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# Improved MCMC method for parameter estimation based on marginal probability density function †

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**Abstract**

In many engineering problems, sampling is often used to estimate and quantify the probability distribution of uncertain parameters during the course of Bayesian framework, which is to draw proper samples that follow the probabilistic feature of the parameters. Among numerous approaches, Markov Chain Monte Carlo (MCMC) has gained the most popularity due to its efficiency and wide applicability. The MCMC, however, does not work well in the case of increased parameters and/or high correlations due to the difficulty of finding proper proposal distribution. In this paper, a method employing marginal probability density function (PDF) as a proposal distribution is proposed to overcome these problems. Several engineering problems which are formulated by Bayesian approach are addressed to demonstrate the effectiveness of proposed method.

*Keywords*: Bayesian approach; Marginal PDF; Markov chain monte carlo (MCMC); Parameter estimation; Sampling method

## 1. Introduction

Parameter estimation is often an essential step in many engineering problems such as in the structural analysis at the design stage or in the health management of the existing structures. At the design stage, material parameters of constitutive model, which significantly affect the validity of the numerical simulation, need to be correctly estimated based on the data by direct or indirect measurements. In the health prognosis for the existing structures, degradation parameters of underlying physical model in the deteriorating structures are to be estimated using the monitored data over times to predict remaining useful life (RUL). In the recent times, Bayesian approach has been widely used as a suitable means to quantify the uncertainty of the parameters existent in the estimation process [1, 2]. The Bayesian approach can be summarized as follows: Construct posterior distribution of the unknown parameters based on the observed data which represents our degree of belief. Draw samples that follow the distribution of the parameters. Obtain the posterior predictive distribution of the responses in concern at the unobserved points or at the future time using the drawn samples of the parameters.

In general, the posterior distribution is given by complex or implicit expression in terms of parameters, of which the sample drawing is cumbersome, and prohibiting the use of standard techniques of probability functions. Several methods have been developed in this direction. In the simplest practice, inverse cumulative distribution function (CDF) method is employed to draw samples after computing PDF values at a grid of points over an effective range [3]. This method, however, has drawbacks such as the difficulty in identifying the range, scaling of the grid points and costly computation when the number of parameters increases. The rejection sampling method is to repeat samples's 'acceptance' and 'rejection' by using an arbitrary proposal distribution multiplied by a weight factor [4]. This method cannot produce proper results if the proposal distribution is not wide enough or the weight is too small or too high. More numerous approaches are found in the literatures such as sampling importance resampling (SIR) method [5] and weighted likelihood bootstrap (WLB) method [6]. However, these methods have found only a limited success, and not useful for the practical application.

Recently, Markov Chain Monte Carlo (MCMC) method has been recognized as a computationally effective means in this area, which is based on a Markov chain model of random walk with the stationary distribution being the target distribution [7]. Metropolis-Hastings is the most common form within the variants of the MCMC algorithm. The examples of MCMC approaches are found in diverse fields of engineering, which ranges from the risk assessment [1], model validation

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[8] and parameter estimation [9]. Within the approach, however, proper choice of proposal distribution still remains unclear and the success and failure are significantly affected by this distribution. This was also evidenced by the authors in our recent engineering studies. The algorithm failed due to the difficulty in the design of the proposal density particularly in the cases of increased parameters and high correlations. There have been many attempts to overcome this problem in the statistical literature [10], but the successful results in practice are found rare in the context of engineering application. In this study, an improved robust method is proposed that marginal PDF of each parameter from the joint posterior distribution is employed as a proposal distribution. Since the numerical integration to construct the marginal PDF is computationally expensive, latin hypercube sampling (LHS) is applied to obtain the PDF in discrete manner [11]. Several engineering problems that estimates uncertain parameters based on Bayesian framework are addressed to demonstrate the effectiveness of proposed method.

## 2. Conventional MCMC sampling method

MCMC is a strategy for generating samples using a Markov chain mechanism. Markov chain is a sequence of realizations of a random variable, and the probability of drawing a new value only depends on the realization of the one immediate before it. The Metropolis-Hastings (M-H) algorithm is a typical method of MCMC. In the case of a single parameter, the procedure is given in terms of the pseudo-code:

1. Initialise $x^{(0)}$
2. For $i = 0$ to $nm - 1$
   - Sample $u \sim U_{[0,1]}$
   - Sample $x^* \sim q\left(x^* \mid x^{(i)}\right)$
   - if $u < A\left(x^{(i)}, x^*\right) = \min\left\{1, \dfrac{p\left(x^*\right) q\left(x^{(i)} \mid x^*\right)}{p\left(x^{(i)}\right) q\left(x^* \mid x^{(i)}\right)}\right\}$ (1)

     $x^{(i+1)} = x^*$

   else

     $x^{(i+1)} = x^{(i)}$

where $x^{(0)}$ is the initial value of an unknown parameter to estimate, $nm$ is the number of iterations or samples, $U$ is a uniform distribution, $p(x)$ is the posterior distribution (target PDF), and $q\left(x^* \mid x^{(i)}\right)$ is an arbitrary chosen proposal distribution which is used when a new sample $x^*$ is to be drawn conditional on the current point $x^{(i)}$. Common practice of the proposal distribution is to employ symmetric function, i.e., $q\left(x^{(i)} \mid x^*\right) = q\left(x^* \mid x^{(i)}\right)$. Uniform or Gaussian distribution at the current point with finite length or scale are the most common choices among others. As mentioned before, success and failure of MH algorithm relies heavily on a proper design of the proposal distribution. In order to illustrate this, a target distribution of $x$, which was addressed by Andrieu et al. [7], is revisited as follows.

$$p(x) \propto 0.3\exp\left(-0.2x^2\right) + 0.7\exp\left(-0.2(x-10)^2\right). \tag{2}$$

As candidates of proposal distribution, normal distributions with three different standard deviation, $\sigma = 1$, $\sigma = 10$ and $\sigma = 100$, are employed respectively. The shapes of each distribution are compared in Fig. 1 with the mean located at 5. The MCMC sampling results of each three proposal distributions with $nm = 5000$ are shown in Fig. 2. If the standard

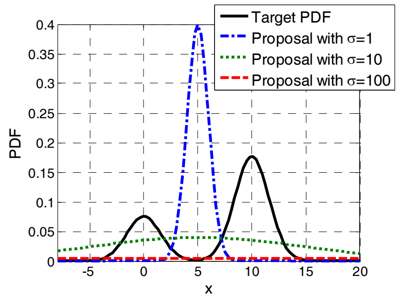
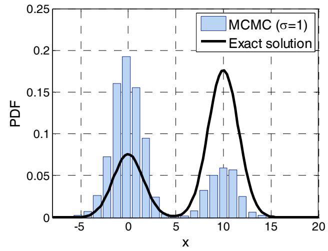
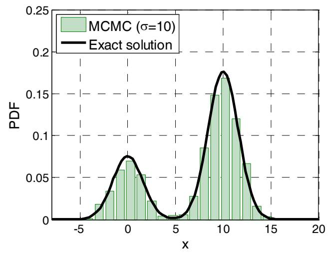


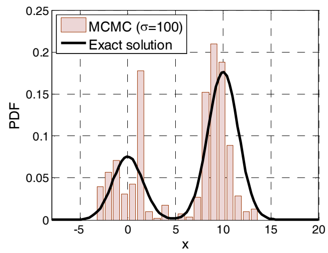

Fig. 1. Target PDF given by Eq. (2) and the proposal PDFs.




(a) When $\sigma$ =1 in the proposal PDF




(b) When $\sigma$ =10 in the proposal PDF




(c) When $\sigma$ =100 in the proposal PDF

Fig. 2. MCMC sampling results of the target PDF given by Eq. (2).

deviation is too small, the proposal distribution does not cover the target PDF well enough. Then the samples are drawn in local region, and the result becomes Fig. 2(a). If the standard deviation is too large, another bad result is obtained like Fig. 2(c) because the rejection rate can be very high. By using proper proposal distribution in between, acceptable result is obtained. This example has illustrated the importance of proposal distribution in the case of single parameter. However, as the number of parameters increase along with the existence of correlation with each other, it is much harder to find out proper scale of proposal distribution that ensures convergent sampling sequence. In fact, the authors have found difficulties with this, and were often unable to obtain adequate samples in our engineering problems.

It is well recognized that assessing convergence of MCMC is a difficult task. Unless the exact solution is available, in this study, the convergence is examined by running MCMC multiple times, from which the trace of Markov chain, histograms and the statistical quantities such as mean and confidence bounds are obtained, and check whether the same result is obtained.

## 3. Improved MCMC sampling method

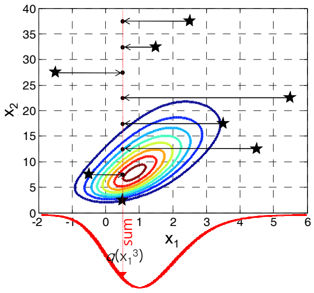
An improved robust MCMC sampling method for multi-dimensional parameters that ensures adequate sampling is proposed in this study, which is to employ a marginal PDF as a proposal distribution. Let us denote the parameters by $\{x_1, x_2, \ldots, x_{np}\}$ with the number of parameters being $np$. The marginal PDF of an arbitrary parameter $x_i$ is defined by the integral of the target joint PDF with respect to all the other parameters except itself, which is given by

$$q(x_i) = \int \cdots \int \int \cdots \int p(x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_{np}) dx_1 \cdots dx_{i-1} dx_{i+1} \cdots dx_{np}. \quad (3)$$

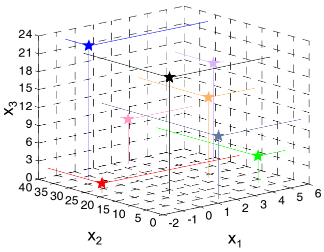
Conventional way to compute this is to assume an effective range for each parameter, divide the range by an equal interval with the number $nl$, and calculate joint PDF at the entire points. Then, at an arbitrary point $x_i^k$, the PDF is given by the following expression.

$$q(x_i^k) \propto \sum_{j_1=1}^{nl} \cdots \sum_{j_{i-1}=1}^{nl} \sum_{j_{i+1}=1}^{nl} \cdots \sum_{j_{np}=1}^{nl} p\left(x_1^{j_1}, \ldots, x_{i-1}^{j_{i-1}}, x_i^k, x_{i+1}^{j_{i+1}}, \ldots, x_{np}^{j_{np}}\right), \quad k = 1, \ldots, nl. \quad (4)$$

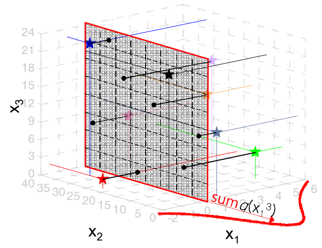
In this approach, the total number of PDF calculations is $nl^{np}$ which becomes computationally expensive as the number of parameters increase. In this paper, a simpler approach, which employs latin hypercube sampling (LHS), is proposed to accommodate efficiency. As an illustration, consider a joint PDF consisting of two parameters $x_1$ and $x_2$ which is repre-



(a) Case of 2 parameters and marginal PDF by LHS method



(b) Case of 3 parameters



(c) Marginal PDF by LHS method

Fig. 3. Illustration of marginal PDF calculation.

sented by contours in Fig. 3(a). Divide both ranges by $nl$ = 8 to obtain $8 \times 8$ = 64 cells, and generate points by the LHS so that only one sample is present at each row and column of the square. The points are indicated by the star marks. Let us compute, for example, the marginal PDF at $x_1$ = 0.5 as in the figure. Conventionally the value can be obtained by summing the PDF values at all the points along the vertical line. In LHS method, the value is summed at the points that have moved from the LHS points with the same $x_2$. The movement is depicted in the figure as arrows. In this 2-D case, which is trivial, both conventional and LHS method are identical albeit explained differently. If the parameters are increased, however, this does not hold as is explained in the case of three parameters. The LHS points are generated in Fig. 3(b) with the number of intervals $nl$ = 8. In order to obtain the marginal PDF value at an arbitrary $x_1$ as is illustrated in Fig. 3(c), conventional method is to sum all the PDF values at $8 \times 8$ = 64 points at the $x_2 - x_3$ plane given by the translucent grey. In the proposed method, however, only 8 points that have moved from the original LHS points with the same $(x_2, x_3)$ are used for the sake of efficiency. Based on this, the marginal PDF of a parameter $x_i$ by the LHS method is given by the following expression.

$$q\left(x_i^k\right) \propto \sum_{j=1}^{nl} p\left(x_1^j,\ldots,x_{i-1}^j,x_i^k,x_{i+1}^j,\ldots,x_{np}^j\right), \quad k=1,\ldots,nl\,. \quad (5)$$

At an arbitrary $x_i^k$, we need $nl$ number of computations, which should be repeated over $k=1,\ldots,nl$. Then we need $nl^2$ computations for a single parameter $x_i$, and $nl^2 \times np$ numbers for the whole parameters, whereas the number is $nl^{np}$ in the conventional method. Comparing these two, the LHS method requires much less computation.

Although demonstrated using a small number $nl$ = 8, the number in practice is often as large as more than ten thousands. For $np$, on the other hand, a few numbers less than 10 are normally considered. In most computing environments, the efficiency can be facilitated by computing all the $nl$ number of PDFs at an arbitrary $x_i^k$ in a single step. Furthermore in practical implementation, the marginal PDF is not computed at every $x_i^k, k=1,\ldots,nl$, which is still too costly. Instead of $nl$, the range of each parameter is divided by much less number $nl_m$ as small as several tens, while all the $nl$ number of PDFs are obtained in a single step as noted above. After all, the total number of computations is reduced to $1 \times nl_m \times np$, which is much more tractable in view of computational efficiency.

The marginal PDF constructed by the LHS method is then employed as a proposal density in order to implement efficient and robust MCMC process. As an illustration, consider following target PDF consisting of two parameters [12].

$$p\left(x_1,x_2\right) \propto \prod_{n=1}^{4} T_n^{B_n}\left(1-T_n\right)^{5-B_n} \quad (6)$$

where

$$T_n = \frac{\exp\left(x_1 + x_2 A_n\right)}{1+\exp\left(x_1 + x_2 A_n\right)},$$
$$A = \left[-0.86,-0.3,-0.05,0.73\right],\ B = \left[0,1,3,5\right].$$

The contours of this PDF is given in Fig. 3(a). The steps of the improved MCMC are explained using this example as follows.

**Step 1: Generate points by the LHS method**

Assuming the number of intervals $nl$ = 8, the generated 8 points are indicated as star marks in Fig. 3(a).

**Step 2: Construct marginal PDF and generate samples**

As was noted earlier, in the two parameters example, there is no difference in constructing the marginal PDF by the LHS and conventional method. Marginal PDFs are obtained over each grid of the parameters using Eq. (5). The resulting PDF shapes for the two parameters $x_1$ and $x_2$ are given in Fig. 4. Once the PDFs are available, samples that follow the marginal PDF can be drawn easily using the inverse CDF method. For more practical illustration, the marginal PDFs are constructed one more time with the number of interval $nl$ = 100 as shown in Fig. 5(a). Due to the large number of intervals, the shapes of the marginal PDFs agree more closely to their exact solutions. Samples can be drawn from each marginal PDF respectively. 5000 numbers of $\left(x_1,x_2\right)$ samples are generated, and the points are superposed with the exact joint PDF in Fig. 5(b). As expected, the result disagrees with the exact PDF because the samples are just obtained from each marginal PDF independently.

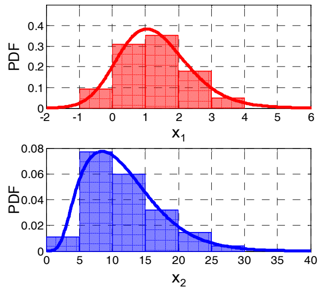
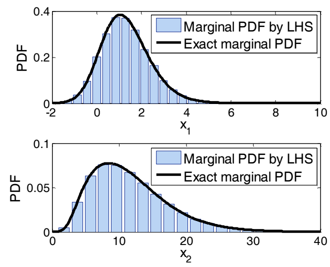
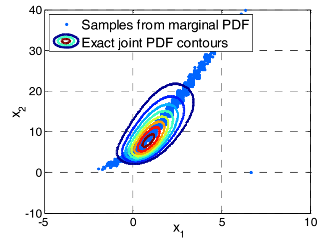



Fig. 4. Marginal PDF illustration in case of $nl$ = 8.




(a) Marginal PDFs




(b) Joint PDF plot

Fig. 5. Marginal PDF in case of $nl$ = 100 and samples from the marginal PDF.

**Step 3: Implement the improved MCMC using the samples of marginal PDF**

As mentioned before, the samples of the marginal PDF are used as the proposal distribution of the MCMC method, that is, a new sample $x^*$ is arbitrarily taken from the samples generated in the step 2. Since the samples distribution follow the marginal PDF as was noticed in Fig. 5(a), the proposal distributions cover the target PDF well enough and much better accept/reject ratio can be expected than any other proposal distributions.

In the improved MCMC, two important points should be remarked. In the conventional MCMC, if the new drawn sample $x^*$ does not satisfy the MH criteria given in Eq. (1), the

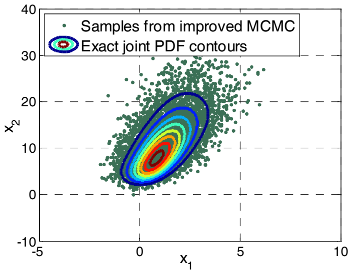



Fig. 6. Sampling result of improved MCMC.

sample is not updated, i.e., the new sample at $i+1$'th step is kept at the previous $i$'th value. In the improved MCMC, however, if the new sample $x^*$ is not accepted, the $i+1$'th sample is not assigned and the sampling is repeated until $i+1$'th sample satisfies the MH criteria. Therefore, the computing time to get the $nm$ number MCMC samples takes longer than the conventional method. The second point is that the uniform distribution, $U_{[0,1]}$ in Eq. (1) is replaced by $U_{[0,c]}$ where $c$ is a constant less than 1. By the authors' experience, it was found that as $c$ gets smaller, the overall time was decreased dramatically, while the obtained samples distribution did not change much. For example, comparing the CPU times with $c$ being 0.2 and 1, the former is found 10 times faster than the latter. In fact, if $c$ becomes less than 1, the acceptance rate increases because new sample $x^*$ having more than $c$ times PDF value comparing to $p\left(x^{(i)}\right)$ always accepted whereas if $c$ is unity the acceptant result depends on the randomness, which results in the increased efficiency. The reason for this efficiency may be attributed to the fact that the marginal PDF that is closer to the target PDF is employed for the proposal distribution. The improved MCMC is summarized in Eq. (7). Compare this with the conventional MCMC in Eq. (1).

$$
\begin{aligned}
&1.\ \text{Initialise } x^{(0)} = mean\left(q(x)\right). \\
&2.\ \text{For } i = 0 \text{ to } nm-1 \\
&\quad -\ \text{Sample } u \sim U_{[0,c]} \\
&\quad -\ \text{Sample } x^* \sim q(x) \\
&\quad -\ \text{if } u < A\left(x^{(i)}, x^*\right) = \min\left\{1, \frac{p(x^*)}{p\left(x^{(i)}\right)}\right\} \\
&\qquad\qquad x^{(i+1)} = x^*,\ i = i+1 \\
&\quad \text{else} \\
&\qquad\qquad i = i
\end{aligned}
\tag{7}
$$

where $q(x)$ is the marginal PDF of $x$. The final sampling results obtained by this method are shown in Fig. 6, which are very close to the exact joint PDF.

## 4. Verification of the improved MCMC sampling method

In this section, the efficiency of the improved MCMC is illustrated by means of several engineering problems that are recently studied by the authors. As our focus is on the discussion of sampling performance in view of engineering application, only a brief outline is given to describe each problem. The results by the proposed method are compared with the conventional MCMC. The process is implemented with the number of LHS $nl$ = 10000 and the number of MCMC iterations $nm$ = 5000 in all the problems. In the conventional MCMC, the uniform distribution with finite length is employed for the proposal density.

Table 1. Tested life data and predicted B1·B10 life of the springs.

| | Test data | | | Predicted life | | |
|---|---|---|---|---|---|---|
| | Actual life 1 | Actual life 2 | Actual life 3 | B1 | B10 | Method |
| Spring type 1 | 1.1438 | 0.8836 | 0.4213 | 0.3087 | 0.4368 | Conv. MCMC |
| | | | | 0.2500 | 0.3674 | Imp. MCMC |
| Spring type 2 | 14.1138 | 9.9230 | 5.3832 | 7.0116 | 9.2448 | Conv. MCMC |
| | | | | 5.1564 | 7.2268 | Imp. MCMC |
| Spring type 3 | 0.2879 | 0.1089 | 0.0954 | 0.0631 | 0.0920 | Conv. MCMC |
| | | | | 0.0543 | 0.0793 | Imp. MCMC |

### *4.1 Three parameters example: spring problem*

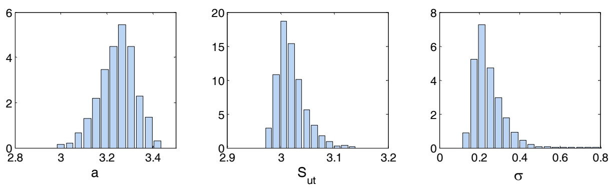
Although the finite element analysis (FEA) is a convenient means to examine the fatigue life of structural parts, it often fails to adequately predict the life due to the inherent uncertainty of the fatigue parameters. By the way, in almost every company, life tests are conducted at the end of the development process for the purpose of quality assurance (QA). Thus, the data are accumulated spontaneously. Motivated by this, a Bayesian procedure to inversely estimate the fatigue-life parameters which utilizes this test data, is developed. The posterior distributions of the parameters are determined conditional on the life data routinely obtained from the QA tests. As more data are accumulated, the degree of uncertainty on the parameters may be further reduced. In this context, a high cycle fatigue problem of a vehicle suspension coil spring is considered [13]. Using the stress-life relation and Goodman formula, the life is predicted by

$$N = \left(\frac{S_a/\left(1 - S_m/S_{ut}\right)}{a}\right)^{1/b} \tag{8}$$

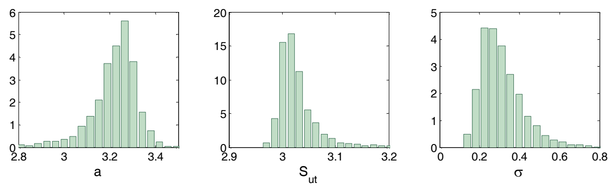
where $a,b$ are the stress-life coefficients, $S_{ut}$ are the ultimate tensile strength, and $S_m$ and $S_a$ are the mean and alternating stresses occurring in the spring during the life test, respectively. For the purpose of illustration, the parameter $b$ is assumed as constant at -0.0725. Then the unknowns are $a$ and $S_{ut}$. Suppose we have total of 9 life test data for the three different springs with the same material as listed in Table 1, which are normalized for convenience. Then the posterior distribution of the unknown parameters is given as follows:

Table 2. Percentile of posterior PDF of three parameters in the spring problem.

| Parameters | Method | Percentile | | | |
|---|---|---|---|---|---|
| | | 5th prctile | median | 95th prctile | 90% C.I. |
| $a$ | Conv. MCMC | 3.1080 | 3.2527 | 3.3703 | 0.2622 |
| | Imp. MCMC | 3.1297 | 3.2454 | 3.3267 | 0.1970 |
| $S_{ut}$ | Conv. MCMC | 2.9855 | 3.0150 | 3.0698 | 0.0843 |
| | Imp. MCMC | 2.9951 | 3.0166 | 3.0598 | 0.0647 |
| σ | Conv. MCMC | 0.1569 | 0.2267 | 0.3821 | 0.2252 |
| | Imp. MCMC | 0.1873 | 0.2811 | 0.4544 | 0.2672 |

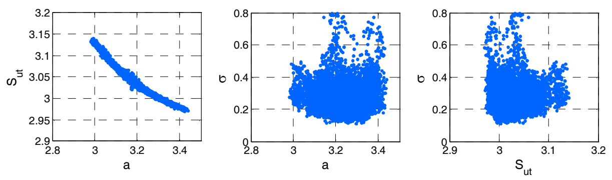



(a) Conventional MCMC

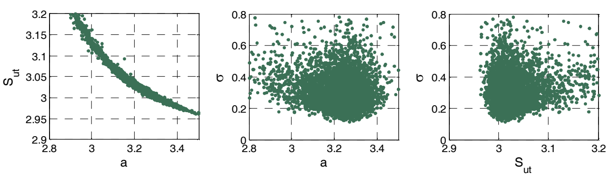



(b) Improved MCMC

Fig. 7. Posterior PDFs of three parameters in the spring problem.




(a) Conventional MCMC



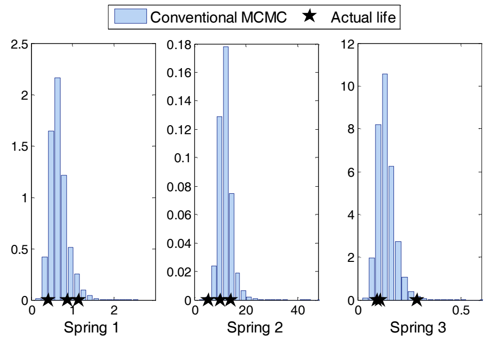

(b) Improved MCMC

Fig. 8. Correlations of three parameters in the spring problem.

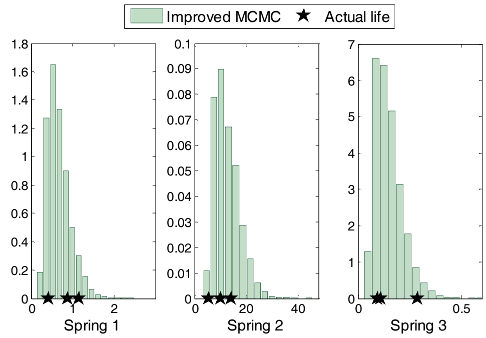
$$p\left(a, S_{ut}, \sigma\right) \propto \sigma^{-11} \exp\left[-\frac{1}{2\sigma^2}\sum_{k=1}^{9}\left(y_k^E - y_k^A\right)^2\right] \quad (9)$$

where $y_k^E$ and $y_k^A$ denote the real life obtained by the test and the predicted life by the FEA respectively. Note that the measurement error $\sigma$ is added to the unknown parameters.

The sampling results of the posterior distribution of the unknown parameters are obtained using the conventional and the




(a) Conventional MCMC



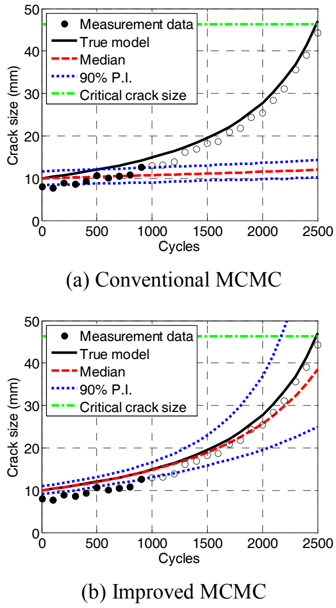

(b) Improved MCMC

Fig. 9. Posterior predictive distribution of fatigue life of the three springs.

improved MCMC. PDF shapes of each parameter and their correlations are given in Figs. 7 and 8, respectively. Percentiles and the confidence interval (C.I.) of the parameters are also listed in Table 2. The posterior predictive distributions of the fatigue life using the obtained samples are given in Fig. 9. Comparing the two results, the PDF shapes are found to agree closely. The correlation feature between $a$ and $S_{ut}$ is also apparent with the same form as shown in Fig. 8. B1 and B10 life are listed in Table 1, in which the two are in modest agreement. It is however remarked that the result by conventional MCMC has been obtained after more than dozens of trial and error with respect to the length of proposal density which is uniform distribution in order to achieve convergence. This has taken more than hours. On the other hand, the improved MCMC produces the same result in just 50 seconds at a single attempt. Moreover, as will be demonstrated in the following problems, the success of conventional MCMC is found only in this problem which is three parameters, and it fails when more than this number. On the other hand, the improved MCMC provides convergent result stably in just a few attempts regardless of the number of parameters.

### *4.2 Four parameters example: crack growth problem*

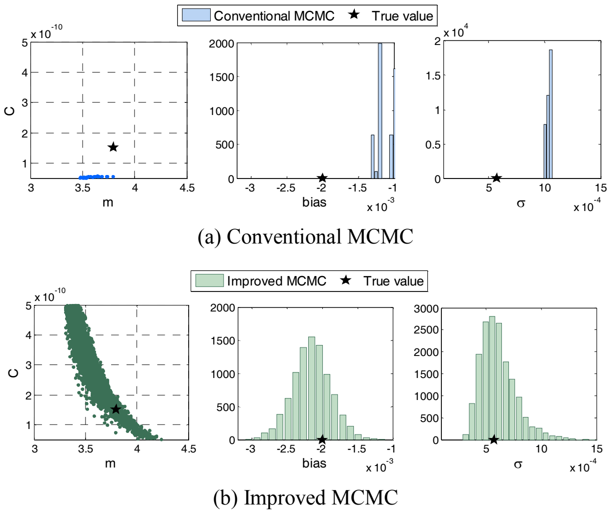
This example is to estimate damage growth parameters in Paris model based on the measured crack size over a number of cycles, which was addressed by Coppe et al. [14]. Due to many uncertainties, the parameters are often widely distrib-




(a) Conventional MCMC

(b) Improved MCMC

Fig. 10. Posterior prediction of the crack growth.




(a) Conventional MCMC

(b) Improved MCMC

Fig. 11. Posterior PDFs of four parameters in the crack growth problem.

uted between nominally identical structures. The Bayesian technique is employed to progressively update the distribution of these parameters. According to the Paris law, the crack size is expressed in terms of the cycle $N$ as

$$a(N)=\left[NC\left(1-\frac{m}{2}\right)\left(\Delta\sigma\sqrt{\pi}\right)^{m}+a_i^{1-\frac{m}{2}}\right]^{\frac{2}{2-m}} \qquad (10)$$

where $C$ and $m$ are the two damage growth parameters that should be estimated, $a_i$ is the initial crack size which is assumed to be known, and $\Delta\sigma$ is the stress range due to the fatigue loading. Assume that we have 10 data set of crack size measurements at a number of different cycles. Then the posterior distribution of the unknown parameters is given by

$$p(m,C,b,\sigma)\propto \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^{10}\exp\left[-\frac{1}{2\sigma^2}\sum_{k=1}^{10}\left(a_{meas_k}-a(N_k)-b\right)^2\right] \times p(m)\times p(C) \qquad (11)$$

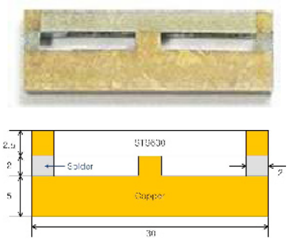
where

$$p(m)=U_{[3.3,4.3]},\ p(C)=U_{\left[\log\left(5\times10^{-11}\right),\log\left(5\times10^{-10}\right)\right]}$$

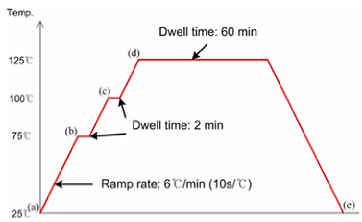
are the prior information of the two parameters. In Eq. (11), two parameters $\sigma$ and $b$ are added to the unknowns, which are the measurement errors due to the noise and bias, respectively. Therefore the number of unknown parameters is four. In this problem, synthetic data is used in order to study the effect of noise and bias. Synthetic measurement data are generated by assuming that the true parameters, $m_{true}$ and $C_{true}$ are known, calculating the true crack sizes according to Eq. (10) for a given $N$, and adding a deterministic bias and random noise intentionally to the true crack data. The true model and synthetic 10 data are plotted as curve and dots in Fig. 10 respectively. The unknown parameters are to be estimated based on this data. Using the conventional MCMC, proper sampling could not be achieved in spite of lot of trials. One instance of such result is given in Fig. 11(a). On the other hand, the result of the improved MCMC is shown in Fig. 11(b), which is obtained in about two minutes at one attempt. The obtained PDF shapes look quite plausible and the correlation between $m$ and $C$ is also identified clearly. The posterior predictive distribution of the crack growth obtained by the sampling results of the unknown parameters is shown in Fig. 10. The solid curve is the true crack growth, the three dashed curves are the median and 90% predictive interval (PI) obtained from the distribution and the green horizontal line denotes critical crack size. As was expected, conventional MCMC fails to predict the growth adequately. On the other hand, the improved MCMC predicts the crack growth quite well, following the true model by correcting the bias.

### *4.3 Five parameters example: solder joint problem*

Last example is to inversely estimate viscoplastic material parameters of the solder joint in microelectronics package. A specimen of solder joint is devised as in Fig. 12(a) so that the joint undergoes similar deformation to the actual package. The specimen is subjected to a thermal cycle given in Fig. 12(b). The deformation is measured using Moire interferometry. Viscoplastic FEA is conducted for the specimen based on the Anand model. The model parameters are inversely determined so that the predicted deformation agrees with the experimental data at five instances of heating and cooling cycle which is depicted in Fig. 12(b). During the procedure, the uncertainties due to the experimental error and insufficient number of experimental data are addressed by using the likelihood estima-



(a) Specimen of solder joint




(b) Thermal cycle

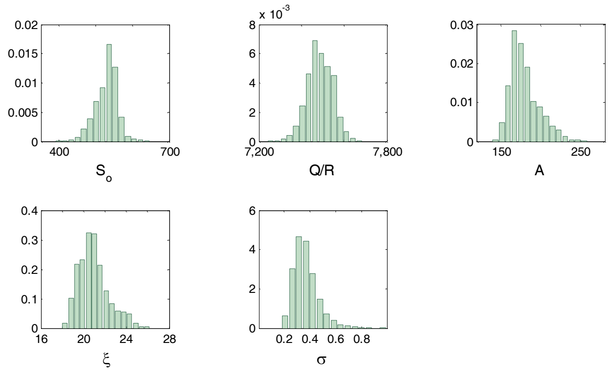
Fig. 12. Illustration of solder joint problem.

tion. Though Anand model requires 9 parameters originally, the number of parameters is reduced to the most influencing 4 after sensitivity study while the others are taken as the constant values. More details can be found in the previous study [15]. After all, the posterior distribution is given as follows:

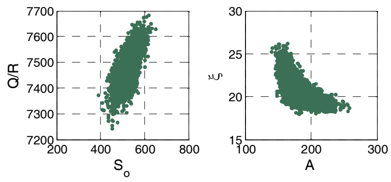
$$p\left(S_0, \frac{Q}{R}, A, \xi, \sigma\right) \propto \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^{13} \exp\left[-\frac{1}{2\sigma^2}\sum_{k=1}^{11}\left(y_k^E - \hat{y}_k^F\right)^2\right] \quad (12)$$

where $S_0, Q/R, A, \xi$ and $\sigma$ are the 4 Anand parameters and the experimental error respectively, which are to be determined based on the measured data. In the equation, $y^E$ and $\hat{y}^F$ denote the displacement of solder obtained by experiment and analytic model respectively. Note that the hat symbol in $\hat{y}^F$ denotes the response surface model that is given by second order polynomial in terms of the four parameters to replace the costly FEA in the process.

The sampling result of the unknown parameters obtained using the improved MCMC, and the PDFs are plotted in Fig. 13(a). Also, the correlations between $S_0$ and $Q/R$ and between $A$ and $\xi$ are identified in Fig. 13(b). The results are obtained in about eight minutes despite the existence of two pairs of complex correlations between the parameters which can make the sample drawing quite difficult. For this problem, the result by the conventional MCMC could not be obtained at all. The posterior predictive distributions obtained by the sampling results are shown Fig. 14. In the figures, the black line with star marks is the experimental result, the blue line with triangle is the FEA result using the material parameters given by Yeo et al. [16], and the red line with circle is the median of the predictive distribution obtained by the improved MCMC. The 90% predictive bounds are also plotted using vertical bars at each instances. From the figures, it is found that the result by the FEA based on the existing literature is quite different from the experimental data. After inversely estimating the material parameters, the median of the predicted distribution gets much closer to the experimental data.

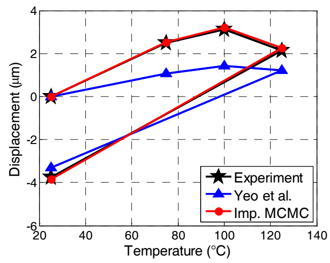



(a) Posterior PDF

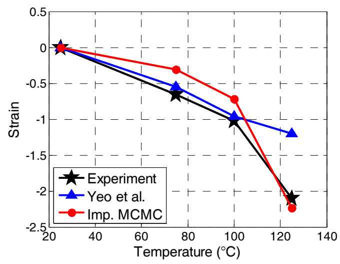



(b) Correlation

Fig. 13. Posterior PDFs and correlations of five parameters in the solder joint problem.




(a) Displacement




(b) Strain

Fig. 14. Posterior prediction of displacement and strain in the solder joint problem.

## 5. Conclusions

Although many sampling methods have been developed, there was no cost-effective and robust method that can handle practical problems in the engineering application. The conventional MCMC is known as the most effective sampling method, but this has also a problem that it does not effectively work if the number of parameters increase and the parameters are highly correlated with each other. In this case, the sampled results vary under different proposal distributions or even the sampling is failed. In order to resolve this issue, an improved MCMC method is proposed by using marginal PDF as a proposal distribution. In this method, additional computation is required for marginal PDF construction before the main MCMC procedure. The computing time increase for this, however, is marginal compared to the whole time of MCMC process. On the contrary, greater efficiency as well as robustness is achieved by this method since we get always convergent samples, i.e., the same samples whenever the method is undertaken, which was not possible using the conventional MCMC. In conclusion, the MCMC in conjunction with the marginal distribution is a very promising approach to tackle the parameter estimation in the case of increased parameters and correlations. The validity of the method is proved by the several practical engineering problems in which adequate samples are obtained for the posterior distribution.

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