

SUPPLEMENTAL MATERIAL
for
Uncertainty Loops in Travel-Time Tomography
from Nonlinear Wave Physics

Erica Galetti,* Andrew Curtis, and Giovanni Angelo Meles

*School of GeoSciences, University of Edinburgh,
The King's Buildings, West Mains Road,
Edinburgh, EH9 3JW, United Kingdom*

Brian Baptie

*British Geological Survey, Murchison House,
West Mains Road, Edinburgh, EH9 3LA, United Kingdom*

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THE RJ-MCMC ALGORITHM

In seismic tomography, recordings of seismic waves are used to infer the structure of the Earth’s subsurface. Typically, a subsurface model \mathbf{m} is estimated from a seismic dataset \mathbf{d} by solving the inverse problem $\mathbf{d} = \mathbf{G}(\mathbf{m})$ for \mathbf{m} , given forward function \mathbf{G} that relates \mathbf{m} to \mathbf{d} . In surface-wave traveltime tomography, \mathbf{d} is often a vector representing first-arriving source-to-receiver traveltimes, and \mathbf{m} a vector of seismic slownesses of different cells in a fixed spatial grid.

In linearized tomography, \mathbf{G} represents multiplication by a two-dimensional matrix whose elements are the length of each ray (traced through a prior estimate of the slowness model) in each grid cell. However, the ray path is itself dependent on the unknown velocity structure of the medium, rendering the relationship in the above equation nonlinear. In addition, while having the advantage of being computationally efficient, traditional linearized tomographic methods which use fixed model parameterization require somewhat arbitrary regularisation to be applied to dampen the effect of noise in the data and to constrain model slowness combinations that are unconstrained by the data. The final solution may also be strongly affected by the initial estimate of the velocity model.

Alternative tomographic methods offer the possibility of adapting the parameterization (the shape and size of the grid) to the spatial distribution of the data [1]. In particular, the self-parameterizing reversible-jump Markov chain Monte Carlo (rj-McMC) algorithm, recently applied to geophysical problems for the first time [2], also allows the number of model parameters to be varied during the inversion. This method uses Bayes’ theorem and Markov chain Monte Carlo to generate a series of velocity models which are distributed according to the Bayesian posterior probability density. Bodin *et al.* [3] show that the method can also estimate data uncertainties when these are unavailable.

The workow of the rj-McMC algorithm we employed for our study, an adapted version of the original algorithm of Bodin and Sambridge [2], is shown in Fig. S1. A velocity model \mathbf{m} is defined over a Voronoi tessellation of the geographical 2D space, and both velocity and data noise parameters have a uniform prior distribution. At each iteration, a new model \mathbf{m}' is proposed as a random perturbation of the current model and the acceptance term $\alpha(\mathbf{m}'|\mathbf{m})$ (see equation (18) in Bodin and Sambridge [2]) is calculated, allowing the algorithm to either accept or reject the proposed model. The acceptance term α promotes natural parsimony

(tending to use fewer model parameters if more are unnecessary) and ensures that all models that improve data fit are accepted, while those that do not are randomly accepted or rejected depending on their likelihood. Rather than providing a single best-fitting solution \mathbf{m} , the result of rj-McMC is an ensemble of models which are samples of the posterior probability distribution of the number of cells, velocities at each point of the model space, and data uncertainties. Since it is the *whole* ensemble of models, and not each model taken separately, that represents a solution to the inverse problem, statistics such as the ensemble average and standard deviation at each geographical location can be calculated: while each single velocity model in the ensemble is discontinuous and unrealistic, the average velocity map is a smooth representation of the true mean velocity field, and the standard deviation map then provides an indication of the uncertainty distribution as shown in Fig. 1. Note that maps of statistical moments of higher order, such as skewness or kurtosis, may also be extracted from the ensemble of models [4].

For UK tomography, 3 million iterations of the algorithm in Fig. S1 are performed. Every 150th sample after a burn-in period of 1.5 million iterations is considered as a representative sample from the posterior distribution of \mathbf{m} . An average velocity model and a map of the standard deviation at each geographical location are calculated from the model ensemble.

Bodin and Sambridge [2] used a linearized approach as they kept ray paths fixed throughout each run of the Markov chain, only updating the ray geometries after an ensemble average had been calculated. Our transdimensional tomography is fully nonlinear: we calculate source-receiver ray paths for each model proposed in all chains, therefore using the correct ray geometries and traveltimes in the evaluation of the likelihood ratio (compare rays around -2.5°E , 52.5°N in \mathbf{m} and \mathbf{m}' in Fig. S1). Our rays are calculated using the fast marching method (FMM) as an eikonal solver [5] on a refined grid obtained by dividing each $1^\circ \times 1^\circ$ area into 16×16 cells with a further grid refinement (64×64 cells) within a distance of 0.5° from each receiver. From synthetic experiments, this grid parameterization provided a good compromise between ray path accuracy and computation time. Similarly to Bodin *et al.* [3], we assume traveltime uncertainties to be proportional to source-receiver distance: $\sigma_i = a \times d_i + b$, where σ_i is the standard deviation of the data noise along ray path i , d_i is the source-to-receiver length of ray path i (here defined as the *actual* length of ray path i), and a and b are hyperparameters that are also varied and hence estimated during the inversion.

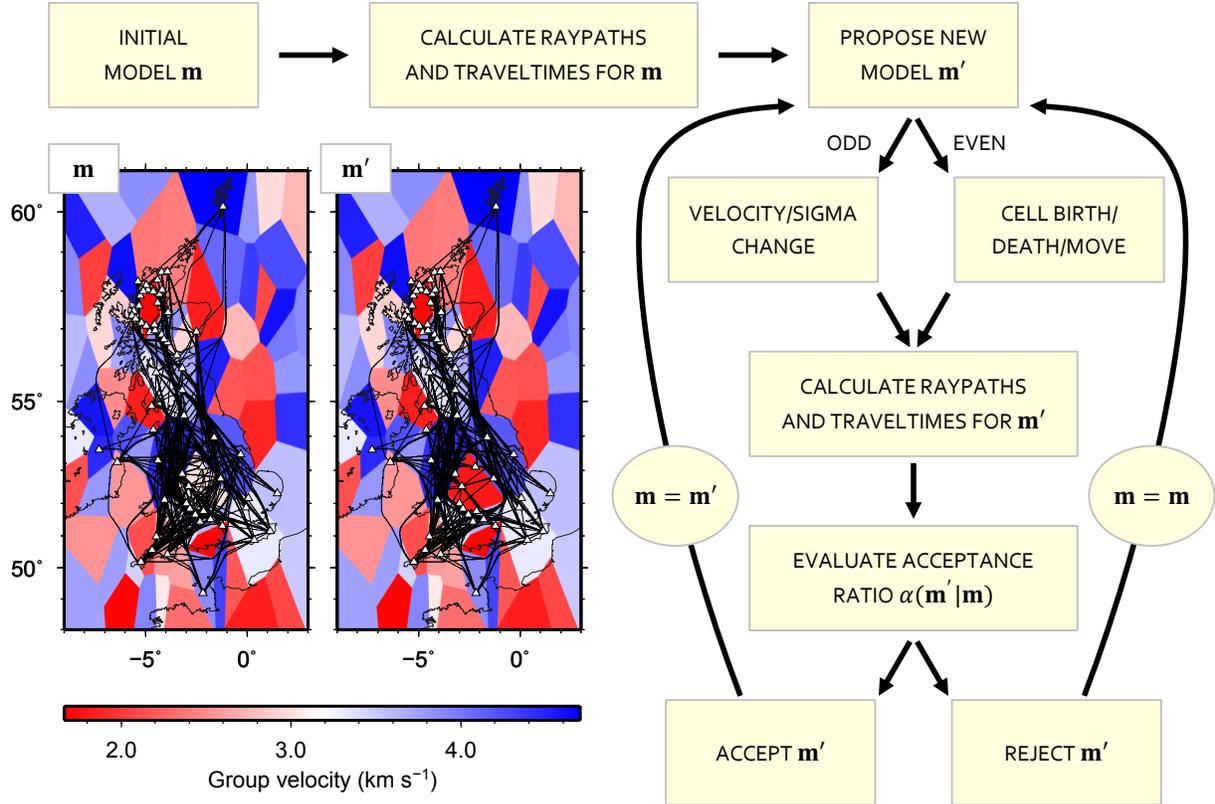


FIG. S1. Workflow of the transdimensional rj-McMC algorithm. This samples the model space by producing an ensemble of Voronoi tessellated models distributed according to the Bayesian posterior probability distribution. For each proposed model, the correct ray paths and traveltimes are calculated and used in the calculation of the likelihood by updating the entire ray geometry. Note how the ray geometry may change dramatically from \mathbf{m} to \mathbf{m}' if one of the model parameters (in this case the velocity value of the cell centred near -2.5°E , 52.5°N) is changed.

* E-mail: erica.galetti@ed.ac.uk

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