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Comparison of Markov Chain Monte Carlo and Sequential Monte Carlo inference techniques for calibrating soil parameters in a braced excavation

Comparaison des techniques d'inférence de chaîne de Markov Monte Carlo et de Monte Carlo séquentielle pour étalonner les paramètres du sol dans une excavation avec soutènement

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ABSTRACT: Data assimilation has gained significant attention for the sequential updating of soil parameters, particularly in the context of automatic back-analysis. Compared to traditional manual calibration methods, continuous Bayesian calibration provides a formal approach to merge measured data with model predictions. The performance of two prevalent inference algorithms, namely the Markov chain Monte Carlo (MCMC) and Sequential Monte Carlo (SMC), are compared in back-analyzing the parameters of a synthetic braced excavation problem. Model parameters are sequentially inferred using inclinometer data calculated during a typical excavation project based in London. The accuracy of the MCMC and SMC samplers in inferring the synthetic ground truth is compared systematically. Results reveal that back-analysis using MCMC is better for problems which involve high-dimensionality in the output space, while SMC yields faster inference results, especially in cases which involve a lower dimensional output space. This study demonstrates the effectiveness of the two methods in sequential Bayesian updating and outlines their benefits and limitations in identifying soil parameters for a synthetic problem.

RÉSUMÉ:. L'assimilation de données a suscité beaucoup d'attention pour la mise à jour séquentielle des paramètres du sol, notamment dans le contexte de la rétro-analyse automatique. Comparée aux méthodes traditionnelles de calibrage manuel, la calibration bayésienne continue offre une approche formelle pour fusionner les données mesurées avec les prédictions du modèle. La performance de deux algorithmes d'inférence prévalents, à savoir la chaîne de Markov Monte Carlo (MCMC) et le Monte Carlo séquentiel (SMC), est comparée dans la rétro-analyse des paramètres d'un problème synthétique d'excavation avec soutènement. Les paramètres du modèle sont inférés séquentiellement en utilisant des données d'inclinomètre calculées lors d'un projet d'excavation typique basé à Londres. L'exactitude des échantillonneurs MCMC et SMC dans l'inférence de la vérité synthétique du sol est comparée de manière systématique. Les résultats révèlent que la rétro-analyse utilisant MCMC est meilleure pour les problèmes impliquant une grande dimensionalité dans l'espace de sortie, tandis que SMC donne des résultats d'inférence plus rapides, notamment dans les cas impliquant un espace de sortie de dimension inférieure. Cette étude démontre l'efficacité des deux méthodes dans la mise à jour bayésienne séquentielle et décrit leurs avantages et limites dans l'identification des paramètres du sol pour un problème synthétique.

Keywords: Data assimilation; Bayesian calibration; excavation; MCMC; particle filter.

1 INTRODUCTION

The use of a probabilistic back-analysis or inverse analysis based on field observations in a braced excavation process has been widely reported (e.g. Hsein et al., 2013; Lo and Leung 2019; Jin et al., 2021). Among the different probabilistic inverse methods, such as maximum likelihood, maximum a posteriori and Monte Carlo, Bayesian updating using the entire probability distribution stands out as the most attractive option as it provides a quantitative framework for updating the probability distributions of input parameters. This is achieved by assimilating prior probability distributions with observed data via the likelihood function. However, as many geotechnical projects are carried out in stages, a recursive updating scheme is often formulated to align with the construction stages. Through a sequential Bayesian calibration approach, the updated soil parameters facilitate the predicted wall deflections with improved confidence with each subsequent excavation stage. This process can be repeated at each stage until the construction is complete.

For any problem which employs a Bayesian framework, the posterior distribution cannot typically be calculated analytically and must, therefore, be approximated numerically. In geotechnical engineering, the prevailing approaches used to estimate the posterior distribution are the family of Markov Chain Monte Carlo (MCMC) methods (see Andrieu et al., 2003 and Murakami et al., 2023 for an overview) and the sequential Monte Carlo approach (SMC) (e.g., particle filter). Despite the numerous studies employing either MCMC and SMC for back-analysis, there have been limited attempts to identify the merits of these two popular approaches at solving typical geotechnical problems.

The aims of this study are two-fold: (1) provide an overview on the principles of MCMC and SMC inference approach, (2) based on an artificial multi-stage excavation with known soil parameters as our ground truth values, assess the feasibility and effectiveness of the two sampling approaches in inferring the model parameters.

2 SAMPLING METHODS

The aim of a sampling algorithm is to approximate the posterior $p(z|y)$ for the soil parameters z given observed data y. Efficient sampling methods are a topic of active research, with numerous techniques proposed in the past few years. (see Murphy, 2022). This study will primarily focus on the two prevailing sampling methods, namely, MCMC and SMC. Both methods follow a straightforward Monte Carlo style approach to estimating the posterior: generate s samples from the *t-th* step posterior, $z_t^s \sim p(z_t|y_t)$, and then use these to aggregate any quantity of interest $\mathbb{E}[f|y_t] \approx \frac{1}{S}\sum_{s=1}^{S} f(z_t^s)$ given suitable function *f*. Any desired level of accuracy of the posterior distribution can be achieved by generating a sufficiently large set of samples.

Both MCMC and SMC can be employed in sequential Bayesian inference for soil parameters in excavation. The overall structure of sequential Bayesian inference is illustrated in Figure 1. Throughout the excavation steps, the posterior of the unknown parameters z_t at the current stage t is fed into the inference as prior at the next stage $t+1$. As new observation y_{t+1} become available, new stage parameters z_{t+1} can be updated. Though MCMC and SMC share the common ingredients during the Bayesian inference, there are some fundamental differences in how samples are proposed and weighted.

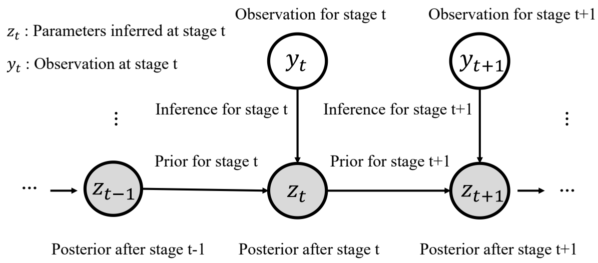

Figure 1. Sequential Bayesian inference for soil parameter.

2.1 Markov Chain Monte Carlo (MCMC)

Markov Chain Monte Carlo (MCMC) algorithms are methods for randomly sampling from an arbitrary distribution based on Markov chains. Different from non-iterative Monte Carlo methods (e.g., rejection sampling or importance sampling), MCMC can build a series of dependent and sequential samples. Instead of drawing samples independently, the samples in the Markov chain depend on the last adjacent sample. Many different MCMC sampling techniques share similar ingredients. For simplicity and clarity, here we take Metropolis–Hastings (MH) algorithm as example, but alternative more effective sampling methods can be also easily implemented.

The basic idea in MH is to define a proposal distribution $q(z_t^{s+1}|z_t^s), s = 1, \ldots, n$, between two adjacent samples from the current sample point z_t^s to the new point z_t^{s+1}. For any given distribution $p(z_t^s)$, we define the acceptance function, which is used to decide whether to accept this move, as follows:

$$f(z_t^{s+1}|z_t^s) = \min(1, \alpha) \quad (1)$$

$$\alpha = \min\left(1, \frac{q(z_t^s|z_t^{s+1})p(z_t^{s+1}|y_t)}{q(z_t^{s+1}|z_t^s)p(z_t^s|y_t)}\right) \quad (2)$$

$$f(z_t^{s+1}|z_t^s) = \min(1, \alpha) = \min\left(1, \frac{p(z_t^{s+1})}{p(z_t^s)}\right) \quad (3)$$

If $\alpha > 1$, which implies $q(z_t^s|z_t^{s+1})p(z_t^{s+1}|y_t) > q(z_t^{s+1}|z_t^s)p(z_t^s|y_t)$, we accept the candidate sampled point from $q(z_t^s|z_t^{s+1})$. If $\alpha < 1$, we accept the candidate point with probability α. A commonly used proposal distribution is Gaussian distribution centered on the current point z_t^s. The acceptance function can be modified as Equation (3). The process of MH sampling is shown in *Algorithm 1*. Typically, convergence improves with the number of paralleled chains and iterative steps used .

In a multi-stage excavation problem, the t-step posterior of the calibrated soil parameters z_t can be readily explored and extracted with paralleled MCMC. Based on these distributions, we can then draw samples for predictive purpose. Additionally, upon acquiring new observations y_{t+1} in the subsequent stage, the $t+1$-step soil parameters z_{t+1} can be updated using obtained samples z_t^s as priors for the next stage, ensuring a continuous calibration for z_{t+1}^s.

2.2 Sequential Monte Carlo (SMC)

SMC, also known as particle filter, is initialized by generating a population of independent particles (each particle corresponding to a possible soil parameter set). It will filter these particles in a way that the final distribution of particles approximates the posterior distribution. This filtering typically consists of three steps: initial samples, weighting, and resampling, which are sequentially applied while a new observation is added.

The recursive filtering process can be treated as a predict-correct step shown in *Algorithm 2*. Each particle generated is assigned a weight, usually proportional to its likelihood $\mathcal{L}(z_t|y_t)$. In the next step, the weights of these particles are reassigned with replacement, with their sampling probabilities given by their normalized weights ω_t^s. This means that particles with low weights (bad fit) tend to be less likely, whereas particles with high weights (good fit) are more likely to be saved. This study adopts a particle filter with sequential importance sampling as described in Nguyen et al. (2014).

Unlike MCMC samplers, where new soil parameter sampling point z_t^{s+1} is generated based on the current z_t^s, SMC sampling points $z_t^{1:s}$ can be processed simultaneously.

Algorithm 1 Metropolis Hastings algorithm at t-th step

Initialize z_t^0;
for $s = 0,1,2,\dots n$ **do**
  Candidate sample $z_t^{s+1} \sim q(z_t^{s+1}|z_t^s)$;
  Compute acceptance probability α;
    Compute $f(z_t^{s+1}|z_t^s) = \min(1,\alpha)$;
  Sample $u \sim U(0,1)$;
  Set new sample to

$$z_t^{s+1} = \begin{cases} z_t^{s+1} & if\ u < f(z_t^{s+1}|z_t^s) \\ z_t^s & if\ u \geq f(z_t^{s+1}|z_t^s) \end{cases}$$

Algorithm 2 Particle filtering

for $s = 1,2,\dots n$ **do**
  Draw $z_t^s \sim q\left(z_t^s|z_{t-1}^s, y_t\right)$;
  Compute weight $\omega_t^s \propto \omega_{t-1}^s \frac{p(y_t|z_t^s)p(z_t^s|z_{t-1}^s)}{q(z_t^s|z_{t-1}^s, y_t)}$;
Normalized weights: $\omega_t^s = \frac{\omega_t^s}{\sum_{s=1}^{S}(\omega_t^s)}$;

3 MODEL SETUP

The ground stratigraphy and construction sequence is modelled based on an excavation project described by Chen (2020). An artificial and symmetric 2D FE excavation model has been set up using Imperial College Finite Element Program (ICFEP). The excavation was modelled using bottom-up construction method in nine stages (with a final excavation depth of 28.9m) with the support of concrete diaphragm walls and steel props. The wall is modelled as a beam element, and the props are modelled as bar elements only accounted for axial force. The soil elements adopt modified Cam Clay model with small strain stiffness model. The soil profile and the excavation depth in each stage are shown in Figure 2. In order of increasing depth below ground level, the soil profile has six layers: made ground, Terrace Deposits, London clay A-3, London clay A2, Lambeth Group Upper Mottled Clay and Lambeth Group Lower Mottled Clay. The excavation width is 27.0m and the extension length for the mesh is 100m to avoid boundary effect. In these analyses, Bayesian updating was employed to determine the best-estimate small-strain stiffness soil parameters, G_0, to replicate measured wall deflection. Details for the model setup and construction stages can be found in Chen (2020) and Fu (2023).

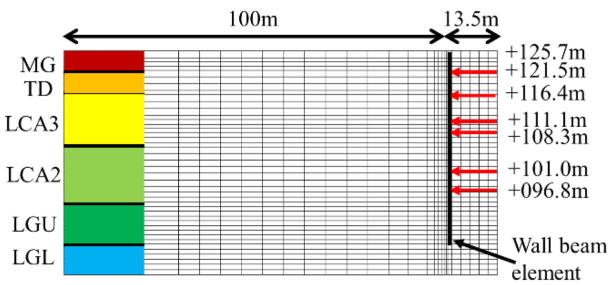

Figure 2. Detailed configurations of the excavation.

As the Bayesian updating process becomes significantly more difficult with increasing number of soil layers and complexity. The number of parameters to be calibrated should be carefully balanced with the amount computational resources available. As this study focuses on the differences of MCMC and SMC samplers in excavations problems, only a smaller number of parameters are treated as random variables in order to preserve the effect of individual soil layers while exploring the influence of the sampling methodology. In order to focus on the ability of the methods to capture the non-linear shear stiffness profile of the soil response, only the maximum shear modulus of each layer, namely G_1 to G_6, is consider. The remaining parameters, such as shear stiffness degradation parameters, limiting stiffness and plastic parameters, are kept constant. Table 1 summarize the soil parameters varied in the analysis. The ranges for the input parameters are deliberately assumed to be very large as to be difficult to back-analyze without prior knowledge of the solution. To establish comparability between MCMC and SMC, the same run outputs were used as the training dataset for both methods. An artificial solution (ground truth) was obtained by adding 3% Gaussian noise to a synthetic run of the simulation with known input values within the prior range. The artificial run is excluded from the training data set, thereby excluding the exact solution from both MCMC and SMC. Differences in the ground truth values between Case A and Case B are a result of the different seeds upon initializing.

Typically, the total number of runs is controlled by the computational time of the FE model, and as such, there are no fixed rules in place. In this study, Latin hypercube sampling is used for a balance approach to draw from the prior distribution. To ensure comparability is achieved between the two methods, emulated outputs are generated using a surrogate model at each stage over the prior range of parameters (experimental design space). The performance of each of the surrogates have been validated with mean square error percentage and are found to have an error of less than 0.1%. It is noted that although a surrogate is not mandatory for SMC updating, it is employed to ensure that the number of particles in SMC are comparable to the number of samples evaluated using MCMC. The use of surrogate model also allows the MCMC resampling scheme to interpolate particles on the fly, without the need for the expensive FE model. For the SMC scheme used in this study, a unique set of emulated particles are evaluated using the surrogate models every stage to replicate the behaviour of a traditional PF scheme.

4 RESULTS AND DISCUSSION

4.1 Case A

To demonstrate the working principles between SMC and MCMC in greater detail, Case A only considers two stiffness input variables. To determine the most appropriate pair of input parameters, sensitivity analysis was performed using Sobol's indices. Results showed that the first-order index for G_3 and G_4 were the greatest among the 6 possible parameters at 66% and 34%, respectively. A simple analysis consisting of only 30 runs was therefore performed with only these two parameters as random variables. Figures 3 and 4 shows the evolving distributions of these two parameters using either MCMC and SMC for the sequence of excavation.

Figures 3(a) and 3(b) illustrate the evolution of the mean value (μ) and the standard deviation (σ) of G_3 and G_4 with respect to the excavation stages. Both SMC and MCMC are shown to reliably converge towards the artificial ground truth. By the final excavation stage, parameters determined by SMC and MCMC result in a root mean square errors of 0.6% and 1.0% respectively.

In SMC method as shown in Figure 4(a)-(c), the underlying principle is to iteratively filter a population of particles with respect to their fit to new observations. The color change in the figure reflects the resampling weight assigned to the particles, which gradually narrows down the confidence range until only a few particles with the highest weight remain. The samples with the red ellipse show the one standard deviation confidence interval ($\mu \pm \sigma$). Practically, the reweighting procedure of SMC is achieved using all the data at once. This non-iterative nature leads to particles being independent of each other. Consequently, it is necessary to generate all potential particles before the updating process. Particle positions therefore remain unchanged during the calibration process, as the updates primarily affect the weights assigned to the particles, rather than the particles themselves.

Unlike SMC, MCMC treats samples from posterior equally and specifies a random walk-in parameter space. Further, the samples in MCMC are not predefined and are constructed in a correlated manner. A uniform distribution is chosen as the non-informative prior, as shown Figure 4(d). As new observation is incorporated, as shown in Figure 4(e), newly generated samples tend to be clustered near the vicinity of the *maximum a posteriori* estimation, while samples in less likely regions will be disregarded during the burn-in process. After multiple stages of random walk and burn-in, corresponding to the construction sequences, a region where the parameters are most likely expected is established.

In terms of computational efficiency, the models were executed on a PC equipped with a 32-core Intel(R) Xeon(R) Silver 4216 CPU @ 2.10GHz and 256GB of memory. SMC, employing 5000 particles, completes the analysis in mere 10 minutes. In contrast, MCMC, with 800 steps and 30 chains, takes over 30 minutes to achieve the same results.

From the comparison, we can see that in a low dimensional problem, the main differences between the two methods is in the speed at which stable confident estimate is achieved. It is shown that, the SMC approach is substantially quicker than the MCMC approach at a achieving a unique solution.

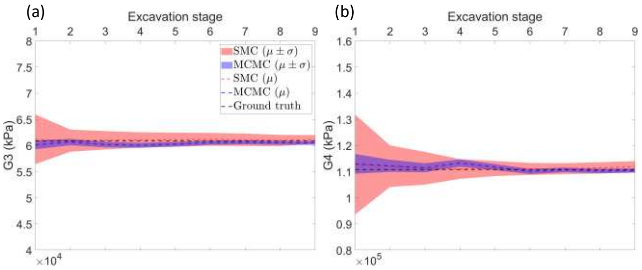

Figure 3. Summary for SMC and MCMC with excavation stages (a) G_3 parameter (b) G_4 parameter.

4.2 Case B

In Case B, the performance of MCMC and SMC is compared for a problem with a higher-dimensional input space; this problem now involves six soil parameters as outlined in Table 1. Sensitivity analysis reveals that G_2 (17.3%), G_3 (76.3%), and G_4 (2.6%) are the most influential variables among the 6 parameters. In this study, despite the importance of a few, all parameters from G_1 to G_6 are recognised to increase the complexity of the inference process. Figure 5 summarizes the mean (μ) and one standard deviation (σ) confidence range for both MCMC and SMC as excavation progresses through various stages. Notably, G_1, G_5, and G_6 struggle to approximate the ground truth due to their low Sobol's indices.

As shown in Figures 5(b)-5(d), both MCMC and SMC initially exhibit wider result spreads at the beginning of the analysis, which gradually narrow as excavation progresses. While SMC yields a smaller variance, MCMC proves more adept at exploring samples in high-dimensional spaces. As shown in Figures 5(b)-5(d), as we acquire new observational data, the posterior distribution obtained through MCMC effectively encompasses the true underlying information. In contrast, SMC does not converge to the same ground truth and demonstrates a more pronounced bias.

5 CONCLUSIONS

This study conducted a comparative analysis of the performance of Markov Chain Monte Carlo (MCMC) and Sequential Monte Carlo (SMC) methods for calibrating soil parameters in the context of an artificial braced excavation. Both methods demonstrated their effectiveness in updating soil parameters, particularly in low-dimensional settings.

MCMC, with its random walk approach, showcased its proficiency in exploring high-dimensional parameter spaces, making it a suitable choice for complex and multifaceted problems. On the other hand, SMC, with its non-iterative nature, offered the advantage of parallel processing, significantly enhancing computational efficiency. This attribute makes SMC a favourable option when quick results are imperative. However, it is crucial to consider that SMC, while delivering rapid outcomes, might exhibit a narrower variance in results and may not guarantee the same level of accuracy as MCMC in high-dimensional scenarios. Therefore, the choice between these methods should be guided by the specific needs and priorities of the analysis, whether precision or computational efficiency takes precedence.

CODE AVAILABILITY

Sampling methods for Markov Chain Monte Carlo and Sequential Monte Carlo are both based on MATLAB software. MCMC is performed using an open-source toolbox UQLAB available at https://www.uqlab.com/. SMC is available at https://github.com/luan-th-nguyen/ParticleFilter.

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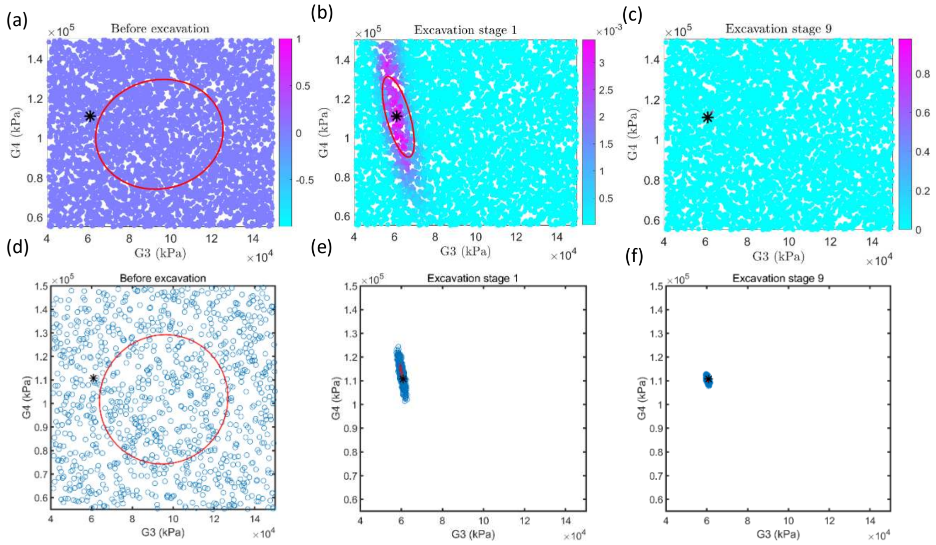

Figure 4. Bayesian Calibration of SMC and MCMC: (a)-(c) for SMC, (d)-(f) for MCMC.

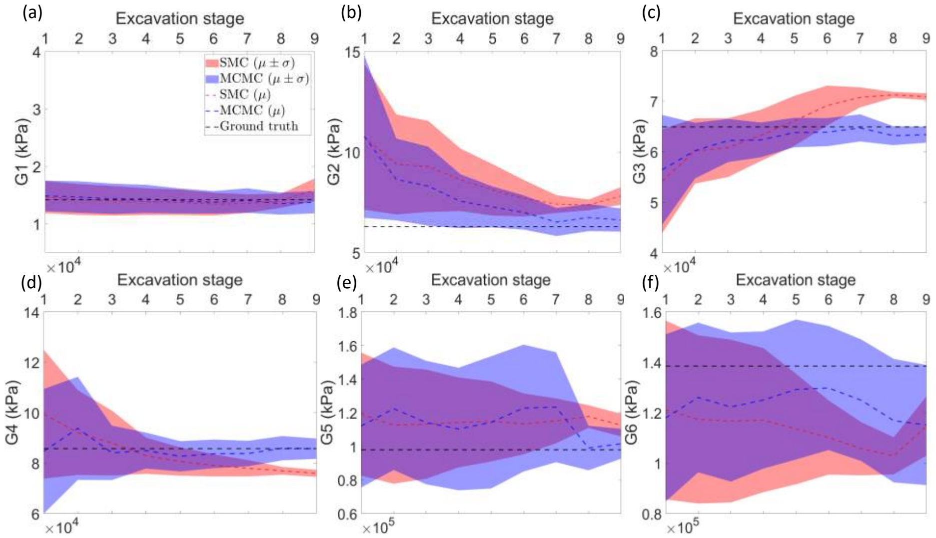

Figure 5. Summary for SMC and MCMC on parameters: (a) G_1, (b) G_2, (c) G_3, (d) G_4, (e) G_5, (f) G_6,.

Table 1. Summary of analysis and soil parameters for calibration.

Case	**Input parameter range (MPa)**		**Ground truth (MPa)**	**Sampler method**	**FE Simulation runs**
A	G_3	38.9-150	60.8	MCMC/SMC	30
	G_4	53.5-150	110.8	MCMC/SMC	
B	G_1	10-20.2	14.213	MCMC/SMC	120
	G_2	53-227.4	62.915	MCMC/SMC	
	G_3	38.9-150	64.906	MCMC/SMC	
	G_4	53.5-150	85.774	MCMC/SMC	
	G_5	55-183	97.856	MCMC/SMC	
	G_6	55-183	138.519	MCMC/SMC	