Estimation of Three-Dimensional Basin Boundary Shape Using a Random Search Method

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SUMMARY:
Waveform inversion is an effective way to construct the deep subsurface structure that can reproduce the observed seismic waveform. A waveform inversion method for estimating the layer interfaces of three-dimensional (3D) sedimentary basins was proposed by Aoi (2002), in which the inverse problem is quasi-linearized on the assumption of weak nonlinearity between the data and model. One of the major difficulties of the inversion method is the nonuniqueness of the solution that is inevitable in such optimization procedures, which can cause problems such as strong dependency on the initial model and failure of convergence. In this study, we formulate the basin topography waveform inversion using a random (Monte Carlo) method. Instead of searching for one best-fitting model by quasi-linearized inversion, we take a global optimization process using a Markov Chain Monte Carlo (MCMC) method, in which the statistical characteristics of the sampled model parameters can be analysed by Bayesian approach.

Keywords: subsurface structure, ground motion simulation, inverse problem, Monte Carlo method

1. INTRODUCTION

In this study, we focus on the sedimentary basins in the deep subsurface structure, or the region between the seismic bedrock and the engineering bedrock. Sedimentary basin structure has strong influence on ground motion because of the drastic changes in medium properties. It is well known that long-period ground motions with large amplitude and long duration are observed during large earthquakes in distant sedimentary basins, which can be several hundreds of kilometres apart from the earthquake sources. Excitation of ground motion inside a sedimentary basin is caused not only by amplification due to soft sediments with low seismic velocities but also by complicated wave propagations due to the two- or three-dimensional lateral variation of the structure.

Subsurface velocity structure models for ground motion prediction are often constructed and calibrated through compiling geological information and data-fitting of various geophysical data, such as reflection/refraction exploration, microtremor observations, etc. (e.g. Koketsu *et al.*, 2009). Meanwhile, waveforms of earthquake ground motion should be an appropriate target of such data-fitting, since the main purpose of constructing velocity structure models is to simulate earthquake ground motion. In other words, waveform inversion is an effective way to calibrate subsurface structure models that can reproduce the observed seismic waveform.

1.1. Quasi-linearized waveform inversion

Aoi (2002) proposed a waveform inversion method for estimating 3D layer interfaces of sedimentary basins, in which the inverse problem is quasi-linearized on the assumption of weak nonlinearity between the data and model. In this method, the observation equation

$$u(\boldsymbol{m}) = u^{\text{obs}} \tag{1.1}$$

is quasi-linearized around the initial model at l-th iteration

$$u(\boldsymbol{m}^l) + \sum_k \frac{\partial u}{\partial m_k} \delta m_k^l \bigg|_{\boldsymbol{m}=\boldsymbol{m}^l} \sim u^{\text{obs}} \tag{1.2}$$

where $\boldsymbol{m}$ is the model parameter vector that defines the topography of the basin boundary (i.e. sediment/bedrock interface), $u(\boldsymbol{m})$ is the synthetic velocity waveform under $\boldsymbol{m}$, u^{obs} is the observed waveform, and k is the counter for the model parameters. The system is iteratively solved for $\delta\boldsymbol{m}^l$ until waveform misfit converges in the least squares sense.

The waveform inversion method is a potentially useful tool to construct or calibrate the deep subsurface velocity structure models worldwide. However, its dependence on the initial model can be a shortage. Since the quasi-linearized inversion process is based on the partial derivative (sensitivity function) of the objective function, it generally converges to a local optimum point. Therefore the initial model should be close enough to the global optimum point; however, appropriate initial model is not always available.

Iwaki and Iwata (2011) applied the quasi-linearized waveform inversion method to real seismic data observed in the Osaka sedimentary basin, Japan. They revised an existent 3D velocity structure model of Osaka basin area, and suggested the high potential of the method for practical uses. They used the velocity structure model by Iwata *et al.* (2008) as an initial model, which is relatively a well-calibrated model for ground motion prediction. In order to demonstrate the dependency of the scheme on the initial model, Iwaki and Aoi (2011) have tried the same waveform inversion under exactly the same condition as Iwaki and Iwata (2011) but with a different initial model that is obviously different from realistic Osaka basin model, and ended up different insufficient result. This experiment revealed its dependency on the initial model.

On the other hand, taking global optimization process, such as Monte Carlo methods, can avoid such difficulties addressed above. Monte Carlo methods are experiments that involve random numbers for solving problems. They are often used in inverse problems to search the global model space. Although they require a larger amount of computation, the inverse process is more robust and it depends less on the initial model.

In this paper, we formulate the basin topography waveform inversion using a Monte Carlo method. Instead of searching for one best-fitting model by quasi-linearized inversion, we take a global optimization process using a Markov Chain Monte Carlo (MCMC) method, in which the statistical characteristics of the sampled model parameters can be analysed by Bayesian approach.

2. INVERSION BY A MONTE CARLO METHOD

2.1. Markov Chain Monte Carlo Method

According to the Bayesian theorem, the solution to an inverse problem $\boldsymbol{d}^{\text{obs}} \approx g(\boldsymbol{m})$ is given by a posterior probability density function (PDF) that is expressed as follows (e.g. Tarantola, 2005)

$$\sigma_M(\boldsymbol{m}) = k\rho_M(\boldsymbol{m})L(\boldsymbol{m}) \tag{2.1}$$

where $\rho_M(\boldsymbol{m})$ is the prior probability density function of the model parameters and $L(\boldsymbol{m})$ is the likelihood function. If a uniform distribution within a model space is assumed for ρ_M, then the posterior PDF is proportional to the likelihood function $L(\boldsymbol{m})$, which measures the waveform fitting between the data and synthetics.

In MCMC method, the models $\{\boldsymbol{m}_1, \boldsymbol{m}_2, \ldots\}$ that form the posterior PDF $\sigma_M(\boldsymbol{m})$ are sampled in order from the model space according to an accept-rejection sampling algorithm. Markov Chain means that the sampling of a model at a step depends on the model sampled at the previous step. Here, we use the Metropolis algorithm (e.g. Tarantola, 2005) as follows:

(1) Let the model $\boldsymbol{m}_i$ at a given step *i*.
(2) Choose $\widetilde{\boldsymbol{m}}$, a candidate of $\boldsymbol{m}_{i+1}$, randomly from a proposal distribution around $\boldsymbol{m}_i$
(3) Take ratio of likelihood $\alpha = L(\widetilde{\boldsymbol{m}})/L(\boldsymbol{m}_i)$.
If $\alpha \geq 1$, then accept the candidate (i.e. $\boldsymbol{m}_{i+1} = \widetilde{\boldsymbol{m}}$). Go to step *i*+1.
If $\alpha < 1$, then take a random number. With probability α, accept the candidate $\boldsymbol{m}_{i+1} = \widetilde{\boldsymbol{m}}$ and go to step *i*+1. With probability $(1-\alpha)$, reject the candidate and go to (2).

The repeating process (1)(2)(3) with sufficient number of steps samples the target distribution $\sigma_M(\boldsymbol{m})$.

2.2. Numerical Test

We perform a preliminary analysis using a virtual basin model as a target in order to examine the applicability of a MCMC method for boundary topography inversion. The waveforms computed from the target model are referred to as "observed waveforms" hereafter.

2.2.1 Settings

The target model is a virtual 3D basin model with irregular boundary shape whose size is 25 km x 20 km and the maximum bedrock depth is 2500 m (Fig. 2.1, left). The MCMC inversion starts with the initial model that has flat floor as shown in Fig. 2.1 (right). The basin is composed of two sedimentary layers surrounded by seismic bedrock. The depth of the top surface of the second sedimentary layer is proportional to that of the bedrock; it is 0.41 times the bedrock depth. The material properties of the structure are listed in Table 1.

Receivers are located on the ground surface with 2.5 km interval as drawn in Fig. 2.2 left. The basin boundary topography is parameterized by 35 nodes distributed with 2.5 km interval as shown in Fig. 2.2 (right). The basin boundary topography, or the distribution of seismic bedrock as a function of space, is expressed in terms of the difference from the initial topography:

$$z(x,y) = z^0(x,y) + \sum_{k=1}^{K} m_k b_k(x,y) \tag{2.2}$$

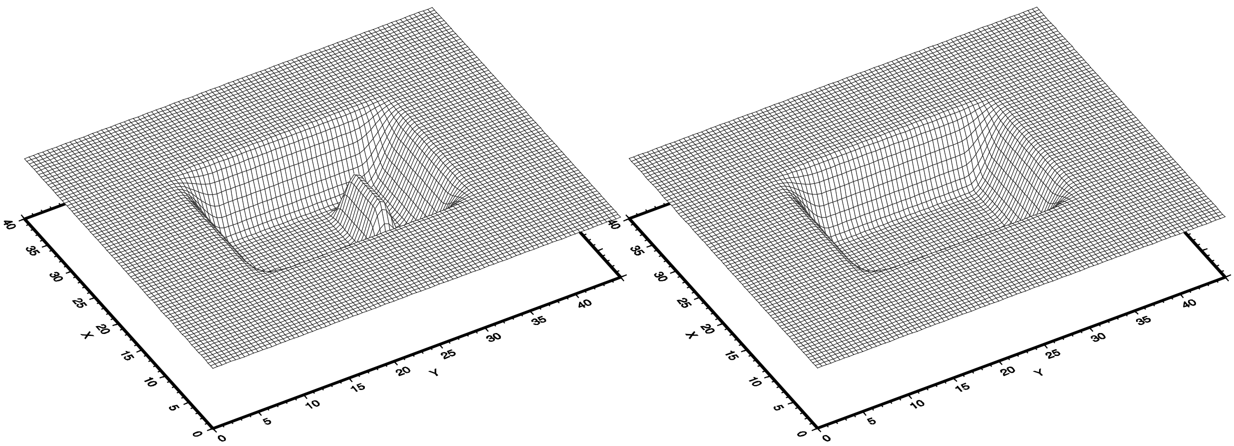
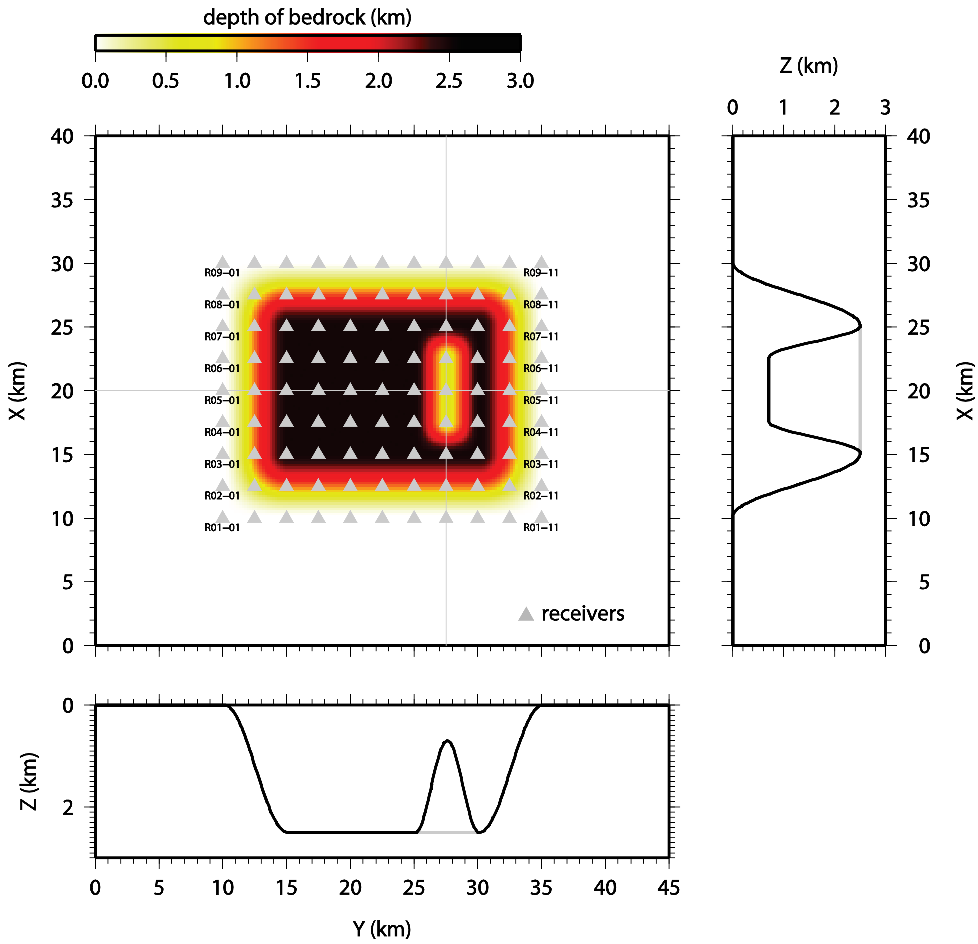


Figure 2.1. Bird's-eye view of the basin boundary topography (i.e. bedrock depth distribution) of the target model (left) and the initial model (right).



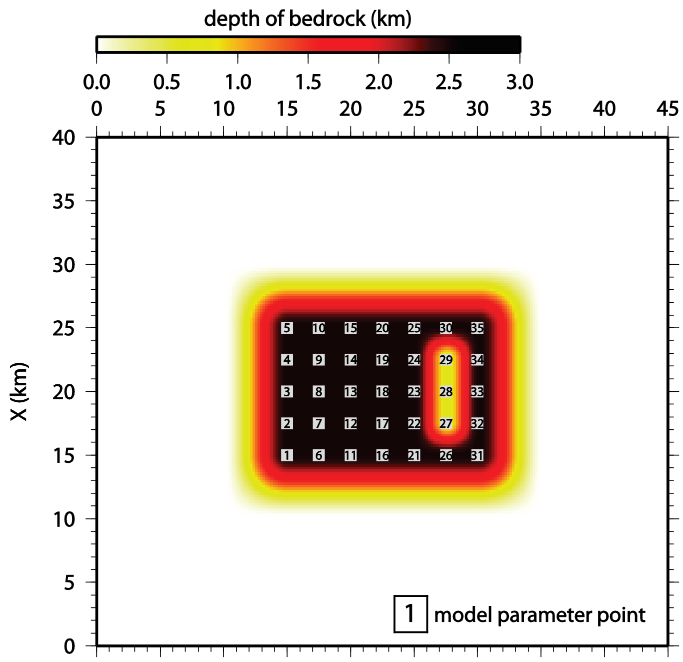


Figure 2.2. Distributions of the receivers denoted by triangles (top) and the model parameter points (nodes) denoted by squares with parameter numbers inside (bottom). The cross section views show the basin boundary topography of the target model (black line) and initial model (gray line).

where $z^0(x,y)$ is the initial depth distribution, K=35 is the number of nodes, m_k, the model parameter, is the change in bedrock depth at k-th node, and $b_k(x,y)$ is the basis function. Note that value of z is positive downwards. The basis function is defined as

$$b_k(x,y) = \begin{cases} \left[\cos\left(\frac{\pi|\boldsymbol{r}-\boldsymbol{r}_k|}{R}\right)+1\right]/2 & \text{if } |\boldsymbol{r}-\boldsymbol{r}_k| \le R \\ 0 & \text{otherwise} \end{cases} \tag{2.3}$$

where $\boldsymbol{r} = (x,y)$ is the position vector, $\boldsymbol{r}_k = (x_k, y_k)$ is the position of k-th node, and R is the interval of the nodes, which is equal to 2.5 km. Schematic view of the expression of the bedrock depth distribution is shown in Fig. 2.3.

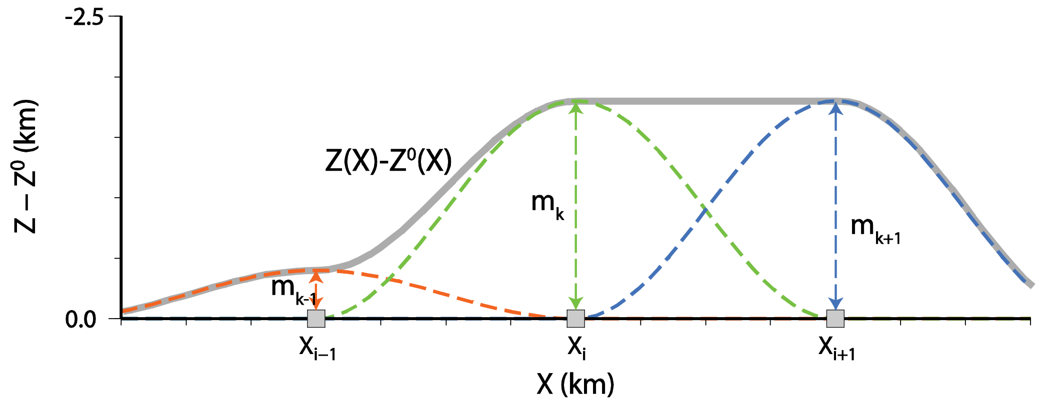


Figure 2.3. Schematic view of the difference in bedrock depths $z - z^0$ (gray line) denoted by equations (2.2) and (2.3). Gray squares on the x-axis denote the nodes, which are apart from each other by R = 2.5 km. The model parameters m_{k-1}, m_k, and m_{k+1} are the differences in bedrock depth from the initial model at the corresponding nodes, which are interpolated by the basis functions b_{k-1}, b_k, b_{k+1} (orange, green, and blue lines, respectively).

Table 1. Material properties of the model.

	V_P (m/s)	V_S (m/s)	ρ (kg/m^3)	Q	Depth (km)
Sediment 1	1800	550	1800	275	–
Sediment 2	2500	1000	2100	500	const × z
Bedrock	5500	3200	2700	500	$z(x,y)$

2.2.2. MCMC Inversion

In MCMC inversion, we sample posterior PDF of the model parameter $\sigma_M(\boldsymbol{m})$ according to the metropolitan algorithm described in subsection 2.1. The prior PDF for model parameter $\rho_M(\boldsymbol{m})$ is assumed to have a uniform distribution between the minimum and maximum values of -0.4 km and +2.2 km, respectively. The acceptance ratio α, or the ratio of likelihood is computed as

$$\alpha = \exp\left[-\frac{1}{2}\left(S(\widetilde{\boldsymbol{m}}) - S(\boldsymbol{m}_i)\right)\right] \tag{2.5}$$

where $S(\boldsymbol{m})$ is the squared difference between the synthetic waveforms computed from the model $\boldsymbol{m}$ and the observed waveforms. The Gaussian distribution with $\sigma = 0.2$ km is assumed as a proposal distribution. The value of σ decides the range from which the candidate model is chosen, and therefore the rate of acceptance or reject.

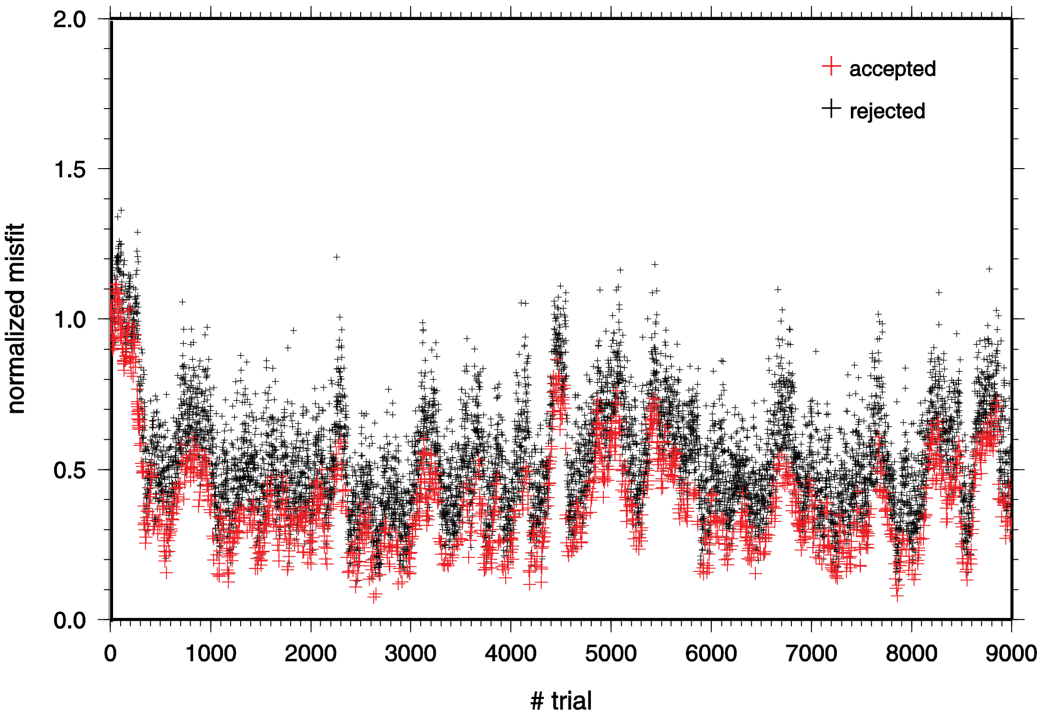


Figure 2.4. Normalized waveform misfit of all the models chosen during the sampling process. The red and black crosses denote the accepted and rejected models, respectively.

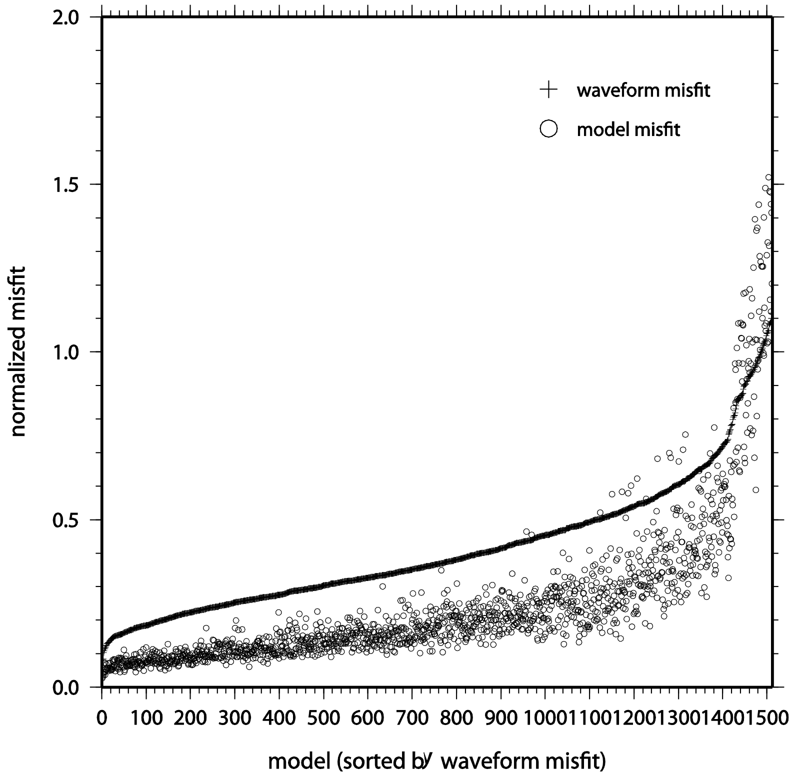


Figure 2.5. Waveform misfit (black crosses) and model misfit (green circles), sorted by the value of waveform misfit in ascending order. Only the accepted models (denoted by red crosses in Fig. 2.4.) are plotted.

Waveforms are computed by the 3D finite-difference method with discontinuous grids by Aoi and Fujiwara (1999) up to 0.33 Hz. The computation area is 40 km by 45 km in horizontal directions and has depth of 18 km. The finest grid spacing is 0.2 km in horizontal directions and 0.1 km in vertical direction.

We tried a total of 9000 models, from which 1513 models are accepted by the accept-rejection algorithm. The waveform misfit values, normalized by that of the initial model, for both the accepted and rejected models are plotted in Fig. 2.4. The waveform misfits of the accepted models are plotted, sorted in ascending order, in Fig. 2.5., together with the model misfit, defined as the squared difference between the bedrock depth of the target and the corresponding model summed over the space. The waveform and model misfits correlate well with each other where the waveform misfit is sufficiently small.

All the accepted model parameters are plotted as probability density in Fig. 2.6. at 35 nodes. The best solution that best represents the target model should be m_k = 1.8 km at k = 27, 28 ,29 and m_k = 0.0 km otherwise. The mean value μ at each node has an acceptable value that is near to the best solution. We constructed the "mean model" by taking the mean value at each node. The basin boundary topography of mean model is drawn Fig. 2.7, which is similar to the target model.

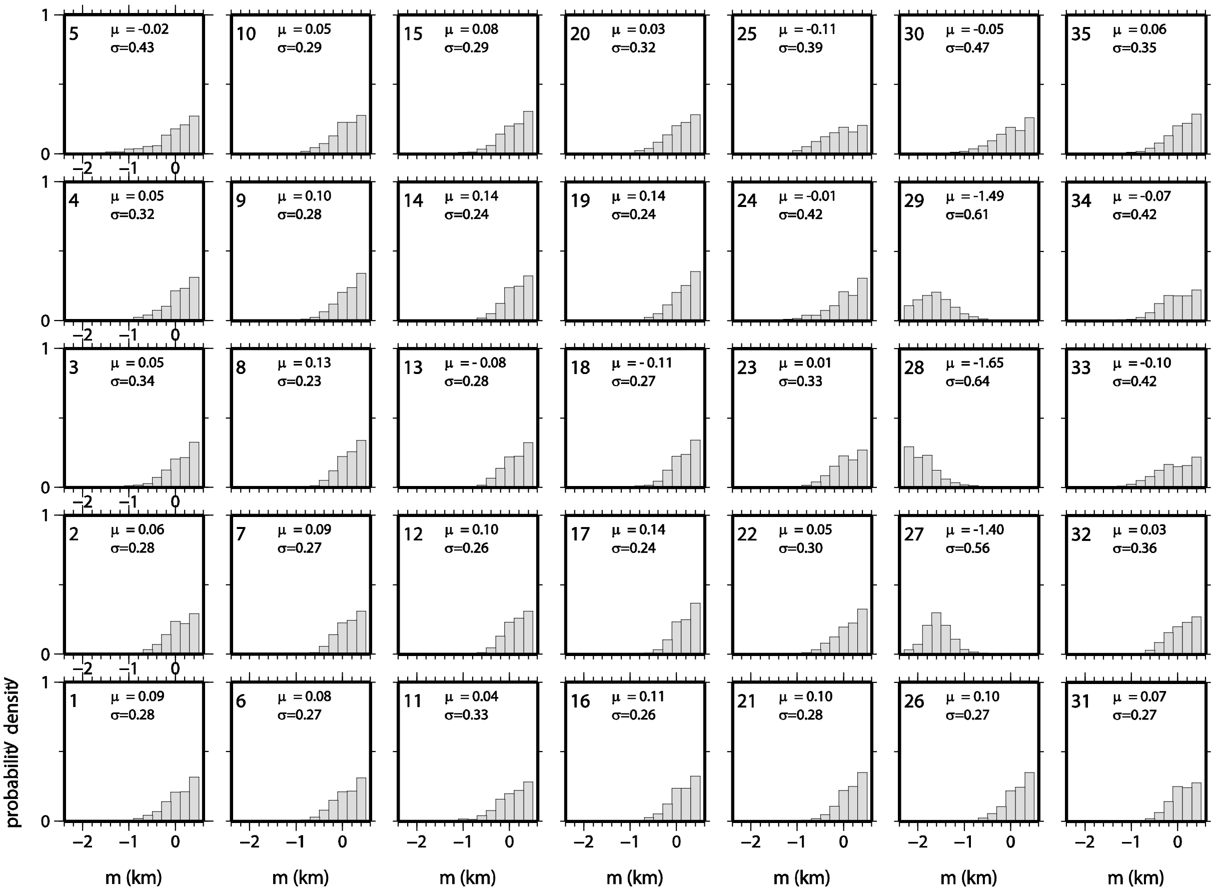


Figure 2.6. Probability density, mean and standard deviation values of the sampled model parameters at each node.

3. CONCLUSIONS

We formulated waveform inversion of the three-dimensional basin boundary topography through fitting of ground motion waveforms recorded inside the basin, using a Markov Chain Monte Carlo (MCMC) method. In order to investigate the applicability of MCMC method to be used in construction of the deep subsurface structure models, we performed a numerical test using a virtual basin model as a target model, from which the virtual observed waveforms are computed. We took the mean and standard deviation of the sampled posterior probability density function of the model parameters, which corresponds to the solution of the inverse problem. We took the mean and standard deviation of the sampled model parameters, and obtained a mean model that is sufficiently close to the target model.

We introduced waveform inversion of 3D basin boundary topography by two ways: one by quasi-linearized inversion as shown by Aoi (2002) and Iwaki and Iwata (2011), and the other by MCMC method described in this paper. Main advantages of MCMC method in construction of subsurface structure models is that: (1) it has weak dependency on the initial model and therefore does not require a well-calibrated model to start with, (2) it provides a solution in the form of probability density function so that its statistical properties can be examined. It is suggested that MCMC inversion can be used to obtain a global optimum solution when only poor initial model is provided, and can be combined with a local search such as quasi-linearized waveform inversion.

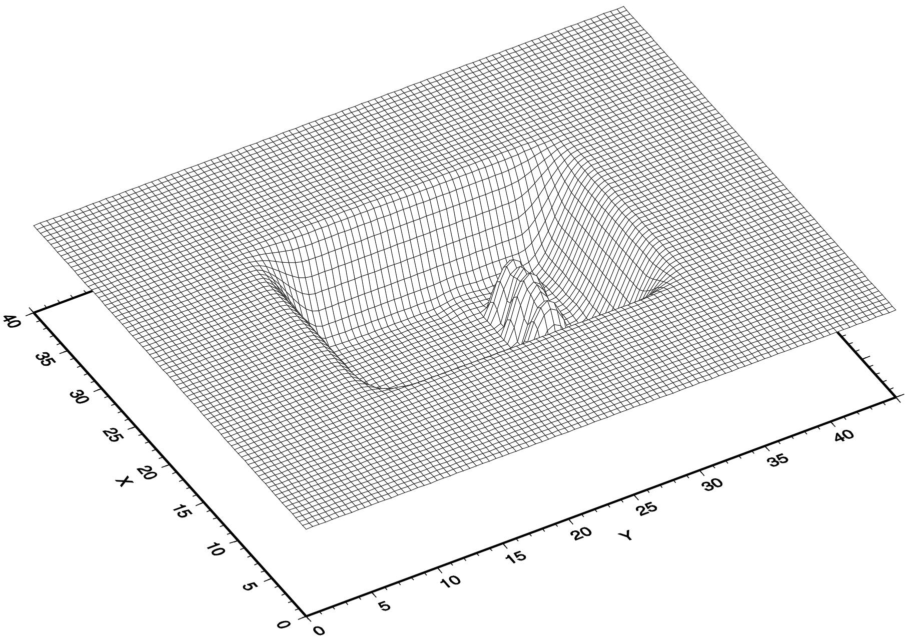


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Figure 2.7. Bird's-eye view of the basin boundary topography of the mean model.

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