Comparison between the Hamiltonian Monte Carlo method and the Metropolis-Hastings method for coseismic fault model estimation

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Research Article

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Posted Date: February 24th, 2022

DOI: <https://doi.org/10.21203/rs.3.rs-1368527/v1>

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Title page:

Full paper

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Abstract

A rapid source fault estimation and quantitative assessment of the uncertainty of the estimated model can elucidate the occurrence mechanism of earthquakes and inform disaster damage mitigation. The Bayesian statistical method that addresses the posterior distribution of unknowns is significant for uncertainty assessment. Particularly, the Metropolis-Hastings (M-H) method, a kind of the Markov chain Monte Carlo (MCMC) method, generally has many applications, including coseismic fault estimation. However, this method exhibits a trade-off between the transition distance and the acceptance ratio of parameter transition candidates and requires a long mixing time, particularly in solving high-dimensional problems. This necessitates a more efficient Bayesian method. In this study, we developed a fault estimation algorithm using the Hamiltonian Monte Carlo (HMC) method, which is generally considered to be more efficient than the other MCMC method but not sufficiently feasible, to estimate the coseismic fault for the first time. HMC can conduct sampling more intelligently with the gradient information of the posterior distribution. We applied our algorithm to the 2016 Kumamoto earthquake (M_j 7.3), and its sampling converged in 2×10^4 chains, including 1×10^3 burn-in chains.

The estimated models satisfactorily accounted for the input data; the variance reduction was approximately 88 %, and the estimated fault parameters and event magnitude were consistent with those reported in previous studies. HMC could acquire similar results using only 2 % of the M-H chains. Moreover, the power spectral density (PSD) of each model parameter's Markov chain showed that this method exhibited a low correlation with the subsequent sample and a long transition distance per step. These results indicate that HMC has advantages in terms of chain length than M-H, expecting a more efficient estimation for a high-dimensional problem that requires a long mixing time or a problem using non-linear Green's function, which has a large computational cost.

Keywords

Hamiltonian Monte Carlo, global navigation satellite system, Markov chain Monte Carlo, real-time GEONET Analysis system for rapid deformation, Bayesian inversion

Main Text

1. Introduction

To minimize earthquake and tsunami damage, the details of the coseismic fault must be estimated rapidly. Surface displacement data supplied by the global navigation satellite system (GNSS) can provide a stable estimation without underestimating the magnitude, considering that the measurement of a seismometer can be saturated when a megathrust occurs (e.g., Ohta et al. 2012). GNSS data are used in the real-time GEONET analysis system for rapid deformation monitoring (REGARD) (Kawamoto et al. 2017), which was jointly developed by the Geospatial Information Authority of Japan and Tohoku University. This system analyzes a GNSS carrier phase in real-time to detect seismic events and automatically and rapidly estimate the fault model. Fault models were automatically estimated, for example, the 2016 Kumamoto earthquake (M_{JMA} 7.3) (Kawamoto et al. 2016), the 2019 Yamagata-Oki earthquake (M_{JMA} 6.7), and the 2021 Fukushima-Oki earthquake (M_{JMA} 7.3). These rapid inferences of REGARD include the slip distribution model on a plate interface in a subduction zone and a single rectangular fault estimation to address non-interplate earthquakes, such as inland and intra-slab earthquakes. The fault models predicted by REGARD were also adopted as part of the

real-time tsunami inundation and damage forecast system operated by the Cabinet Office,
Government of Japan (Musa et al. 2018; Ohta et al. 2018). In other words, it is important
to accurately understand the estimation uncertainty of the estimated fault models to
predict tsunamis and other natural disasters.

For the uncertainty evaluation, a method based on Bayesian statistics is generally used
to solve the inverse problem. This method is used to quantitatively assess the uncertainty
of the prediction using the posterior probability density function (PDF) of model
parameters while explicitly integrating prior information. Amey et al. (2018) applied the
Bayesian inversion method to the inference of the slip distribution in the 2014 Napa
Valley earthquake with self-similarity of the fault slip (Mai and Beroza 2002) as prior
information. In addition, many previous studies have used Bayesian inversion (e.g.,
Sambridge and Mosegaard 2002; Fukuda and Johnson 2008; Dettmer et al. 2014; Ohno
et al. 2022).

In the case of non-interplate earthquakes such as the 2019 Yamagata-Oki earthquake or
the 2008 Iwate-Miyagi Nairiku earthquake (M_{JMA} 7.2), fault geometries are complex or
unknown, and many earthquakes are difficult to assume the fault geometry in advance

(Ohta et al. 2008; Ohno et al. 2021). The assumption of fault geometry required in the slip distribution model can make inferences ambiguous and affect the inferred result (e.g., Fukahata and Wright 2008; Fukuda and Johnson 2010; Duputel et al. 2014; Agata et al. 2021; Dutta et al. 2021).

There are some previous studies which are satisfied the two requirements above, rapid estimation and quantitative uncertainty assessment; for example, Minson et al. (2014) developed a real-time estimation method using Bayesian linear regression including the fault geometry selection with the assessment of its uncertainty and the slip distribution estimation on that geometry. Ohno et al. (2021) also developed Bayesian fault estimation methods that acquire the uncertainty of the fault parameters of a single rectangular fault by directly drawing the PDF using the Markov chain Monte Carlo (MCMC) method. Their method incorporates parallel tempering (Swendsen and Wang 1986; Geyer 1991) and an algorithm to automatically determine hyperparameters for real-time and fully automatic fault estimation.

One of the MCMC sampling methods typically used in the context of Bayesian fault estimation is the Metropolis-Hastings (M-H) method (Metropolis et al. 1953; Hastings

1970). M-H forms a Markov chain based on the judgment of acceptance or rejection depending on the ratio of the posterior distribution between a current parameter set and a transition candidate sampled randomly. Because of its simplicity, this algorithm has been applied to many studies in various fields, including fault estimation. However, M-H exhibits a disadvantageous trade-off relationship between the transition distance of the parameters and the acceptance ratio. In other words, M-H sampling is appropriate to decrease its acceptance ratio in proportion to the transition distance in the parameter space, especially for the sampling after the burn-in. Although the transition distance is often adjusted based on an acceptance ratio of approximately 30–50 %, this low acceptance makes the inference inefficient. Furthermore, with respect to the higher dimensional problems with vast parameter space, the acceptance ratio cannot be improved (the curse of dimensionality), and the transition distance is further shortened. To address the trade-off problem, the M-H method requires a relatively long chain and mixing time.

Considering this problem, we focus on the Hamiltonian Monte Carlo (HMC; Duane et al. 1987) method instead of the M-H method. The HMC method requires a relatively short Markov chain to converge a sampling because this method can transition long distances

while maintaining an acceptance ratio that is nearly 100 % by utilizing the gradient information of the posterior PDF. Fichtner and Simute (2018) applied the weakly nonlinear problem of source point determination and developed an efficient and accurate algorithm. This study also proposed application to higher dimensional problems to capitalize on the efficiency of HMC; in fact, HMC is frequently used in the study of seismic tomography (e.g., Fichtner et al. 2019; Gebraad et al. 2020; Muir and Tkalcic 2020). Nevertheless, HMC has not been applied to fault estimation problems in the past, and its applicability needs to be verified.

In this study, as an application test, we developed an algorithm for a single rectangular fault estimation using HMC. To evaluate its performance, the algorithm was applied to the 2016 Kumamoto earthquake. Furthermore, to examine the estimation accuracy and efficiency of the HMC method, the results were compared with those of the conventional M-H method. We mainly discuss the applicability of HMC to the estimation of earthquake source fault models and briefly discuss the computational time for real-time usage.

2. Method

2.1 Bayes' theorem

Bayesian inversion is based on Bayes' theorem (e.g., Tarantola 2005; Gelman et al. 2021) on a model parameter vector, $\boldsymbol{\theta}$, and a data vector, $\mathbf{d}$, used in estimation.

$$f(\boldsymbol{\theta}|\mathbf{d}) = \frac{f(\boldsymbol{\theta})f(\mathbf{d}|\boldsymbol{\theta})}{f(\mathbf{d})} \quad (1)$$

where $f(\boldsymbol{\theta}|\mathbf{d})$ is the posterior PDF, $f(\boldsymbol{\theta})$ is the prior PDF, $f(\mathbf{d}|\boldsymbol{\theta})$ is the likelihood function, and $f(\mathbf{d})$, which does not depend on the model parameters, is the normalization constant. According to Equation (1), the posterior PDF is proportional to the prior PDF and the likelihood function.

2.2 Sampling method

2.2.1 Hamiltonian Monte Carlo method

We developed a method for single rectangular fault estimation using the HMC method (Duane et al. 1987; Neal 2011) and evaluated its ability in this study. First, in the HMC method, an auxiliary parameter vector $\mathbf{p}$ with the same dimensions as the model

parameter vector, $\boldsymbol{\theta}$, is introduced. Then, the Hamiltonian H is expressed by Equations (2) and (3) in the phase space at position $\boldsymbol{\theta}$ and momentum $\mathbf{p}$.

$$H(\boldsymbol{\theta}, \mathbf{p}) = h(\boldsymbol{\theta}) + \frac{1}{2} \mathbf{p}^T \mathbf{p} \quad (2)$$

$$h(\boldsymbol{\theta}) = -\log(f(\boldsymbol{\theta}|\mathbf{d})) \quad (3)$$

where $h(\boldsymbol{\theta})$ is the potential energy as a function of position $\boldsymbol{\theta}$, and the Hamiltonian H is calculated using the set of $\boldsymbol{\theta}$ and $\mathbf{p}$. Subsequently, the transition in the phase space is performed while keeping the Hamiltonian H constant. In the HMC method, the leapfrog method, a numerical integration method, is used for the simulation because it realizes volume-preservation, time-reversible sampling, and sampling that allows for a detailed balance. The standard procedure for a single step of the leapfrog method is as follows:

$$p_i\left(t + \frac{1}{2}\right) = p_i(t) - \frac{e}{2} \frac{\partial h(\boldsymbol{\theta}(t))}{\partial \theta_i} \quad (4)$$

$$\theta_i(t + 1) = \theta_i(t) + e p_i\left(t + \frac{1}{2}\right) \quad (5)$$

$$p_i(t + 1) = p_i\left(t + \frac{1}{2}\right) - \frac{e}{2} \frac{\partial h(\boldsymbol{\theta}(t + 1))}{\partial \theta_i} \quad (6)$$

161

162 where θ_i and p_i are the i th unknown and auxiliary parameters, respectively, e is the
163 step size, t is the current step number, and L is the total step size. Equations (4)–(6) are
164 iterated from $t = 1$ to L , where L is the total step size of the leapfrog. Furthermore, e
165 and L are hyperparameters, and their initial settings are important for efficient estimation.
166 Subsequently, a numerical error, including the final parameters θ_L and p_L , is evaluated
167 using the acceptance ratio p_{accept} .

168

169
$$p_{accept} = \min(1, r) \quad (7)$$

170
$$r = \exp\left(H(\boldsymbol{\theta}^{(\tau)}, \mathbf{p}^{(\tau)}) - H(\boldsymbol{\theta}^{(\tau')}, \mathbf{p}^{(\tau')})\right) \quad (8)$$

171

172 $(\boldsymbol{\theta}^{(\tau)}, \mathbf{p}^{(\tau)})$ represent the current parameter ($t = 1$ in leapfrog), where τ is the current
173 sample number and $(\boldsymbol{\theta}^{(\tau')}, \mathbf{p}^{(\tau')})$ dose the candidate parameter ($t = L$). In Equation (8),
174 the Hamiltonian is theoretically preserved, and only a small numerical error affects
175 Equation (8); therefore, r is always close to 1, and a high probability of acceptance is
176 realized. Despite the challenge posed by an increase in calculation time, a very small e

is required to decrease the numerical error.

The HMC method enables sampling that transitions a long distance in parameter space with a high acceptance ratio through the above procedure. Generally, this procedure is carried out as follows:

- 1) An initial parameter $(\boldsymbol{\theta}^{(1)})$, total sample size (T), and hyperparameters ϵ and L are set.
- 2) Random numbers are generated from a standard normal distribution and set to $\mathbf{p}^{(\tau)}$.
- 3) Transition from the current point $(\boldsymbol{\theta}^{(\tau)}, \mathbf{p}^{(\tau)})$ to the candidate point $(\boldsymbol{\theta}^{(\tau')}, \mathbf{p}^{(\tau')})$ is performed using the leapfrog method and hyperparameters ϵ and L (Equations (4)–(6)).
- 4) The candidate point is accepted or rejected using the acceptance ratio p_{accept} .
- 5) 2) – 4) are iterated from $\tau = 1$ to T .

Figure 1 shows an example of exploration using the HMC method. As seen in the figure,

HMC acts on the settings where the hyperparameters are $(e, L) = (10^{-3}, 10)$.

2.2.2 No-U-Turn Sampler

The HMC method requires hyperparameters e and L , which have a significant effect on the sampling efficiency. Therefore, optimization is needed to use this method efficiently. If L is too large, the leapfrog will generate "U-Turn" trajectories; therefore, the final transition length can become shorter than the middle one. To solve this problem, we employed the No-U-Turn Sampler (NUTS; Hoffman and Gelman 2014), the extended method of the HMC.

While the usual HMC uses the constant L throughout the sampling, the NUTS does not have the capability to set a constant L value. Instead, the leapfrog transition is terminated based on the detection of "U-Turn". "U-Turn" in phase space defines the shortening of distance Q between a leftmost point, θ^+ , and a rightmost point, θ^- , of leapfrog transition, and then, it is determined using the time derivative of Q .

$$Q = \frac{1}{2}(\theta^+ - \theta^-)^T(\theta^+ - \theta^-) \quad (9)$$

$$\frac{dQ}{d\tau} = (\boldsymbol{\theta}^+ - \boldsymbol{\theta}^-)^T \mathbf{p}^+ < 0 \text{ or } (\boldsymbol{\theta}^+ - \boldsymbol{\theta}^-)^T \mathbf{p}^- < 0 \quad (10)$$

210

211 where the current sample number τ represents the time in the phase space, and
 212 $\mathbf{p}^+$ and $\mathbf{p}^-$ are the momentum at $\boldsymbol{\theta}^+$ and $\boldsymbol{\theta}^-$, respectively.

213 The above method enables the flexible escape of U-Turn, but the arbitrary stop of the
 214 leapfrog breaks the time reversibility. The NUTS algorithm overcomes this issue to
 215 introduce a procedure such as the slice sampling, one of the MCMC methods; this is done
 216 by exploring from the current point $\boldsymbol{\theta}^{(\tau)}$ by building a binary tree to a random time
 217 direction (a sign of ϵ), selecting the candidate state set C based on the condition below,
 218 and eventually selecting the subsequent states from C uniformly.

219

$$C = \{\boldsymbol{\theta}' \mid \boldsymbol{\theta}' \in B \cap H(\boldsymbol{\theta}', \mathbf{p}') < u\} \quad (11)$$

221

222 where B is the set of all the visited state and u is the so-called slice generated as a
 223 uniform random number between 0 and the current posterior probability
 224 $\exp(-H(\boldsymbol{\theta}^{(\tau)}, \mathbf{p}^{(\tau)}))$.

2.2.3 Comparison with Metropolis-Hastings

To verify the accuracy and efficiency of our method, we used the random-walk M-H that was adopted by Ohno et al. (2021) to compare the estimation by the HMC method to that by the M-H method (Metropolis et al. 1953; Hastings 1970), which is often used to solve the geophysical problem (Fukuda and Johnson 2008; Ito et al. 2012; Dettmer et al. 2014; Minson et al. 2014; Ohno et al. 2022). Although Ohno et al. (2021) introduced an automatic determination method for likelihood variance and parallel tempering, we use the same variance value as HMC and estimate using only a single Markov chain for a single parameter to compare both methods strictly. Another part of M-H conforms to that of Ohno et al. (2021).

2.3 Settings of a single rectangular fault estimation

We estimated parameter θ of the single rectangular fault model in Okada (1992) from permanent displacement data $\mathbf{d}$ based on real-time GNSS by the HMC and NUTS algorithms. In this section, we describe the setting of the estimation, such as the prior distribution or likelihood function.

2.3.1 Prior distribution

We prepare a normal distribution as a prior of latitude and longitude and a uniform distribution as a prior of others. We also set a uniform distribution, which is assumed to exclude the fault that has an extreme stress drop value, for the stress drop and the ratio of the fault length and width, which is assumed to have a shorter length than its width, to improve the efficiency of exploration. Table 1 shows all prior distributions.

2.3.2 Likelihood function

The likelihood function is expressed by Equations (12) and (13).

$$f(\mathbf{d}|\boldsymbol{\theta}) = \frac{1}{\sqrt{2\pi\sigma_h^2}^{2N}} \exp\left(\frac{-1}{2\sigma_h^2} \mathbf{r}_h^T \mathbf{r}_h\right) \times \frac{1}{\sqrt{2\pi\sigma_v^2}^N} \exp\left(\frac{-1}{2\sigma_v^2} \mathbf{r}_v^T \mathbf{r}_v\right) \quad (12)$$

$$\mathbf{r}_i = \hat{\mathbf{d}}_i(\boldsymbol{\theta}) - \mathbf{d}_i \quad (13)$$

where N is the number of stations, and $\hat{\mathbf{d}}_i(\boldsymbol{\theta})$ is the surface displacement of model $\boldsymbol{\theta}$ calculated by the method of Okada (1992). Subscripts h and v represent the components of the horizontal and vertical displacements, respectively, and we assumed

that they were independent. Equation (12) is based on the assumption that the residuals, including the model and observational error, follow the normal distribution with mean 0 and variance σ_i^2 .

2.3.3 Change in variables

HMC and NUTS use a gradient of posterior PDF to transition parameters. We observed the gradients of latitude and longitude to be significantly large, except for seven parameters, resulting in the very low efficiency of the exploration. A potential method for correcting the gradients is the application of an adjustment hyperparameter, e , which is the coefficient of the gradient, but parameter e is common; therefore, addressing our case is complicated by the differences among each gradient. Therefore, we applied a change of variables to the seven parameters to change the parameter scale. In addition, certain previous tests have shown that a diminution in exploration efficiency can occur in the area near the parameter's domain boundary, so we adopted log and logit translation as the change of variables to enlarge the definition domain. The depth, fault length, and fault width were applied to log translation (Equation (14)), and the strike, dip, and rake angles

272 were applied to logit (Equation (15)).

273 log translation from $x \in (a, \infty)$ to $x' \in (-\infty, \infty)$:

274
$$x' = \log(x - a) \quad (14)$$

275 logit translation from $x \in (a, b)$ to $x' \in (-\infty, \infty)$:

276
$$x' = \text{logit}(x) = \log\left(\frac{x - a}{b - x}\right) \quad (15)$$

277

278 Equations (14) and (15), for example, $Depth \in (0, \infty)$ is translated to $Depth' =$

279 $\log(Depth)$ and $Strike \in (0, 360)$ to $Strike' = \log\{Strike/(360 - Strike)\}$.

280 These scale changes improve the efficiency of exploration and expand the domain of the

281 parameters. To correct our PDF using the Jacobian formula along with change variables,

282 we estimated the following PDF by adding Jacobian $\mathbf{J}$ (Tarantola 2005; Gelman et al.

283 2021).

284

285
$$f(\boldsymbol{\theta}|\mathbf{d}) = f(\boldsymbol{\theta}) \times f(\mathbf{d}|\boldsymbol{\theta}) \times |\mathbf{J}| \quad (16)$$

286
$$|\mathbf{J}| = e^{Depth'} e^{Length'} e^{Width'} e^{Slip'} \frac{360e^{Strike'}}{(1 + e^{Strike'})^2} \frac{90e^{Dip'}}{(1 + e^{Dip'})^2} \frac{360e^{Rake'}}{(1 + e^{Rake'})^2} \quad (17)$$

287

Note that we set the parameter's domain as $Strike \in (0,360) [^\circ]$, $Dip \in (0,90) [^\circ]$,
and $Rake \in (-180,180) [^\circ]$, respectively.

2.4 Convergence test

In this study, the convergence of each Markov chain was evaluated using two criteria.
First, we confirmed the smoothness of the histograms for each model parameter. Although
it is a subjective perspective, it is required for convenience in later discussions using
statistics such as mode. Second, we utilized the method of convergence decision by
Gelman (1996) for objective judgment. This method can be used to determine the
convergence by comparing a chain's variance between a full chain and a divided one. We
applied this test to all model parameters individually and confirmed their convergence.

If the Markov chain whose length is T excluded burn-in, it is divided into K equal
chains, and T/K length chains are prepared. Then, the following two indices of a chain's
variance are calculated, where $\bar{\theta}$ and $\bar{\theta}_k$ ($k = 1, 2, \dots, K$) are the mean values of a
parameter in the full chain and the k th divided chain, respectively.

$$\text{VAR}_B = \frac{T}{K-1} \sum_{k=1}^K (\bar{\theta}_k - \bar{\theta})^2 \quad (18)$$

$$\text{VAR}_W = \frac{1}{K(T-1)} \sum_{k=1}^K \sum_{t=1}^T (\theta_k^{(t)} - \bar{\theta}_k)^2 \quad (19)$$

Equations (18) and (19) roughly represent the variance among the chains and the average variance of each chain, respectively. Then, the index of a convergence decision using the two indices above is expressed as follows:

$$R = \sqrt{\frac{T-1}{T} + \frac{1}{T} \frac{\text{VAR}_B}{\text{VAR}_W}} \quad (20)$$

The R value is almost 1 on the converged chain; in fact, limitless sampling may yield a converged Markov chain; it is explicit for Equation (20) that the R value converges to 1, where $T \rightarrow \infty$. In this study, the threshold of convergence is given as $R < 1.1$, according to Gelman (1996).

2.5 Data and the setting of hyperparameters

We applied our method to the 2016 Kumamoto earthquake (Mw 7.0), which occurred at 16:25:05 (UTC) in the Kyusyu region, southwestern Japan. The ground displacement data including three components (east-west, north-south, and up-down) were obtained using the REGARD system (Kawamoto et al. 2016) in real-time, and we used the data at 60 s after the mainshock at 200 stations near the source (Figure 2).

Table 2 shows the settings of the hyperparameters in both methods, HMC and M-H estimation. The total step size, L , was optimized in each leapfrog step using the NUTS algorithm explained above. In contrast, the step size of leapfrog e was determined using trial and error. The length of the entire chain was determined using the convergence test explained above, and the length of the burn-in chain was determined by evaluating the trace plot of parameters, especially variance reduction (VR). Figures S1 and S2 show the results of the convergence test and the entire trace plot of each parameter, respectively.

We continued the HMC sampling by 20,000 chains because parameters should satisfy both criteria; nevertheless, these figures indicate the convergence at 6,000 chains. The burn-in chain is often determined using a trace plot of VR or posterior probability (e.g.,

Amey et al. 2018); therefore, we also removed the first 5 % of the chain similarly.

Although the observation error of GNSS may appear to result from the horizontal error

being smaller than the vertical error, we assumed the standard deviation of likelihood, σ_h

and σ_v , representing the same error value, $\sigma_h = \sigma_v = 2\text{cm}$ to simplify the inversion.

Table 2 also shows the hyperparameters in terms of M-H sampling. The entire burn-in

chain length was determined in the same way as the HMC, a factor of 50, compared to

HMC (Figure S1, S2). Note that the M-H method requires other hyperparameters and the

maximum transition size for each parameter.

3. Results

3.1 Expression of posterior probability density functions

For geophysical interpretation, the posterior PDFs regarding the fault parameters are required. However, we can obtain the rescaled PDFs directly using this method because of the change in variables (detailed in 2.3.3). Moreover, the application of log and logit projection, whose Jacobian matrix is complex, for unknown parameters complicates the restoration of their scale. Therefore, we suggest special plotting for log and logit translation that maintains the frequency of each class and inversely changes its upper and lower limits. Then, we can obtain the expected PDFs that represent the correct posterior probability and each parameter scale. The change in appearance following the use of our expression method is shown in Figure S3.

3.2 Results of the application for Kumamoto earthquake

Figure 3 shows the posterior PDFs of each unknown parameter (latitude, longitude, depth, strike, dip, rake angle, fault length, fault width, and slip amount) and certain seismic parameters (moment magnitude (M_w), stress drop and VR) computed for each

sample inferred by HMC and M-H.

The results of HMC in Figure 3 denote a shallow right-lateral fault dipping toward the northwest, and the displacement predictions calculated from each sample are consistent with the data (VR~88 %). The distribution of Mw is a reasonable estimation with a peak of approximately 7.0, which is consistent with previous studies (Asano and Iwata 2016; Kawamoto et al. 2016; Yarai et al. 2016; Tanaka et al. 2019).

Figure 3 shows considerable features that PDFs obtained using HMC accord with by M-H in the shape of PDFs or statistics, nevertheless, both methods estimate independently. This means that HMC can be applied to the single rectangular fault estimation. Conversely, there are a few differences in PDF of depth, it can affect by log translation, which implicitly assumes a non-zero for depth. Its width is extremely narrow, and its statistics are approximately 0. The estimation of VR using HMC is also similar to that using M-H. Therefore, the non-zero assumption with log translation seems to be sufficiently available for a practical application.

For a comparison of the surface deformation, Figure 4 (a) shows the rectangular fault of a mode model (the so-called maximum a posteriori model) solved by HMC, and the

predicted displacement at each station assumed the model with the displacement data we
used. Figure 4 also shows a mode model solved by M-H. As already mentioned, the HMC
mode model adequately explains the displacement data and is consistent with the M-H
model. As illustrated in figure 4 (b), which is drawn using a method proposed by Ohno et
al. (2021), we exhibited the spatial frequency of the fault rectangular. This figure includes
the color scale considering overlaps among the rectangles of each HMC sample on the
map. The HMC models likely contain only a small uncertainty of estimation because the
color scale expands in a significantly narrow region.

4. Discussion

4.1 Comparison of initial exploration

Figure 5 shows the Markov chains of the first 1,000 samples in the HMC and M-H methods. The exploration of HMC can produce estimates that are approximately the same as the final products within 40 chains and a VR of 88 %. In contrast, the trace plots of M-H appear to seek a more optimized solution even at 1,000 chains, and then, approximately 20,000 chains are spent to improve VR (Figure S2). Although we showed only a single case comparing both the methods, our results are important in being able to ensure efficient convergence of HMC, where HMC required less than 1 % chains of M-H's for model exploration. To fully utilize this efficiency, this method should be applied to high-dimensional problems such as slip distribution estimation or inversion using non-linear Green's function, which incurs a high computational cost in one step.

The motion of exploration appearing in trace plots also denotes an obviously high efficiency. The rake angle or slip amount chains using the M-H method initially move in the opposite direction of the final statistics, but the chains using the HMC method directly select the plausible direction. This shows that the HMC method is superior than the M-H

method because of the transition using gradients of the posterior PDF. The chains of latitude or strike denote that even if HMC passes by following the final statistics, a quick return to the same value is expected. It is an interesting exploration tendency showing the ability of the HMC method to explore a wide range of parameters in one step and aim at a minimum posterior immediately. These features cannot be realized by the M-H method, whose transition is performed by adding only a small amount and whose acceptance ratio is generally low.

Figure 6 shows the marginal PDFs appearing in pairs of parameters fault length, fault width and slip amount. The figures using all parameters are shown in Figure S4-S7. Figures 6a (HMC) and 6b (M-H) display the marginal PDFs including the burn-in chains, indicating that the HMC method can reach the high probability area effectively with straight and stepping trace. This method only trace in the plausible area because of the larger white area, which has never been explored, rather than the M-H method. Considering that Figures 6c (HMC) and 6d (M-H) show that the HMC method can generate a similar correlation to the M-H among parameters, and we confirmed the lean sampling of the HMC method.

However, the HMC or other MCMC methods have the problem of ensuring minimum global exploration. One of the methods to certainly and efficiently explore more broadly in parameter space is parallel tempering (e.g., Dosso et al. 2012; Sambridge 2013; Dettmer et al. 2014; Hallo and Gallovič 2020; Ohno et al. 2021,2022). In future work, we will develop a method that introduces this expanding method to the HMC and realize a more efficient and stable fault estimation.

4.2 Comparison regarding the autocorrelation of Markov chains

As mentioned previously, the M-H method conducts the sampling of parameter exploration by slightly perturbing model parameters. In contrast, HMC transitions from place to place and visits plausible samples if they are far away. Given these sampling characteristics, we analyzed the autocorrelation of Markov chains generated by both methods.

Figure 7 shows the power spectral densities of the Markov chain regarded as a time series and its inclination ("a" value in the figure) using log approximation. In this figure, the results of the M-H method explicitly denote the inverse proportion to frequency

432 f [/count] and show random walk tendency; the inclination is roughly f^{-2} . The
 433 inclination in the zone over 1,000 chains appears to be flat, similar to white noise.
 434 Conversely, the results of the HMC method denote an inclination of less than 0.5, and a
 435 white noise-like tendency for almost all parameters. Only the result of the depth parameter
 436 denotes a larger inclination than the HMC's other results, nearly 1.5, although it is slightly
 437 smaller than that of the M-H method. This high autocorrelation is considered to be caused
 438 by the exploration near the domain. Hallo and Gallovič (2020) address similar problems
 439 using the unique prior PDF that is reflected in the parameter domain.

440 Generally, for MCMC sampling, a higher autocorrelation tends to induce deterioration
 441 of sampling efficiency and complicates the achievement of the proper posterior PDFs by
 442 finite-length chains (Geyer 2011). As discussed above, M-H sampling is often highly
 443 correlated between close samples. The thinning method, which discards all but every k th
 444 sampled value, is likely to address this problem (Link and Eaton 2012), but it does not
 445 guarantee improved estimation efficiency (Geyer 2011; Link and Eaton 2012). In addition,
 446 even if we adopt this method to introduce to M-H, we must abandon several thousand
 447 samples for one sample because the PSD analysis shows a high autocorrelation in the

zone over 1,000 chains. Therefore, it is conceivable that the HMC method can efficiently achieve lower autocorrelation sampling without wasting samples.

4.3 More optimized utilization of the HMC

As discussed above, at the point of the number of chains, compared to the M-H method, the HMC method can estimate posterior PDFs more efficiently in the Bayesian analysis of seismic fault estimation. However, the HMC can also be less efficient at the point of the calculation time in general, especially in the case of applying to the problem where one chain's computational cost of the forward calculation is low, such as in our problem.

To reduce the calculation time, a method for optimizing hyperparameter ϵ , which represents the step size of the leapfrog, should be developed. For example, the Stan algorithm (Hoffman and Gelman 2014) employs the dual averaging method developed by Nesterov (2009), a stochastic gradient descent method, which is expected to optimize in the same way as our method does.

In addition to the hyperparameter, the calculation time of the estimation relies on the number of model parameters. It is difficult for the random walk M-H method to conduct

efficient sampling in a parameter space that consists of many parameters because the space is vast and ambiguous for model exploration (Roberts 1998, Ringer 2021). However, as reported by Fichtner and Simute (2018), the HMC method can maintain the calculation time because of the differentiation of the posterior PDF, which contributes to ensuring the transition to the high posterior probability region. Therefore, the HMC can be superior and play an important role in solving high-dimensional problems such as slip distribution estimation or problems that require copious amounts of resources for forward computation.

5. Conclusion

We developed a fault estimation algorithm using the HMC method; this was the first attempt to use the HMC method for fault estimation. The developed method performs efficiently following the adjustment of each parameter scale by changing the variables, making good use of the log and logit functions. We then applied the developed method to the 2016 Kumamoto earthquake ($M_j 7.3$) and assessed its feasibility for the single rectangular fault estimation and its exploration efficiency through comparison with the M-H method.

We found that the HMC method estimates the informative model that reproduces the observation data and substantially corresponds to the fault model predicted by the M-H method, although both algorithms perform the estimation independently. This indicates that the HMC method can be utilized for the single rectangular fault estimation. The length of the Markov chain required for the HMC sampling was approximately 2 % of that of the M-H method, and the 1 % chains were needed to explore the high VR fault models (VR~88 %). We also clarified that the HMC method works as a low autocorrelation and a long transition in one step, as described by the PSD analysis of

489 Markov chains of each parameter. These results are attributed to the theoretical
490 characteristics of the HMC method, which allows for efficient search following the
491 gradient of the posterior distribution. This reasonable HMC sampling appears to be valid
492 for high-dimensional problems such as slip distribution estimation or problems using
493 nonlinear Green's function, which incurs high computational costs for one chain.

494 In contrast, the HMC method requires a longer calculation time for one chain than the
495 M-H method. This indicates that the use of the M-H method is more suitable than that of
496 the HMC for single rectangular fault estimation, a low-dimensional problem. Therefore,
497 the choice between the M-H or HMC methods depends on the cost of forwarding
498 calculation and the number of unknown parameters in the applied problem.

499

Declarations

List of abbreviations

HMC: Hamiltonian Monte Carlo

PDF: Probability Density Function

M-H: Metropolis-Hastings

MCMC: Markov Chain Monte Carlo

REGARD: REal-time GEONET Analysis system for Rapid Deformation

monitoring

GNSS: Global Navigation Satellite System

VR: Variance Reduction

PSD: Power Spectral Density

Availability of data and materials

All 30-s GEONET raw data for post-processing can be obtained via the GSI website. Other data used and/or analyzed in this study are available from the corresponding author upon reasonable request.

516

517 **Competing interests**

518 The authors declare that they have no competing interests.

519

520 **Funding**

521 This work was supported by the JST FOREST Program (grant number:
522 JPMJFR202P, Japan). This study was also supported by the Ministry of
523 Education, Culture, Sports, Science and Technology (MEXT) of Japan, under its
524 “The Second Earthquake and Volcano Hazards Observation and Research”
525 Program (Earthquake and Volcano Hazard Reduction Research) and the Next
526 Generation High-Performance Computing Infrastructures and Applications
527 R&D Program by MEXT. This study was supported by the Japan Society for the
528 Promotion of Science Grant-in-Aid for Scientific Research (KAKENHI; grant:
529 21H05001).

530

531 **Authors' contributions**

TY, KO and YO designed the study, developed the programs, and analyzed the data. All authors read and approved the final manuscript.

Acknowledgements

This work was supported by the JST FOREST Program (grant number: JPMJFR202P, Japan). This study was also supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan, under its “The Second Earthquake and Volcano Hazards Observation and Research” Program (Earthquake and Volcano Hazard Reduction Research) and the Next Generation High-Performance Computing Infrastructures and Applications R&D Program by MEXT. This study was supported by the Japan Society for the Promotion of Science Grant-in-Aid for Scientific Research (KAKENHI; grant: 21H05001).

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687

688 **Table Legends**

689 **Table 1.** Prior parameter for fault parameters and certain calculated parameters. A mean

690 of normal distribution for latitude and longitude is assumed as their initial parameter. A

691 reference point of latitude and longitude is a fault center, and depth is fault top. $N(\mu, \sigma^2)$,

represents a normal distribution with mean μ , variance σ^2 and $U(a, b)$ represents a uniform distribution with a lower limit a and upper limit b .

Table 2. Setting of hyperparameters.

Figure Legends

Figure 1. Example of sampling using the Hamiltonian Monte Carlo (HMC) method. The contours show the constant Hamiltonian and their values. Triangles, circles, and squares show start points, transition points, and endpoints of each leapfrog transition, respectively. The blue triangle particularly represents the initial point of the sampling. In addition, the orange line shows the jump to the next momentum generated by standard normal distribution after acceptance of the candidate point.

Figure 2. Location of stations. A bigger map shows the red rectangular area in a smaller one depicting the whole of Japan. Red triangles represent the 200 GNSS stations for

estimation.

Figure 3. Inferred posterior probability density function (PDF) due to Hamiltonian Monte Carlo (HMC) and Metropolis-Hastings (M-H) estimation. Both results of HMC and M-H are shown by blue and red lines, respectively. Each y-axis represents the frequency of Markov chain Monte Carlo (MCMC) samples written by the same color as histograms. Then the insert values represent statistics (the mean, median, mode, and length of 95 % confidence interval of PDFs from top to bottom) similarly presented in blue or red.

Figure 4. Map view results. (a) Each rectangular denote the mode model; the red and blue ones filled with slanted lines are inferred using M-H and HMC, respectively. In this figure, gray lines show known active faults; black and white arrows show the data and the mode model's horizontal displacements, respectively. Residuals between the data and the model's vertical displacements are also shown in a color scale. (b) The frequency of fault rectangular drawn using each HMC sample. The color scale represents the frequency, whose warm color denotes a region of high frequency, and the region that is not colored

indicates no estimation.

Figure 5. Trace plots of the first 1,000 samples. The chains of nine model parameters (latitude, longitude, depth, strike, dip, rake angle, fault length, fault width, and slip amount) and three calculated parameters (Mw, stress drop, and VR) are shown in each figure. The blue and red solid lines indicate the traces produced by HMC and M-H, respectively. Note that the black broken lines indicate the mode value of full chains produced by HMC.

Figure 6. Two dimensional (2D)-marginal posterior PDFs of the HMC and M-H sampling. Each figure indicates the correlation among part of the fault parameters (fault length, fault width and slip amount). Upper figures show the marginal PDFs via the HMC (a) and M-H (b) including burn-in exploration whose starting point is indicated by red star. Lower figures also show the marginal PDFs via the HMC (c) and M-H (d) but excluded burn-in samples.

Figure 7. Power spectral density (PSD) of Markov chains of nine model parameters. In

740 each figure, red and blue show the results of M-H and HMC, respectively. The light color
741 line shows PDF and the heavy color line shows the moving average of PDF (the average
742 of 25 points on the right and left side). The result of the log approximation is visually
743 shown by the straight line and its estimated inclination is inserted on the bottom left of
744 each figure(upper red: M-H, lower blue: HMC).

Figures

Figure 1

Example of sampling using the Hamiltonian Monte Carlo (HMC) method. The contours show the constant Hamiltonian and their values. Triangles, circles, and squares show start points, transition points, and endpoints of each leapfrog transition, respectively. The blue triangle particularly represents the initial point of the sampling. In addition, the orange line shows the jump to the next momentum generated by standard normal distribution after acceptance of the candidate point.

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