} as given in
 988 equation 13), (d) 2, (e) 2.3937 (i.e., $\Delta\mu/\sqrt{2\pi}$), (f) 4. Where visible, the vertical dashed lines denote $\delta\mu$ equal
 989 to σ_{bd} , $2\sigma_{bd}$ and $3\sigma_{bd}$ as in Figure 19.

999 6 Conclusions

1000 We have described a method for electrical resistivity tomography which uses the reversible-
 1001 jump Markov chain Monte Carlo algorithm and model parameterisation with Voronoi cells
 1002 to produce an ensemble of solutions to the inverse problem which are distributed accord-
 1003 ing to the posterior probability density function. The advantage of this approach lies in the
 1004 fact that, by never linearising the physics of the forward modelling problem and allowing
 1005 the model parameterisation to vary freely during inversion, we reduce both modelling- and
 1006 parameterisation-related biases to a minimum while efficiently exploring the model space.
 1007 In addition, since no actual matrix inversion is involved in the inversion process, this method
 1008 obviates the need for any user-defined regularisation – the variation and smoothness of the
 1009 solution is constrained by noise in the data. More importantly, both synthetic and observa-
 1010 tional examples showed that depth resolution increases when non-linearities are correctly
 1011 accounted for during the inversion.

1012 Each of the models in the ensemble solution is defined by a tessellation of Voronoi
 1013 cells with different resistivity. While each of these models is unrealistic when taken on its
 1014 own, the full ensemble of solutions provides a probabilistic representation of subsurface
 1015 resistivity structures and of their uncertainties. Statistical moments such as the arithmetic
 1016 mean, the harmonic mean, the median, the mode and the root-mean-square can be computed
 1017 through the ensemble to obtain a visual representation of the subsurface resistivity field.
 1018 Each of these moments is sensitive to different properties of the ensemble (see Section B.5
 1019 in the Appendix) and, despite the discontinuous nature of the underlying Voronoi models,
 1020 provides a smooth representation of subsurface resistivity.

1021 In addition, compared to an optimisation approach, a sampling-based probabilistic solu-
 1022 tion has the inherent advantage that uncertainties can be directly evaluated from the pos-
 1023 terior probability density function. Within this paper, we considered standard deviation and
 1024 entropy as measures of uncertainty, and found that their magnitude is not only dictated by the
 1025 resolution provided by the data, but also by the true underlying resistivity structure. In fact,
 1026 both synthetic and observational data examples showed that the density of Voronoi nuclei is
 1027 greater where the variability of the true resistivity field is larger and where structures are of
 1028 smaller scale.

1029 **A: Forward modelling**

1030 The flow of electrical current in the Earth's subsurface is governed by Ohm's law,
1031 which states that at each point the current density \mathbf{J} is directly proportional to the electric
1032 field intensity \mathbf{E} and inversely proportional to the resistivity of the medium ρ :

$$1033 \quad \mathbf{J} = \frac{1}{\rho} \mathbf{E} \quad (\text{A.1})$$

1034 If the electric field \mathbf{E} is stationary in time, it can be expressed in terms of a scalar potential Φ
1035 as

$$1036 \quad \mathbf{E} = -\nabla\Phi \quad (\text{A.2})$$

1037 which allows us to re-write equation A.1 as

$$1038 \quad \mathbf{J} = -\frac{1}{\rho} \nabla\Phi \quad (\text{A.3})$$

1039 By the principle of conservation of charge and the equation of continuity, we obtain the fol-
1040 lowing expression,

$$1041 \quad \nabla \cdot \mathbf{J} = \frac{\partial q}{\partial t} \delta(\mathbf{x} - \mathbf{x}_S) \quad (\text{A.4})$$

1042 where \mathbf{x}_S is the location of a point source of charge density q , and $\delta(\mathbf{x} - \mathbf{x}_S)$ is the Dirac delta
1043 function centred at the current source location \mathbf{x}_S . By combining equations A.3 and A.4, and
1044 expressing current I as the change of charge density over time ($I = \partial q / \partial t$), we obtain the
1045 domain equation [*Dey and Morrison, 1979a,b; Pridmore et al., 1981*]

$$1046 \quad \nabla \cdot \left[\frac{1}{\rho(\mathbf{x})} \nabla\Phi(\mathbf{x}) \right] = -I \delta(\mathbf{x} - \mathbf{x}_S) \quad (\text{A.5})$$

1047 which describes the distribution of the electrical potential generated by a point source of
1048 electrical current at location \mathbf{x}_S . Solving this equation to determine the potential Φ which is
1049 generated by the injection of electrical current from an electrode located at \mathbf{x}_S and observed
1050 at \mathbf{x} , given a certain distribution of resistivity $\rho(\mathbf{x})$ in the subsurface, corresponds to most of
1051 the *forward* problem. The data usually recorded in ERT are differences in the electrical po-
1052 tential at pairs of locations; calculating these differences for the potential Φ completes the
1053 forward problem.

1054 **B: Mathematical details for the rj-McMC algorithm**

1055 **B.1 The likelihood**

1056 The likelihood function $p(\mathbf{d}^{obs} | \mathbf{m})$ can be thought of as a measure of the misfit be-
1057 tween observed and predicted data. Using a Gaussian distribution to represent data uncer-
1058 tainty, the likelihood function can be expressed as

$$1059 \quad p(\mathbf{d}^{obs} | \mathbf{m}) = \frac{1}{\sqrt{(2\pi)^K |\mathbf{C}_d|}} \exp \left\{ -\frac{1}{2} (\mathbf{d}^{obs} - \mathbf{d}^{pred})^T \mathbf{C}_d^{-1} (\mathbf{d}^{obs} - \mathbf{d}^{pred}) \right\} \quad (\text{B.1})$$

1060 where $\mathbf{d}^{pred} = \mathbf{g}(\mathbf{m})$, \mathbf{C}_d is the data covariance matrix and $|\mathbf{C}_d|$ represents its determinant.

1061 If data noise is uncorrelated, \mathbf{C}_d in equation B.1 is a diagonal matrix whose elements
1062 are the variances (i.e., squared standard deviations) of the data uncertainties. The data misfit
1063 function $\psi(\mathbf{m})$ can then be defined using the L_2 norm (chi-squared error) as

$$1064 \quad \psi(\mathbf{m}) = \sum_{k=1}^K \left(\frac{d_k^{obs} - d_k^{pred}}{\sigma_k} \right)^2 \quad (\text{B.2})$$

1065 where K represents the total number of data points, d_k^{pred} is the k^{th} datum predicted from
 1066 model \mathbf{m} , and σ_k is the standard deviation of the uncertainty associated with datum d_k^{obs} .
 1067 Combining equations B.1 and B.2 yields

$$1068 \quad p(\mathbf{d}^{obs}|\mathbf{m}) = \frac{1}{\prod_{k=1}^K (\sqrt{2\pi} \sigma_k)} e^{-\psi(\mathbf{m})/2} \quad (\text{B.3})$$

1069 B.2 The prior

1070 Since all inferences about the posterior PDF are relative to the prior distribution, priors
 1071 have great importance in Bayesian inversion schemes as the final result may be heavily influ-
 1072 enced by the choice of an inappropriate prior. In order to minimise the contribution of prior-
 1073 related biases that are introduced into the solution, we choose Uniform prior distributions
 1074 with wide bounds for all model parameters in the examples herein. Given that all parameters
 1075 are independent and have different dimensions, the model prior can then be divided into the
 1076 product of four terms:

$$1077 \quad p(\mathbf{m}) = p(n) p(\mathbf{c}|n) p(\boldsymbol{\mu}|n) p(\mathbf{h}) \quad (\text{B.4})$$

1078 where n is the number of Voronoi nuclei, $p(n)$ is the prior on the number of Voronoi nu-
 1079 clei/cells, $p(\mathbf{c}|n)$ is the prior on Voronoi nuclei location, $p(\boldsymbol{\mu}|n)$ is the prior on cell log(resistivity),
 1080 and $p(\mathbf{h})$ is the prior on noise hyperparameters.

1081 The prior on the number of Voronoi cells $p(n)$ is a discrete Uniform distribution be-
 1082 tween a minimum (n^{min}) and a maximum (n^{max}) number of Voronoi nuclei, such that

$$1083 \quad p(n) = \begin{cases} \frac{1}{\Delta n} & \text{if } n \in \mathcal{N} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.5})$$

1084 where $\mathcal{N} = [n^{min}, n^{min} + 1, \dots, n^{max} - 1, n^{max}]$ and $\Delta n = (n^{max} - n^{min} + 1)$.

1085 In order to evaluate the prior on Voronoi cell locations $p(\mathbf{c}|n)$, we define a rectangular
 1086 area bounded in x and z by $[x^{min}, x^{max}]$ and $[z^{min}, z^{max}]$ within which Voronoi nuclei may
 1087 be located. For simplicity, let us assume that this rectangle can be discretised into a fictitious
 1088 grid of N points at which Voronoi nuclei can be located (where $N = N_x \times N_z$). For n Voronoi
 1089 nuclei there then exist $\frac{N!}{n!(N-n)!}$ ways in which the nuclei can be arranged, all having the same
 1090 probability. Hence, the prior on Voronoi nuclei location is given by

$$1091 \quad p(\mathbf{c}|n) = \begin{cases} \left(\frac{N!}{n!(N-n)!}\right)^{-1} & \forall i \in [1, n], x_i \in \mathcal{X} \text{ and } z_i \in \mathcal{Z} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.6})$$

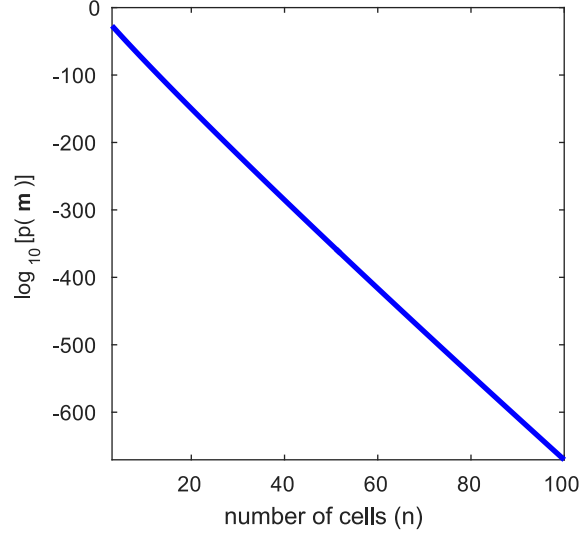
1092 where $\mathcal{X} = [x^{min}, x^{max}]$ and $\mathcal{Z} = [z^{min}, z^{max}]$. Alternatively, the prior on Voronoi cell
 1093 locations may be set to a Dirichlet distribution as discussed by *Steininger et al.* [2013], which
 1094 precludes the need for a fictitious grid to be defined.

1095 The prior on cell resistivity is a continuous Uniform distribution bounded by a mini-
 1096 mum (μ^{min}) and a maximum (μ^{max}) log(resistivity) value, such that for each cell i

$$1097 \quad p(\mu_i|n) = \begin{cases} \frac{1}{\Delta\mu} & \text{if } \mu_i \in \mathcal{M} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.7})$$

1098 where $\mathcal{M} = [\mu^{min}, \mu^{max}]$ and $\Delta\mu = (\mu^{max} - \mu^{min})$. Since the resistivity of each cell is
 1099 independent of that of any other cell, the prior over log(resistivity) for all cells is

$$1100 \quad p(\boldsymbol{\mu}|n) = c_\mu \prod_{i=1}^n p(\mu_i|n) \quad (\text{B.8})$$



1120 **Figure B.1.** Prior $p(\mathbf{m})$ as a function of number of cells n , calculated using equation B.11 and the prior
 1121 parameters from the synthetic example in Section 3.1. Note that the y-axis uses a logarithmic scale.

1101 where c_μ is a normalising constant, and $p(\mu|n)$ is only greater than zero if the log(resistivity)
 1102 of every cell falls within the interval $[\mu^{min}, \mu^{max}]$.

1103 Similarly, the prior on the set of noise hyperparameters \mathbf{h} is assigned assuming that
 1104 all hyperparameters are mutually independent (in other words, without imposing any depen-
 1105 dence between hyperparameters a priori). The prior on each hyperparameter h_j is described
 1106 by a continuous Uniform distribution between a minimum (h_j^{min}) and a maximum (h_j^{max})
 1107 value such that

$$1108 \quad p(h_j) = \begin{cases} \frac{1}{\Delta h_j} & \text{if } h_j \in \mathcal{H}_j \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.9})$$

1109 where $\mathcal{H}_j = [h_j^{min}, h_j^{max}]$ and $\Delta h_j = (h_j^{max} - h_j^{min})$. Since each hyperparameter is indepen-
 1110 dent of all the others, the prior over all hyperparameters is

$$1111 \quad p(\mathbf{h}) = c_h \prod_{j=1}^J p(h_j) \quad (\text{B.10})$$

1112 where c_h is a normalising constant and J is the total number of hyperparameters.

1113 By combining equations B.5, B.6, B.8 and B.10 as in equation B.4, the full prior prob-
 1114 ability density function can be expressed as

$$1115 \quad p(\mathbf{m}) = \frac{c_m n! (N - n)!}{N! (\Delta\mu)^n \Delta n \left(\prod_{j=1}^J \Delta h_j \right)} \quad (\text{B.11})$$

1116 where $c_m = c_\mu c_h$, provided that all parameters fall within the boundaries of their respective
 1117 priors. If one of the parameters falls outside of the range of its prior, the full prior in equation
 1118 B.11 becomes zero. As an example, the prior calculated from equation B.11 using the prior
 1119 parameters from the synthetic example in Section 3.1 is shown in Figure B.1.

1122 B.3 Proposal distributions

1123 At each step of the Markov chain, a perturbed model \mathbf{m}' is drawn from a proposal dis-
 1124 tribution $q(\mathbf{m}'|\mathbf{m})$, which is only dependent on the present model \mathbf{m} and which might take

the form

$$q(\mathbf{m}'|\mathbf{m}) \propto \exp\left\{-\frac{1}{2}(\mathbf{m}-\mathbf{m}')^T \mathbf{C}^{-1}(\mathbf{m}-\mathbf{m}')\right\} \quad (\text{B.12})$$

representing a Gaussian distribution with mean \mathbf{m} and with a typically diagonal covariance matrix \mathbf{C} . In practical applications, in order to create a new model \mathbf{m}' from the current model \mathbf{m} the i^{th} component of \mathbf{m} may be perturbed according to the proposal distribution as

$$\mathbf{m}' = \mathbf{m} + u\sigma_i \mathbf{e}_i \quad (\text{B.13})$$

where u is a random deviate from a standard normal distribution (a Gaussian with mean of 0 and variance of 1), σ_i is the standard deviation of the proposal (step size), and \mathbf{e}_i is a unit vector in the i^{th} direction. Overall, five types of perturbations can be performed on the model \mathbf{m} used here:

- A *resistivity* step perturbs the resistivity of a randomly-selected cell. If the resistivity of cell i is to be perturbed, a new log(resistivity) value μ'_i for the cell can be obtained from

$$\mu'_i = \mu_i + u\sigma_r \quad (\text{B.14})$$

where μ_i is the present log(resistivity) of cell i , and σ_r is the step size of the proposal for a change in cell log(resistivity).

- A *move* step changes the position of a randomly-selected Voronoi nucleus. If the location of cell i is to be perturbed, a new location \mathbf{c}'_i (given by coordinates x'_i and z'_i) for the cell nucleus can be obtained from

$$\begin{aligned} x'_i &= x_i + u\sigma_c \\ z'_i &= z_i + u\sigma_c \end{aligned} \quad (\text{B.15})$$

where x_i and z_i are the current x and z coordinates of nucleus i , and σ_c is the step size of the proposal for a change in cell location.

- A *death* step removes a randomly-selected Voronoi cell nucleus from the model vector \mathbf{m} .
- A *birth* step adds a Voronoi cell nucleus to the current model. If a new cell is added at a random location \mathbf{c}'_{n+1} , the log(resistivity) of the new cell is obtained from

$$\mu'_{n+1} = \mu_i + u\sigma_{bd} \quad (\text{B.16})$$

where μ_i is the present log(resistivity) at location \mathbf{c}'_{n+1} , and σ_{bd} is the step size of the resistivity proposal in the case of birth and death steps.

- A *noise* step perturbs a randomly-selected data noise hyperparameter. If noise hyperparameter h_j is perturbed (while the resistivity structure of the model remains unchanged), a new hyperparameter h'_j can be obtained from

$$h'_j = h_j + u\sigma_{h_j} \quad (\text{B.17})$$

where h_j is the current value of hyperparameter j , and σ_{h_j} is the step size of the proposal for a change in h_j .

B.4 The acceptance parameter α

The use of $\alpha(\mathbf{m}'|\mathbf{m})$ as an acceptance parameter in step 6 of the TERT algorithm ensures that, for perturbation types of *fixed* dimensionality (i.e., changing resistivity and noise, and moving a Voronoi nucleus), all models that improve the data fit are accepted and those that do not are randomly accepted or rejected depending on their likelihood, while in the case of perturbation types involving a change in model dimension (i.e., birth and death steps) the acceptance of proposed models involves a balance between likelihood, prior and proposal ratios (as discussed in more detail in Section 5.4). *Green* [1995, 2003] showed that this in

1168 turn ensures that the sample population follows the posterior distribution $p(\mathbf{m}|\mathbf{d}^{obs})$ as the
1169 number of iterations tends to infinity.

1170 As can be seen in equation 5, the expression for the acceptance ratio $\alpha(\mathbf{m}'|\mathbf{m})$ involves
1171 the product of prior, likelihood and proposal ratios and the Jacobian of the transformation
1172 from \mathbf{m} to \mathbf{m}' . A detailed derivation of all of these terms can be found in *Bodin and Sam-*
1173 *bridge* [2009] for the case of seismic traveltimes tomography, and the derivation is almost
1174 identical for TERT. Since to the best of our knowledge this transdimensional inversion al-
1175 gorithm has not previously been used in electrical resistivity tomography, here we briefly
1176 introduce each term in equation 5.

1177 The calculation of the prior ratio involves the evaluation of the prior for \mathbf{m} and \mathbf{m}' using
1178 equation B.11. In the case of perturbation types of *fixed* dimensionality, $p(\mathbf{m}) = p(\mathbf{m}')$,
1179 hence the prior ratio is unity provided that the proposed values fall within the support of their
1180 respective priors (the support is the set of values for which the probability is non-zero):

$$1181 \left[\frac{p(\mathbf{m}')}{p(\mathbf{m})} \right]_{fixed} = \begin{cases} 1 & \text{if } \mathbf{m}' \in \mathcal{N}, \mathcal{M}, \mathcal{X}, \mathcal{Z}, \mathcal{H} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.18})$$

1182 For perturbation types which involve a jump in dimensionality, the prior ratio for a birth step
1183 is

$$1184 \left[\frac{p(\mathbf{m}')}{p(\mathbf{m})} \right]_{birth} = \begin{cases} \frac{n+1}{(N-n)\Delta\mu} & \text{if } \mathbf{m}' \in \mathcal{N}, \mathcal{M}, \mathcal{X}, \mathcal{Z}, \mathcal{H} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.19})$$

1185 and for a death step is

$$1186 \left[\frac{p(\mathbf{m}')}{p(\mathbf{m})} \right]_{death} = \begin{cases} \frac{(N-n+1)\Delta\mu}{n} & \text{if } \mathbf{m}' \in \mathcal{N}, \mathcal{M}, \mathcal{X}, \mathcal{Z}, \mathcal{H} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.20})$$

1187 For perturbations that change the resistivity structure of the model, the evaluation of
1188 the likelihood ratio involves the computation of the electrical potential Φ generated by each
1189 pair of current electrodes through the Voronoi tessellation of \mathbf{m} and \mathbf{m}' , and the calculation
1190 of potential differences (and data uncertainties if necessary – equation 4) for all required
1191 combinations of current and potential electrodes. For noise perturbations it requires only the
1192 calculation of new data uncertainties. Once all potential differences and/or noise parameters
1193 have been calculated, the likelihood function may be evaluated using equation B.3, giving

$$1194 \frac{p(\mathbf{d}^{obs}|\mathbf{m}')}{p(\mathbf{d}^{obs}|\mathbf{m})} = \left(\prod_{k=1}^K \frac{\sigma_k}{\sigma'_k} \right) \exp \left\{ -\frac{\psi(\mathbf{m}') - \psi(\mathbf{m})}{2} \right\} \quad (\text{B.21})$$

1195 where σ_k and σ'_k are the current and proposed uncertainties associated with the k^{th} datum,
1196 respectively.

1197 The proposal probability $q(\mathbf{m}'|\mathbf{m})$ expresses the probability to move from \mathbf{m} to \mathbf{m}' ,
1198 while $q(\mathbf{m}|\mathbf{m}')$ expresses the probability for the reverse move, from \mathbf{m}' to \mathbf{m} . In the case of
1199 perturbation types which do not involve a change in dimension, $q(\mathbf{m}'|\mathbf{m})$ and $q(\mathbf{m}|\mathbf{m}')$ are
1200 symmetrical distributions, hence their ratio is unity:

$$1201 \left[\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})} \right]_{fixed} = 1 \quad (\text{B.22})$$

1202 For perturbation types which involve a jump in dimension, the proposal distributions $q(\mathbf{m}'|\mathbf{m})$
1203 and $q(\mathbf{m}|\mathbf{m}')$ are not symmetric and we obtain different proposal ratios depending on the
1204 type of perturbation. For a birth step which creates a new cell at location \mathbf{c}'_{n+1} the ratio is

$$1205 \left[\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})} \right]_{birth} = \frac{\sqrt{2\pi}(N-n)}{n+1} \sigma_{bd} \exp \left\{ \frac{(\mu'_{n+1} - \mu_i)^2}{2\sigma_{bd}^2} \right\} \quad (\text{B.23})$$

1206 where μ'_{n+1} is the log(resistivity) of the added cell, μ_i is the present log(resistivity) at loca-
 1207 tion \mathbf{c}'_{n+1} , and σ_{bd} is defined in equation B.16. For a death step which involves the deletion
 1208 of cell i the proposal ratio is

$$1209 \quad \left[\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})} \right]_{death} = \frac{n}{\sigma_{bd} \sqrt{2\pi} (N - n + 1)} \exp \left\{ -\frac{(\mu'_j - \mu_i)^2}{2\sigma_{bd}^2} \right\} \quad (\text{B.24})$$

1210 where μ'_j is the log(resistivity) at \mathbf{c}_i in the new tessellation (i.e., after the deletion of cell i).

1211 The Jacobian term $|\mathbf{J}|$ accounts for scale changes occurring in the case of transdimen-
 1212 sional perturbations by normalising the difference in volume of the two model spaces of dif-
 1213 ferent dimension [Green, 2003]. Besides being equal to one in the case of model perturba-
 1214 tions which do not involve a change in dimension, Bodin and Sambridge [2009] show that $|\mathbf{J}|$
 1215 is unity even for birth and death steps, hence can be ignored.

1216 By substituting the expressions for the Jacobian and for the prior, likelihood and pro-
 1217 posal ratio into equation 5, an expression for $\alpha(\mathbf{m}'|\mathbf{m})$ can be obtained for each type of model
 1218 perturbation. For model perturbations which do not involve a change in dimension, the prod-
 1219 uct of ratios in equation 5 becomes simply the ratio of likelihoods in the proposed and cur-
 1220 rent model since the prior and proposal ratios are both unity:

$$1221 \quad \alpha(\mathbf{m}'|\mathbf{m})_{fixed} = \begin{cases} \min \left[1, \left(\prod_{k=1}^K \frac{\sigma_k}{\sigma'_k} \right) \exp \left\{ -\frac{\psi(\mathbf{m}') - \psi(\mathbf{m})}{2} \right\} \right] & \text{if } \mathbf{m}' \in \mathcal{N}, \mathcal{M}, \mathcal{X}, \mathcal{Z}, \mathcal{H} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.25})$$

1222 For model perturbations involving a change in dimension, for a birth step

$$1223 \quad \alpha(\mathbf{m}'|\mathbf{m})_{birth} = \begin{cases} \min \left[1, \frac{\sigma_{bd} \sqrt{2\pi}}{\Delta\mu} \left(\prod_{k=1}^K \frac{\sigma_k}{\sigma'_k} \right) \exp \left\{ \frac{(\mu'_{n+1} - \mu_i)^2}{2\sigma_{bd}^2} - \frac{\psi(\mathbf{m}') - \psi(\mathbf{m})}{2} \right\} \right] & \text{if } \mathbf{m}' \in \mathcal{N}, \mathcal{M}, \mathcal{X}, \mathcal{Z}, \mathcal{H} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.26})$$

1224 and for a death step

$$1225 \quad \alpha(\mathbf{m}'|\mathbf{m})_{death} = \begin{cases} \min \left[1, \frac{\Delta\mu}{\sigma_{bd} \sqrt{2\pi}} \left(\prod_{k=1}^K \frac{\sigma_k}{\sigma'_k} \right) \exp \left\{ -\frac{(\mu'_j - \mu_i)^2}{2\sigma_{bd}^2} - \frac{\psi(\mathbf{m}') - \psi(\mathbf{m})}{2} \right\} \right] & \text{if } \mathbf{m}' \in \mathcal{N}, \mathcal{M}, \mathcal{X}, \mathcal{Z}, \mathcal{H} \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.27})$$

1226 Note that, since equations B.25–B.27 do not contain variable N (previously defined in equa-
 1227 tion B.6), the priors over x and z are here given over the continuous ranges $\mathcal{X} = [x^{min}, x^{max}]$
 1228 and $\mathcal{Z} = [z^{min}, z^{max}]$.

1229 B.5 Statistical solutions

1230 At the end of the inversion, maps showing different statistical properties of the subsur-
 1231 face resistivity field may be obtained from the ensemble by calculating a number of statistical
 1232 moments through a regular grid of discrete points $[\bar{x}_i \ \bar{z}_i]$ over the M samples in the ensem-
 1233 ble. These statistical properties may include (but are not limited to) the following measures:

- 1234 • the *arithmetic mean* (i.e., the average or first statistical moment), given by

$$1235 \quad \bar{\mu} = \frac{1}{M} \sum_{m=1}^M \mu_m \quad (\text{B.28})$$

1236 This statistic is ideal in purely Gaussian PDFs, but may be heavily affected by outliers
 1237 or by the tails of the distribution when the posterior is not Gaussian.

- 1238 • the *harmonic mean*, given by

$$1239 \quad \text{HM}(\mu) = \frac{1}{\frac{1}{M} \sum_{m=1}^M \frac{1}{\mu_m}} \quad (\text{B.29})$$

- 1240 Since the harmonic mean involves taking the inverse of each value, this statistic is
 1241 more sensitive to low resistivities within the ensemble than is the arithmetic mean.
 1242 • the *root-mean-square*, given by

$$1243 \text{RMS}(\mu) = \sqrt{\frac{1}{M} \sum_{m=1}^M \mu_m^2} \quad (\text{B.30})$$

- 1244 Since the root-mean-square involves squaring each value, this statistic is more sensi-
 1245 tive to high resistivities within the ensemble than the arithmetic mean.
 1246 • the *median*, which can be defined as the parameter value that separates the lower half
 1247 from the upper half of probabilities in the PDF. It is a robust statistic which is less
 1248 affected by extremely large or small values than the arithmetic mean.
 1249 • the *mode*, or *maximum-a-posteriori* value, which can be defined as the parameter
 1250 value appearing most often in the ensemble, and hence which has the largest value of
 1251 the posterior PDF. Compared to the previous statistics, it tends to preserve the discrete
 1252 character of the underlying Voronoi cells in the ensemble, hence maps of this statisti-
 1253 cal moment are normally characterised by sharp discontinuities between structures of
 1254 different resistivity.
 1255 • the *standard deviation* (i.e., the square root of the second statistical moment), given by

$$1256 \sigma_\mu = \sqrt{\frac{1}{M} \sum_{m=1}^M (\mu_m - \bar{\mu})^2} \quad (\text{B.31})$$

1257 This statistic is particularly useful within a stochastic inversion scheme as it provides a
 1258 direct measure of the uncertainty in the solution.

- 1259 • *entropy*, given by

$$1260 \text{Entropy}(\mu) = \sum_{j=1}^J [-p_j \log_2(p_j)] \quad (\text{B.32})$$

1261 where J is the number of bins in a histogram representing the posterior PDF on $\log(\text{resistivity})$
 1262 at location $[\bar{x}_i \bar{z}_i]$ (see Figure 6), and p_j is the probability of $\log(\text{resistivity}) \mu_j$
 1263 in the posterior PDF. Entropy can be described as a measure of disorder (lack of in-
 1264 formation), hence it is high at locations where the PDF resembles the Uniform prior
 1265 (e.g., Figure 6(a)), and low where the posterior PDF is represented by sharp and well-
 1266 defined peaks (e.g., Figure 6(e)).

- 1267 • *skewness* (i.e., the third statistical moment), given by

$$1268 \text{Skewness}(\mu) = \frac{1}{\sigma_\mu^3} \left(\frac{1}{M} \sum_{m=1}^M \mu_m^3 - 3\bar{\mu} \frac{1}{M} \sum_{m=1}^M \mu_m^2 + 2\bar{\mu}^3 \right) \quad (\text{B.33})$$

1269 This statistic provides information on the asymmetry of the PDF, with negatively-
 1270 skewed distributions having a longer tail to the left and positively-skewed distributions
 1271 having a longer tail to the right. Since a Gaussian distribution is symmetric around its
 1272 arithmetic mean, purely Gaussian PDFs have zero skewness.

- 1273 • *excess kurtosis* (i.e., the fourth statistical moment), given by

$$1274 \text{ExKurtosis}(\mu) = \frac{1}{\sigma_\mu^4} \left(\frac{1}{M} \sum_{m=1}^M \mu_m^4 - 4\bar{\mu} \frac{1}{M} \sum_{m=1}^M \mu_m^3 + 6\bar{\mu}^2 \frac{1}{M} \sum_{m=1}^M \mu_m^2 - 3\bar{\mu}^4 \right) - 3 \quad (\text{B.34})$$

1275 This statistic can be used to obtain information on the ‘peakedness’ of the PDF, with
 1276 negative excess kurtosis indicating broader and flatter distributions (such as a Uniform
 1277 distribution), and positive excess kurtosis indicating more ‘pointy’ distributions with
 1278 flatter tails and narrower peaks (such as a Laplacian distribution). In addition, nega-
 1279 tive kurtosis can also indicate bimodal distributions which may be observed at sharp
 1280 discontinuities (e.g., Figure 8).

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Supporting Information for “Transdimensional Electrical Resistivity Tomography”

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1. Observational data experiments: Slovakia dataset

In this experiment, we inverted an observational dataset (donated courtesy of Tina Wunderlich at Kiel University) recorded at an archaeological site in the western Small Carpathians (Slovakia). A detailed investigation involving multiple geophysical techniques was carried out by *Wilken et al.* [2015] at this site with the purpose of imaging the ruins of a number of chapels belonging to the abandoned Franciscan monastery of Katarínka. *Wilken et al.* [2015] found that the combined interpretation of results from different methods (magnetics, ground penetrating radar and ERT) was particularly beneficial in that each technique complemented the others. Given that the same anomalies were imaged using

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multiple techniques, this dataset provides an ideal setting to test our inversion method on observational data.

We inverted a dataset recorded using a Wenner-alpha configuration and 51 electrodes with spacing 0.5 m (gray rectangles in Figures S1–S3), giving 408 measured potential differences in total. We assumed data noise to be unknown, hence also inverted for parameters a and b in equation 3 in the main text. A simplified model showing the interpretation of the profile by *Wilken et al.* [2015] is shown in Figure S1.

We assumed Uniform priors on the number of Voronoi cells as $[5, 6, \dots, 200]$, on $\mu = \log(\rho)$ as $[0.5, 4.5]$, on the x and z coordinates of model boundaries as $[-2, 27]$ and $[0, 10]$, respectively, and on noise parameters a as $[0.0001, 0.2001]$ and b as $[0.1, 1.1]$, respectively. We ran 32 tempered Markov chains (of which 16 were at the target temperature $T_0 = 1$) in parallel for 1×10^6 iterations allowing two randomly-chosen chains to swap models at each iteration according to equation 7 in the main text. Every 100th sample at the target temperature after a burn-in period of 2.5×10^5 iterations was considered as a representative model from the posterior PDF, giving an ensemble of 120×10^3 valid samples.

The results from the inversion using the TERT algorithm are shown in Figure S2. In this case, since the prior on $\log(\text{resistivity})$ does not cross 0, we also include the harmonic mean among the statistical maps produced with TERT. Figure S3 shows the inversion results obtained using the linearised code *R2*, where data noise was assumed to be proportional to the measured resistances according to equation 3 in the main text, and a and b were obtained from the posterior calculated with TERT (Figure S4).

In all cases (a)–(e), a high resistivity anomaly is imaged near $[12, 2]$ m, together with a thin high-resistivity layer near the surface to its left. The central high-resistivity anomaly

corresponds to an anomaly which is also imaged with ground penetrating radar (see *Wilken et al.* [2015] for details), and was originally interpreted as a pot-shaped structure of high resistivity embedded in soil by *Wilken et al.* [2015] (Figure S1). The resistivity of the background medium is resolved differently by different statistical moments: as expected, the harmonic mean map is more sensitive to low resistivities in the ensemble and the root-mean-square map is more sensitive to high resistivity values, while both the arithmetic mean and the median seem to fall somewhere in between.

In terms of uncertainty, the standard deviation and entropy maps show that resolution is limited below 2 m depth. As expected, the density of Voronoi nuclei within the ensemble peaks near the surface, specifically near the thin, high-resistivity layer to the left of the central anomaly. This is intuitively correct since a large number of small Voronoi cells are required to describe smaller-scale structures.

Since we considered data noise as an unknown in the inversion, the posterior on noise hyperparameters a and b are shown in Figure S4. While parameter b peaks at 0.1 (i.e., the lower prior boundary, suggesting that the prior should have probably been extended below 0.1), parameter a peaks around 0.04, suggesting that the level of noise in this dataset is $\sim 4\%$.

The thin high-resistivity layer and the central anomaly are also resolved by the iterated-linearised inversion with code *R2*. However, while sensitivity can be calculated (Figure S3(b)), a map of uncertainty is not produced with this code so it is not possible to associate a measure of the accuracy of the reconstructed structure in Figure S3(a). In addition, some of the maps retrieved through TERT (i.e., Figure S2(a)–(e)) seem to indicate the presence of a high-resistivity structure near [20, 3] m which is not resolved at

all by linearised inversion. Although it is located in an area of high standard deviation and entropy (Figure S2(g)–(h)), the synthetic examples in Section 3 of the main text showed that mean structure may be correctly retrieved with TERT even in regions of high uncertainty, hence it is possible that this anomaly represents a high-resistivity body embedded in soil.

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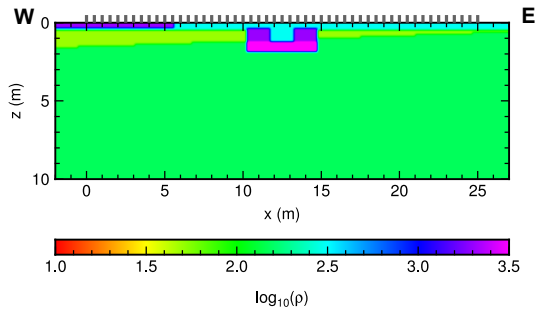


Figure S1. Simplified model showing *Wilken et al.* [2015]’s interpretation of the profile that we imaged using the TERT algorithm. A u-shaped high-resistivity anomaly embedded in low-resistivity material (i.e., soil) is visible near the centre of the profile, together with a thin, high-resistivity layer near the surface to the west of the anomaly. Re-plotted after Figure 11(c) in *Wilken et al.* [2015]. The grey ticks at $z = 0$ m denote electrode locations used in our inversion.

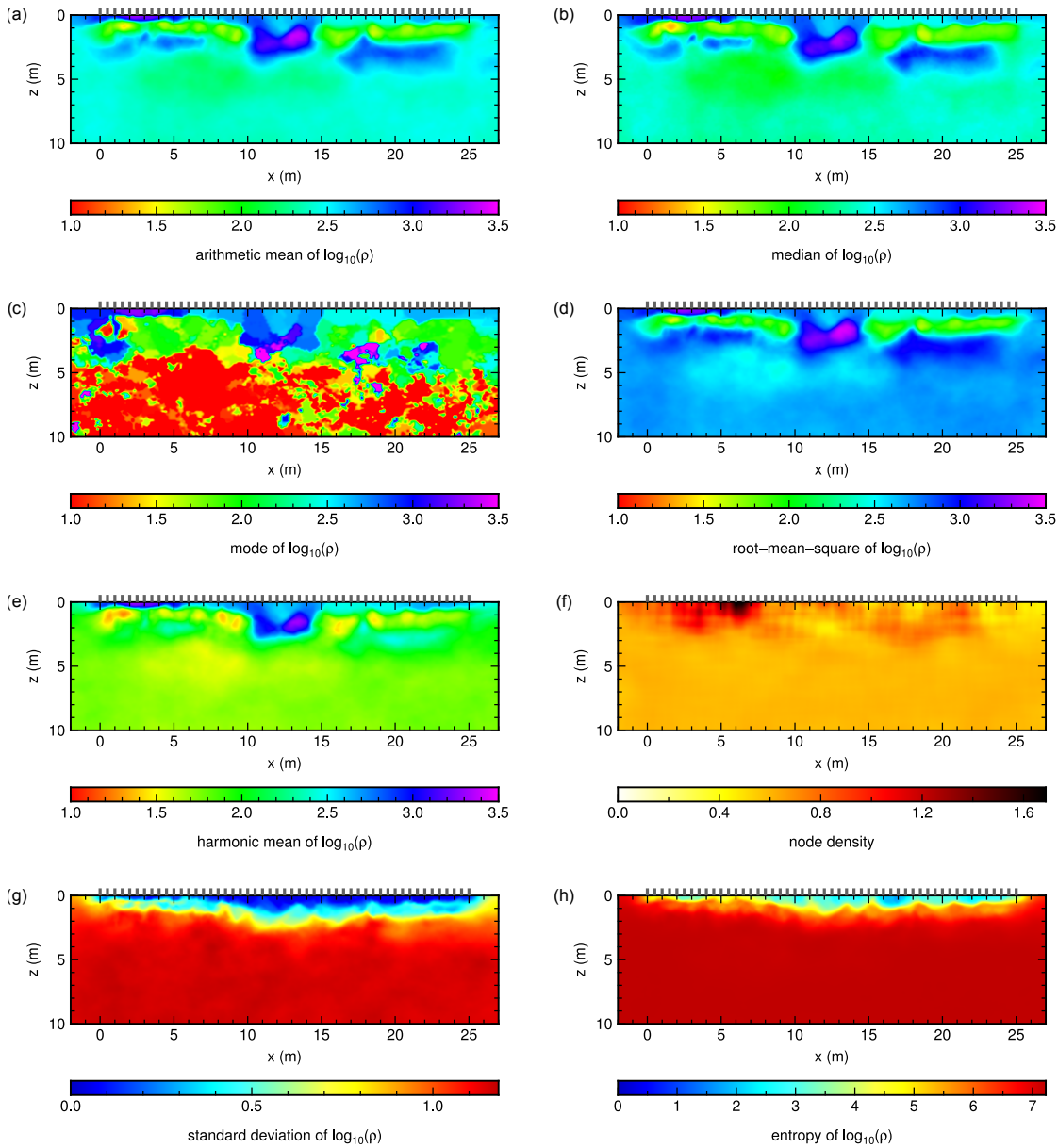


Figure S2. Inversion results for the Slovakia observational dataset found using the TERT algorithm. (a) Arithmetic mean. (b) Median. (c) Mode (i.e., maximum-a-posteriori). (d) Root-mean-square. (e) Harmonic mean. (f) Node density (measured within a $2 \text{ m} \times 2 \text{ m}$ square sector centred on each pixel). (g) Standard deviation. (h) Entropy. Note that the colour scale in (a)–(e) is clipped between 1 and 3.5 to aid visualisation. In all panels, the grey ticks at $z = 0 \text{ m}$ denote electrode locations.

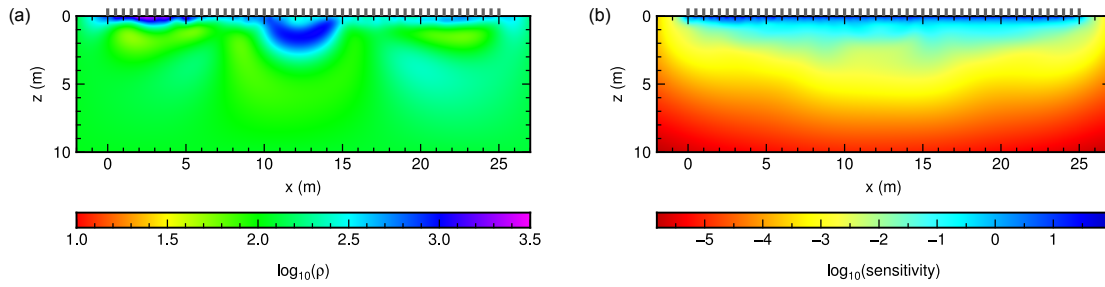


Figure S3. Inversion results for the Slovakia observational dataset found using the iterated-linearised code *R2* by *Binley* [2013]. (a) Best-fit resistivity map. (b) Sensitivity map. In both panels, the grey ticks at $z = 0$ m denote electrode locations.

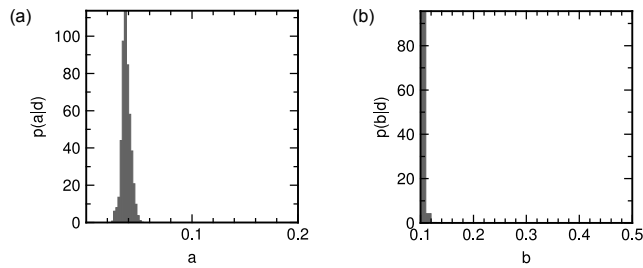


Figure S4. Posterior PDF on noise hyperparameters (a) a and (b) b for the Slovakia observational dataset obtained from TERT.