Trans-dimensional MCMC for fatigue prognosis model determination, updating, and averaging

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ABSTRACT

In this paper, a general Bayesian framework for fatigue model determination, updating and averaging using trans-dimensional Markov Chain Monte Carlo (MCMC) simulations is presented. Uncertainties introduced by model choice, mechanism modeling, model parameter, and response measures are systematically included. Additional response measures are used to update the model probabilities and the parameter distributions associated with each of the models simultaneously via one trans-dimensional MCMC simulation in the general state space. The averaging of model predictions can readily be performed using the simulation samples. The results of Bayes factors serve as a reference for model comparisons and determinations. To improve the simulation efficiency, we incorporate a new algorithm to construct the dimension matching densities and bijection functions. A fatigue crack growth example with experimental data is presented for methodology demonstration and validation.*

1 INTRODUCTION

Material fatigue crack damage is one of the major failure modes caused by usage and aging in many engineering systems, such as aircraft, bridges, railroads, rotors, and electronic circuit assemblies (Schijve, 2003; Cui, 2002; Fatemi and Yang, 1998; Dimarogonas, 1996; Merchant et al., 1999). For high reliability, the severity of fatigue crack damage must be identified and the remaining useful life should be predicted for safety assessments. Deterministic fatigue crack growth predictions are not appropriate under realistic service conditions due to various uncertainties in the fatigue crack propagation process. These uncertainties include, but may not be limited to, model choice uncertainty, model parameter uncertainty, and response measurement uncertainty. The model choice uncertainty refers to the situations where more than one parameterized mechanism models are available to explain an observable phenomenon. The comparisons and determinations among these models are sometimes required for decision making. For example, several models exist for predicting the fatigue crack growth, such as Paris' equation (Paris & Erdogan, 1960), Forman's equation (Forman *et al.,* 1967), and Newman's crack closure model (Newman, 1981). These models may differ in the number of parameters. For a specific model, the associated parameters also exhibit the statistical uncertainty. Different mechanism models may be valid for specific problems or regimes and the justification of using a particular model is case-dependent. One method for model comparisons and determinations is by computing the *Bayes factor* in a Bayesian hypothesis test context (Jeffreys, 1961). For complex high-dimensional models, the closed form solutions for Bayes factors are not available. Analytical approximations or simulation methods are usually employed to obtain the required accurate results for drawing conclusions. Analytical approximations, such as Laplace's method and its variants can produce accurate answers if the posterior distribution is highly peaked about its mode (Kass & Raftery, 1995). In cases where this condition is not assured, the approximation would fail to represent the distribution. Another possible difficulty in applying Laplace's method in complex Bayesian models is that the computations of

the log-likelihood Hessian are either intractable or too costly to evaluate numerically. Another approximation approach is the numerical simulation, such as the Monte Carlo (MC) simulation. The main issue with the direct MC simulation is the low efficiency for high dimensional problems. Importance sampling technique can improve the efficiency but requires familiarity with the prior and posterior space structures (Tokdar & Kass, 2001; Neal, 2001). A more flexible and efficient simulation method, Markov Chain Monte Carlo (MCMC), is usually adopted (Metropolis *et al.,* 1953; Hastings, 1970). When applying these simulation methods, the marginal likelihood for each of the models requires an individual estimation. Multiple simulations are unavoidable and are computationally expensive. Recent study on MCMC computation with Bayesian model determination includes, but is not limited to, jump diffusion samplers (Grenander & Miller, 1994) and pseudo-prior (Carlin & Chib, 1995). Additional information on analytical and simulation-based approximations of Bayes factors can be found in (Kass & Raftery, 1995). The trans-dimensional MCMC (also referred to as the reversible jump Markov chain Monte Carlo) proposed in (Green, 1995) is a generalized MCMC method across models with variable parameter dimensions. The trans-dimensional MCMC method has been applied to mixture models and it has been shown to be very efficient and flexible to handle variable dimension Bayesian models (Richardson & Green, 1997). One problem with the trans-dimensional MCMC is that the dimension matching densities and bijection functions must be carefully chosen and empirically tuned. Otherwise, the rejection rate may be prohibitively high, restricting the usability of trans-dimensional MCMC methods in general multi-model inference problems (Al-Awadhi *et al.,* 2004).

In this paper, we formulate a Bayesian framework for fatigue model determination, updating and averaging. All the computations are implemented via one trans-dimensional MCMC in the general state space. More than one available mechanism model can be flexibly included in the formulation. Additional crack size measurements are used to update the initial judgment on model choice as well as the parameter distributions associated with each of the models. Bayes factors are readily computed as a reference to select the appropriate models. A new algorithm is developed to construct the dimension matching densities and the bijection functions required in the trans-dimensional MCMC simulations. The paper is organized as follows. First, the framework for model determination, updating, and averaging is formulated using the Bayes theorem. Then, the trans-dimensional MCMC simulation is briefly summarized and a new algorithm to construct the dimension matching densities and the bijection functions is described. Next, we demonstrate the overall procedure using a fatigue crack growth problem and compare the results with experimental data. Following this, a few conclusions are drawn based on the current study.

2 PROBABILISTIC MODELING FOR MODEL DETERMINATION, UPDATING AND AVERAGING

Parameterized mechanism models are developed to describe an observable phenomenon in order to infer its future behavior. Many uncertainties exist in the inference process, such as mechanism modeling uncertainty, model parameter uncertainty, and measurement uncertainty. Bayesian probabilistic modeling is capable of managing these uncertainties hierarchically and performing various belief updates. The Bayesian method is usually associated with a specific model M and it is conditional on the assumption that the model is the correct one which can fully describe the physical phenomenon. For convenience, denote $p(\cdot)$ as the probability density function (PDF) or distribution and $P(\cdot)$ the probability. If several models are possible candidates, the Bayesian joint distribution of an event X using model $M_i^{(k_i)}$ associated with a k_i-dimensional parameter vector $\boldsymbol{\theta}_i^{(k_i)} = (\theta_{i,1}, \theta_{i,2}, \ldots, \theta_{i,k_i})$, $\boldsymbol{\theta}_i^{(k_i)} \in \boldsymbol{\Theta}_i^{(k_i)}$ can be expressed as

$$p(X, \boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)}) = P(M_i^{(k_i)}) p(\boldsymbol{\theta}_i^{(k_i)} | M_i^{(k_i)}) p(X | \boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)}) \quad (1)$$

where $P(M_i^{(k_i)})$ is the prior probability assigned to model $M_i^{(k_i)}$, $p(\boldsymbol{\theta}_i^{(k_i)} | M_i^{(k_i)})$ is the prior PDF of the parameter vector given model $M_i^{(k_i)}$, and $p(X | \boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ is the probability distribution of an event X conditional on the model $M_i^{(k_i)}$ and a specific value of $\boldsymbol{\theta}_i^{(k_i)}$. Equation (1) can be interpreted as the product of model probability, parameter PDF, and the likelihood. The global likelihood of the event X, given model $M_i^{(k_i)}$, can be expressed as Eq. (2) using Bayes theorem.

$$P(X | M_i^{(k_i)}) = \int_{\boldsymbol{\Theta}_i^{(k_i)}} p(\boldsymbol{\theta}_i^{(k_i)} | M_i^{(k_i)}) p(X | \boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)}) \mathrm{d}\boldsymbol{\theta}_i^{(k_i)} \quad (2)$$

Given a finite collection of mechanism models $\boldsymbol{M} = \{M_1^{(k_1)}, M_2^{(k_2)}, \ldots, M_n^{(k_n)}\}$, integrating over each model parameter space $\boldsymbol{\theta}_i^{(k_i)}$ and summing up the entire discrete model space yields the total probability of the event X in Eq. (3)

$$P(X) = \sum_{i=1}^{n} P(M_i^{(k_i)}) P(X|M_i^{(k_i)}) = \sum_{i=1}^{n} P(M_i^{(k_i)}) \int_{\boldsymbol{\Theta}_i^{(k_i)}} p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)}) p(X|\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)}) \mathrm{d}\boldsymbol{\theta}_i^{(k_i)} \quad (3)$$

Applying the Bayes theorem again, we obtain the posterior model probabilities shown as Eq. (4)

$$P(M_i^{(k_i)}|X) = \frac{P(M_i^{(k_i)}) P(X|M_i^{(k_i)})}{P(X)} \quad (4)$$

Rather than computing the posterior probability of model $M_i^{(k_i)}$, it is of more interest to calculate the ratio of probabilities of the two models. The ratio is referred to as the *odds ratio* in a Bayesian context, which is expressed as,

$$O_{i,j} = \frac{P(M_i^{(k_i)}|X)}{P(M_j^{(k_j)}|X)} = \frac{P(M_i^{(k_i)})}{P(M_j^{(k_j)})} \frac{P(X|M_i^{(k_i)})}{P(X|M_j^{(k_j)})} \quad (5)$$

where $P(M_i^{(k_i)})/P(M_j^{(k_j)})$ is the prior odds ratio and $B_{i,j} = P(X|M_i^{(k_i)})/P(X|M_j^{(k_j)})$ is the global likelihood ratio which is also called the Bayes factor. With no prior preference, i.e., $P(M_i^{(k_i)})/P(M_j^{(k_j)}) = 1$, the odds ratio is reduced to the Bayes factor. For complex models with a large number of parameters, direct integral evaluation of Eq. (2) is intractable. Simulation-based methods, such as Markov chain Monte Carlo (MCMC) simulations, are usually adopted. A discrete Markov chain is generated in the parameter space and the expectation of the global likelihood $P(X|M_i^{(k_i)})$ is computed using the samples in the chain. The Bayes factor in favor of one model to another model requires the calculation of the global likelihood of the two models. This calculation is usually computationally intensive if multiple model comparisons are required. On the other hand, rearranging Eq. (1) by treating the model itself as a parameter, we can formulate the Bayesian posterior of $(\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ as Eq. (6), which is defined across models in the general state space $\{\cup_{i=1}^{n} (\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})\}$,

$$p(\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)}|X) = p(M_i^{(k_i)}|X) p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)}, X) \quad (6)$$

The required measure for a move across models with different dimensions is not defined for the standard MCMC simulations. Therefore, the parameter space $\boldsymbol{\theta}_i^{(k_i)}$ has to be fixed to k_i. In order to perform the trans-dimensional moves in the general state space, Green (Green, 1995) proposed a method that formulates the detailed balance equation in the general state space by recasting the transition kernel and treating the number of dimension, i.e., the model itself, as a parameter. In this way, the general Metropolis-Hastings random walk algorithm is applicable across models with variable dimensions and the comparisons between models can be achieved with one simulation instead of multiple simulations.

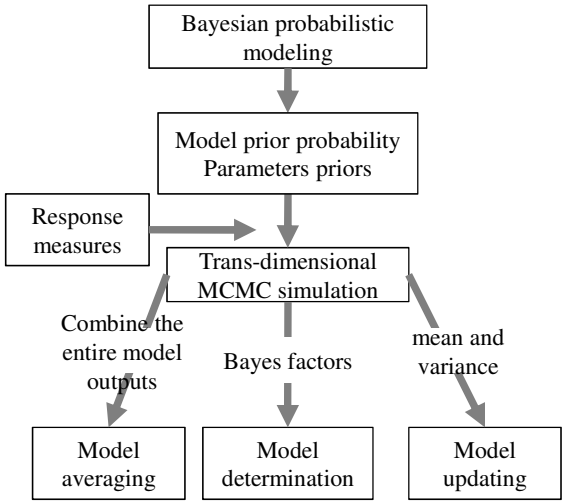

Figure 1: Bayesian model determination, updating and averaging procedure

Combined with the trans-dimensional MCMC simulations, the Bayesian model determination, updating and averaging framework is illustrated in Figure 1. All appropriate mechanism models are probabilistically included by assigning the model probabilities and the parameter PDFs associated with each of the models. These assignments may be based on the empirical judgment or laboratory experiments. When an additional response measure is obtained, the trans-dimensional MCMC simulation generates a discrete Markov chain moving across models in the general state space. The Bayes factor in favor of model $(\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ over model $(\boldsymbol{\theta}_j^{(k_j)}, M_j^{(k_j)})$ is then calculated as the ratio of the number the chain stays in one model $(\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ to another $(\boldsymbol{\theta}_j^{(k_j)}, M_j^{(k_j)})$. For example, suppose a discrete Markov chain with a length of 10,000 is generated in the general state space, and 9,000 samples are in model $(\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ and the rest of 1,000 samples are in model $(\boldsymbol{\theta}_j^{(k_j)}, M_j^{(k_j)})$. The Bayes factor in favor of model $(\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ to model $(\boldsymbol{\theta}_j^{(k_j)}, M_j^{(k_j)})$ is $\sim 9000/1000 = 9$. The derivation of this approximation is shown in Eq. (10). Model probabilities are updated using Eq. (5). The samples of the chain within each of the model candidates are also distributed according to Eq. (7).

$$p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)},X)=\frac{p(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)}|X)}{P(M_i^{(k_i)}|X)} \\ =p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})\frac{P(M_i^{(k_i)})}{P(M_i^{(k_i)}|X)} \tag{7}$$

For a specific model $M_i^{(k_i)}$, the last term of Eq. (7), $P(M_i^{(k_i)})/P(M_i^{(k_i)}|X)$ is a constant, and the samples are distributed according to $\propto p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})$, which is a reproduction of a standard MCMC simulation for model $M_i^{(k_i)}$.

In order to move between two models with different dimensions and maintain the required detailed balance equation, an additional random vector u that matches the difference in the number of dimensions and a corresponding bijection function for the two model coordinates must be designed.

3 MCMC SIMULATION IN THE GENERAL STATE SPACE

In this section, one version of the trans-dimensional MCMC simulations in the general state space is given and a new algorithm is developed to construct the required dimension matching densities and bijection functions automatically.

3.1 MCMC simulations in the general state space

Given an event X, the Bayesian posterior of $(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})$ defined across models in Eq. (6) can be factorized as

$$p(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)}|X) \\ =\frac{p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})p(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})}{\int_{\cup_{i=1}^n\boldsymbol{\Theta}_i^{(k_i)},\boldsymbol{M}}p(\theta_i^{(k_i)},M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})\mathrm{d}(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})} \\ =\frac{P(M_i^{(k_i)})p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})}{\sum_{i=1}^n P(M_i^{(k_i)})\int_{\boldsymbol{\Theta}_i^{(k_i)}}p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})\mathrm{d}\boldsymbol{\theta}_i^{(k_i)}} \\ =\frac{1}{P(X)}P(M_i^{(k_i)})p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)}) \tag{8}$$

For convenience, let i and j denote $(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})$ and $(\boldsymbol{\theta}_j^{(k_j)},M_j^{(k_j)})$, respectively. If the current state (at time t) of the Markov chain S_t is i, one possible version of the trans-dimensional MCMC algorithm is given as follows:

Step 1: Propose a move to j with a probability of $P(i\to j)$. If the proposal is rejected, propose a move within i using a standard MCMC algorithm. Otherwise, continue to step 2.

Step 2: Obtain a sample u from the proposal density $q(u|i,j)$ to match the difference in dimension (u is a vector of size $|k_i-k_j|$).

Step 3: Set the current state in j as $(\boldsymbol{\theta}_j^{(k_j)},u',M_j^{(k_j)})=T_{i\to j}(\boldsymbol{\theta}_i^{(k_i)},u,M_i^{(k_i)})$. $T_{i\to j}$ is a bijection function between two model coordinates $(\boldsymbol{\theta}_i^{(k_i)},u,M_i^{(k_i)})$ and $(\boldsymbol{\theta}_j^{(k_j)},u',M_j^{(k_j)})$

Step 4: Calculate the acceptance probability using the posterior density given in Eq. (8)

$$\alpha_{j,i}= \\ \frac{[P(X)]^{-1}P(M_j^{(k_j)})p(\boldsymbol{\theta}_j^{(k_j)}|M_j^{(k_j)})p(X|\boldsymbol{\theta}_j^{(k_j)},M_j^{(k_j)})}{[P(X)]^{-1}P(M_i^{(k_i)})p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})} \\ \times\frac{P(i\to j)q(u'|i,j)}{P(j\to i)q(u|j,i)}\left|\frac{\partial[T_{i\to j}(\boldsymbol{\theta}_i^{(k_i)},u,M_i^{(k_i)})]}{\partial[\boldsymbol{\theta}_i^{(k_i)},u,M_i^{(k_i)})]}\right| \tag{9}$$

Step 5: generate a random number $\beta\sim U(0,1)$. If $\alpha_{j,i}>\beta$, accept the move from i to j and set the next state $S_{t+1}=j$. Otherwise, reject the move from i to j and set the next state $S_{t+1}=i$.

Looping through Steps 1-5 generates a discrete Markov chain of length L. The global likelihood of model $M_i^{(k_i)}$ is estimated by

$$P(M_i^{(k_i)}|X) \\ =\frac{1}{P(X)}\int_{\boldsymbol{\Theta}_i^{(k_i)}}p(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})p(X|\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})p(\boldsymbol{\theta}_i^{(k_i)}|M)\mathrm{d}\boldsymbol{\theta}_i^{(k_i)} \\ =\frac{1}{P(X)}P(M_i^{(k_i)})p(X|M_i^{(k_i)}) \\ =\frac{1}{L}\sum_{h=1}^{L}1_i(M_h^{(k_h)}) \tag{10}$$

where indicator function $1_i(M_h^{(k_h)})=1$ if $M_i^{(k_i)}=M_h^{(k_h)}$ and zero otherwise. Using this version of trans-dimensional MCMC simulation, the general state space $\{\cup_{i=1}^n(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)})\}$ is explored via the moves across models (according to Eq. (8)). The model parameter space $\boldsymbol{\Theta}_i^{(k_i)}$ is explored via the moves within that model (according to Eq. (7)). The overall structure of the Markov chain can be considered as a primary Markov chain visiting all model candidates $p(\boldsymbol{\theta}_i^{(k_i)},M_i^{(k_i)}|X)$ and a secondary Markov chain moving within each of the models $p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)},X)$.

Despite all the merits of the trans-dimensional MCMC, the dimension matching density $q(u|i,j)$ and the bijection function $T_{i\to j}(\cdot)$ must be carefully chosen for an efficient simulation, particularly in highly parameterized problems. Otherwise, the rejection rates will be prohibitively high. An elaborate design of $q(u|i,j)$ and $T_{i\to j}(\cdot)$ requires the knowledge of the structure of the general state space and empirical tuning, which limit its usability for general problems.

To lessen the difficulty in applying the trans-dimensional MCMC methods, we incorporate a new algorithm to construct the dimension matching densities and the bijection functions automatically. The algorithm is based on the stochastic search mechanisms as detailed next.

3.2 A new algorithm to construct the dimension matching densities and bijection functions

Consider two models $(\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ and $(\boldsymbol{\theta}_j^{(k_j)}, M_j^{(k_j)})$. Without loss of generality, we assume $k_i < k_j$. When the move from i to j is proposed, one additional random vector u of size $k_j - k_i$ has to be generated from $q(u|i,j)$ according to the trans-dimensional MCMC algorithm. Theoretically $q(u|i,j)$ can be any arbitrary PDF. However, $q(u|i,j)$ and $T_{i\to j}(\cdot)$ need to couple well in order to improve the proposal acceptance. For convenience, we use a Gaussian proposal density $u \sim Gauss(0, \sigma_u)$ and this density is independent of $T_{i\to j}(\cdot)$. For example, if $k_j - k_i = 2$, we generate $u = (u_1, u_2)$ according to $u_1 \sim Gauss(0, \sigma_{u_1})$ and $u_2 \sim Gauss(0, \sigma_{u_2})$. Next, we need to construct a suitable $T_{i\to j}(\cdot)$. Starting with one important piece of information on hand, that is the prior PDFs $p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})$ and $p(\boldsymbol{\theta}_j^{(k_j)}|M_j^{(k_j)})$, if the forward and reverse transformations via the bijection $T_{i\to j}(\cdot)$ can concentrate the samples in the region with high probabilities (around the mode of a PDF), the acceptance rate would be relatively high. Suppose the current state of the Markov chain is in i and a move to j is proposed. In order to generate such samples in j, we need a bijection function $T_{i\to j}(\cdot)$ such that after the transformation, the new sample of $(\boldsymbol{\theta}_j^{(k_j)})$ tends to appear around the mode of $p(\boldsymbol{\theta}_j^{(k_j)}|M_j^{(k_j)})$. The transformation should be reversible, that is, if the current state is in j, $q(u|j,i)$ and $T_{j\to i}(\cdot) = T_{i\to j}^{-1}(\cdot)$ can generate a new sample $(\boldsymbol{\theta}_i^{(k_i)})$ around the mode of $p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})$.

Based on the above discussion, we propose an algorithm based on the stochastic search mechanisms. The algorithm is shown in Algorithm 1, where $(\bar{\boldsymbol{\theta}}_i^{(k_i)}, \bar{u})$ is the mode of the dimension matching density $p(\boldsymbol{\theta}_i^{(k_i)}|M_i^{(k_i)})q(u|i,j)$, and $\bar{\boldsymbol{\theta}}_j^{(k_j)}$ is the mode of $p(\boldsymbol{\theta}_j^{(k_j)}|M_j^{(k_j)})$. The basic idea of this algorithm is to randomly generate n matrices based on the initial guess of $T_{i\to j}^{(0)}(\cdot) = [\mathbf{T}^{(0)}]$ and sort them by their performance (norm d), then keep m "outstanding" matrices and use them to update the initial guess of $[\mathbf{T}^{(0)}]$ for the next iteration. The adjustable parameters n and m are used to control the numbers of the generated and reserved matrices. The stopping criteria are chosen based on realistic assumptions. For example, a possible criterion could be that the minimal value of the norm d is less than a specified value. It is worth mentioning that the choice of proposal density for u can be flexibly chosen. Once this choice is fixed, the algorithm ensures the final $T_{i\to j}^{(0)}(\cdot) = [\mathbf{T}^{(0)}]$ will place samples around the modes of the two dimension matching densities. To illustrate the overall methodology, we present a fatigue crack growth problem for demonstration and validation in the next section.

4 A FATIGUE CRACK GROWTH PROBLEM

In this section, the proposed Bayesian framework for model determination, updating and averaging using the trans-dimensional MCMC simulations is demonstrated using a fatigue crack growth problem. Experimental

Algorithm 1: $T_{i\to j}(\cdot)$ construction based on stochastic search mechanism

repeat
  n = 10000, m = 100
  Initiate an array $E[1:\mathrm{n}] = 0$
  Initiate a list $L[1:\mathrm{n}] = NULL$ // store $[\mathbf{T}]$
  for $c = 1$ to N **do**
    $[\mathbf{T}] \leftarrow [\mathbf{T}^{(0)}] + Gauss(0, [\sigma_{\mathbf{T}}])$
    $\boldsymbol{\theta}_j^{(k_j)} \leftarrow [\mathbf{T}](\bar{\boldsymbol{\theta}}_i^{(k_i)}, \bar{u})$ and $(\boldsymbol{\theta}_i^{(k_i)}, u) \leftarrow [\mathbf{T}^{-1}](\bar{\boldsymbol{\theta}}_j^{(k_j)})$
    compute the norm $\mathrm{d} = |(\boldsymbol{\theta}_i^{(k_i)}, u) - (\bar{\boldsymbol{\theta}}_i^{(k_i)}, \bar{u})| + |\boldsymbol{\theta}_j^{(k_j)} - \bar{\boldsymbol{\theta}}_j^{(k_j)}|$
    $L[c] \leftarrow [\mathbf{T}], E[c] \leftarrow \mathrm{d}$
  end for
  Sort array E
  Sort list L according to sorted E
  Update $[\mathbf{T}^{(0)}]$ using the matrices element mean of $L[1:\mathrm{m}]$
  Update $[\sigma_{\mathbf{T}}]$ using the matrices element variance of $L[1:\mathrm{m}]$
until criteria are satisfied

data are used for methodology validation.

4.1 Experimental data

We employ a large crack growth experimental dataset for aluminum alloy 2024-T3 reported in (Virkler *et al.,* 1979) The dataset consists of 68 crack growth trajectories. All specimens have the same geometry, namely, width $w = 152.4mm$, length $l = 558.8mm$, and thickness $t = 2.54mm$ with a center-through initial crack size of $a_i = 9.0mm$. A constant amplitude sinusoidal cyclic load was applied. The variation of stress during one load cycle is $\Delta\sigma = 48.28MPa$ and the stress ratio is $R = 0.2$. The experimental data are shown in Fig. 2(a). Figure 2(b) shows a small portion of the dataset that used for model parameter regression which is described in Paragraph 4.3.

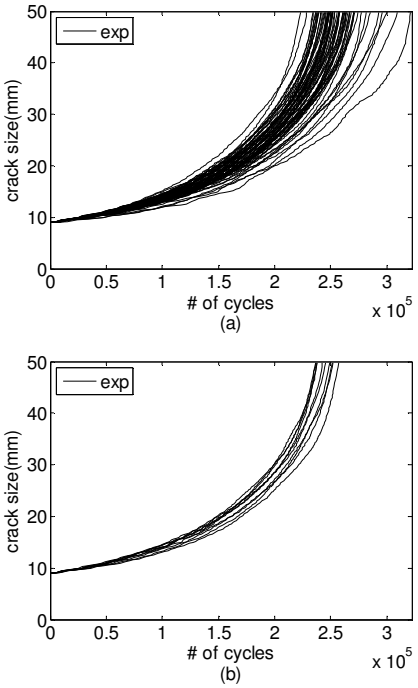

Figure 2: Crack growth curves reported by Virkler et al. (a) the entire 68 crack growth curves; (b) first 10 crack growth curves used for model parameter identification.

4.2 Crack growth models

Three classical crack growth models are included in this example. They are Paris' equation (Paris and Erdogan, 1960), Forman's model (Forman *et al.,* 1967), and McEvily's model (McEvily, 1983). These models are briefly summarized.

Paris' equation:

$$da/dN = C_p(\Delta K)^{m_p} \tag{11}$$

In Eq. (11), a is the crack size, N is the number of loading cycles, and C_p and m_p are model parameters. The suffix "$_p$" denotes "Paris' equation". $\Delta K = \sqrt{\pi a}\Delta\sigma f(\cdot)$ is the variation of the stress intensity factor during one loading cycle. $\Delta\sigma$ is the variation of the applied stress during one loading cycle, and $f(\cdot)$ is the geometry correction function. For a center-through specimen, $f(\cdot) = \sqrt{sec(\pi a/w)}$; $(a/w < 0.7)$. Paris' equation describes only the linear log-log region of the crack growth curve.

Forman's model:

$$\frac{da}{dN} = \frac{C_f(\Delta K)^{m_f}}{(1-R)K_c - \Delta K} \tag{12}$$

where C_f and m_f are model parameters. The suffix "$_f$" denotes "Forman's model". K_c is the critical stress intensity (or fracture toughness) related to the material. Because K_c is determined by the standard ASTM tests and the value is correlated with the material and the specimen geometry. K_c is usually characterized as a random variable instead of a deterministic value. Based on this consideration, Forman's model has three parameters C_f, m_f, and K_c. Forman's model also describes tail region in the crack growth curve due to the introduction of parameter K_c.

McEvily's model:

$$\frac{da}{dN} = C_m(\Delta K - \Delta K_{th})^2\left(1 + \frac{\Delta K}{K_c - K_{max}}\right) \tag{13}$$

In McEvily's model, C_m is the model parameter, where the suffix "$_m$" denotes "McEvily's model". ΔK_{th} is a threshold stress intensity range, below which cracks either propagate at an extremely low rate or do not propagate at all. Knowledge of ΔK_{th} permits the calculation of permissible crack lengths and/or applied stresses in order to avoid fatigue crack growth. Above the threshold value the crack growth rate increases relatively rapidly with increasing ΔK (Janssen *et al.,* 2004). ΔK_{th} and K_c are considered as random variables and McEvily's model has three parameters C_m, ΔK_{th} and K_c.

4.3 Model parameter distributions and model prior probabilities

The first 10 crack growth curves (Fig. 2(b)) from the dataset are chosen to identify the parameter PDFs for each of the three models.

$log(da/dN) \sim log(\Delta K)$ linear regression is used to obtain the parameters in Paris' equation. For convenience, we identify $log(C_p)$ instead of C_p. The parameters in Forman's model and McEvily's model are identified using the nonlinear curve fitting methods. $m_p, m_f, K_c, \Delta K_{th}$ are considered as normal PDFs truncated into the positive regions ($\in R^+$) based on their physical meaning. Both K_c and ΔK_{th} have unit of $MPa\sqrt{mm}$. The means and standard deviations (in the parentheses following the means) of the model parameters are shown in Eq. (14).

$$\text{Paris':} \begin{cases} log(C_p) \sim -26.739(0.774) & \in R \\ m_p \sim 2.974(0.129) & \in R^+ \end{cases} \quad (14\text{-}1)$$

$$\text{Forman's:} \begin{cases} log(C_f) \sim -13.914(1.317) & \in R \\ m_f \sim 1.869(0.239) & \in R^+ \\ K_c \sim 1173.227(76.710) & \in R^+ \end{cases} \quad (14\text{-}2)$$

$$\text{McEvily's:} \begin{cases} log(C_m) \sim -21.273(0.0527) & \in R \\ \Delta K_{th} \sim 22.653(6.056) & \in R^+ \\ K_c \sim 1246.847(67.189) & \in R^+ \end{cases} \quad (14\text{-}3)$$

The mean standard error (standard deviation of the residual error term) of the three models is shown in Fig. 3. Because of the nonlinearity of the models and the measurement noise in the experimental data, the mean standard error is changing throughout the entire crack growth life cycle. In the tail region of the plot (# of cycles > 200,000), the standard error increases rapidly due to the very unstable fatigue crack growth near the point of break, as shown in Fig. 3. The standard error serves as a formal reference to the choice of the standard deviation in the Gaussian likelihood term $p(X|\boldsymbol{\theta}_i^{(k_i)}, M_i^{(k_i)})$ in Eq. (9).

Let M_p, M_f , and M_m denote Paris' equation, Forman's model, and McEvily's model, respectively. Without any information about initial model probabilities, the model prior probability are equally assigned as

$$P(M_p) = P(M_f) = P(M_m) = 1/3 \quad (15)$$

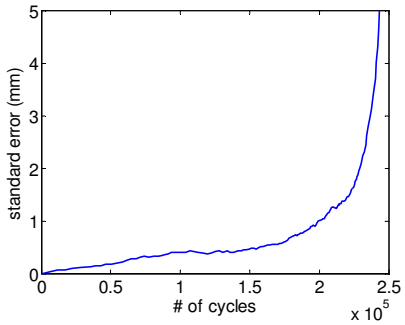

Figure 3: The mean standard error of the three models

4.4 Dimension matching densities and bijection functions for trans-dimensional MCMC

Using the identified parameter PDFs in Eq. (14) and following the stochastic search algorithm described in Algorithm 1, the dimension matching densities and bijection functions can be constructed. As we mentioned earlier, $q(u|i,j)$ can be any density function. A symmetric Gaussian density is a convenient choice. In this problem, we choose $u \sim Gauss(0, 0.01)$. $[\mathbf{T}^{(0)}]$ is initialized as a unit 3×3 matrix and the stopping criterion is configured as the minimal value in the sorted array E (in Algorithm 1) is less than $1e-20$. The following matrices are obtained:

$$[\mathbf{T}]_{f\to p} = \begin{bmatrix} 0.28009 & 0.28873 & -0.019689 \\ 1.7631 & -0.49469 & 0.026004 \\ 1.869 & 3.606 & 0.017712 \end{bmatrix} \quad (16\text{-}1)$$

$$[\mathbf{T}]_{m\to p} = \begin{bmatrix} 0.61893 & 0.46365 & -0.021333 \\ 2.1764 & 0.78516 & 0.020353 \\ 1.1254 & 2.0098 & -0.0281 \end{bmatrix} \quad (16\text{-}2)$$

$$[\mathbf{T}]_{m\to f} = \begin{bmatrix} 1.9149 & 0.43009 & 0.010216 \\ 1.1651 & 1.8069 & -0.021107 \\ 0.72653 & 0.38726 & 0.91859 \end{bmatrix} \quad (16\text{-}3)$$

The suffixes, such as " $_{f\to p}$ ", denote the transformation from Forman's model to Paris' equation. For example, if the current state in trans-

Table 1. Updated model probabilities and model parameters

(crack size, # of cycles)	Paris' equation	Forman's model	McEvily's model
(11.0, 50731)	$\langle P(M_p)\rangle = 0.32792$ $\langle log(C_p)\rangle = -26.798$ $\langle m_p\rangle = 2.9690$	$\langle P(M_f)\rangle = 0.027222$ $\langle log(C_f)\rangle = -14.504$ $\langle m_f\rangle = 1.9405$ $\langle K_C\rangle = 1202.1$	$\langle P(M_m)\rangle = 0.64486$ $\langle log(C_m)\rangle = -21.343$ $\langle \Delta K_{th}\rangle = 29.998$ $\langle K_C\rangle = 1274.7$
(11.0, 50731) (12.6, 81371)	$\langle P(M_p)\rangle = 0.33094$ $\langle log(C_p)\rangle = -26.783$ $\langle m_p\rangle = 2.9677$	$\langle P(M_f)\rangle = 0.008189$ $\langle log(C_f)\rangle = -14.458$ $\langle m_f\rangle = 1.9383$ $\langle K_C\rangle = 1203.8$	$\langle P(M_m\rangle = 0.66087$ $\langle log(C_m)\rangle = -21.351$ $\langle \Delta K_{th}\rangle = 30.752$ $\langle K_C\rangle = 1277.7$

dimensional MCMC at time t is in Forman's model with parameter $(log(C)_f, m_f, K_c)_t$, and the proposal move for time $t+1$ is to Paris' equation, the proposed dimension matching parameters for Paris' equation is obtained by $(log(C)_p, m_p, u)_{t+1} = [\mathbf{T}]_{f\to p} \cdot (log(C)_f, m_f, K_c)_t$. The reverse transformation from Paris' equation to Forman' model uses the inverse of the corresponding matrix.

4.5 Bayesian updating with trans-dimensional MCMC simulations

To illustrate the updating process and validate the methodology, one specimen is arbitrarily chosen from the rest of 58 specimens in the dataset. This specimen represents the "target system" for which we want to perform fatigue crack growth prognosis. The actual crack growth curve of the "target system" and the curves of the ten specimens are shown in Fig. 4(a). The prior deterministic mean predictions of each model and the actual crack growth curve of the "target system" are shown in Fig. 4(b), where we can see that the three models perform equally well.

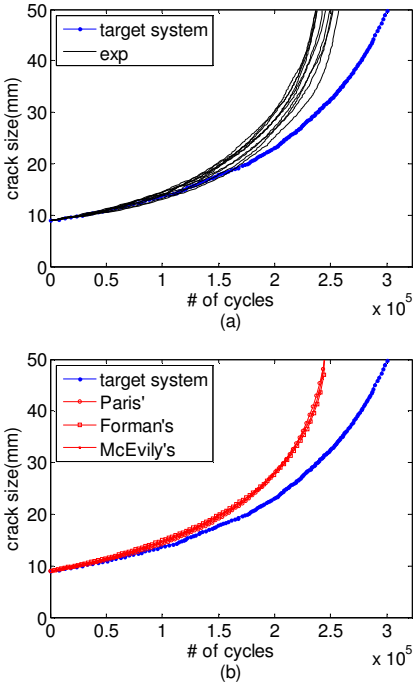

Figure 4: Crack growth curves. (a) 10 specimens for parameter identifications and the "target system"; (b) Prior deterministic mean predictions and the "target system"

Two points (crack size (mm), # of cycles) in the early stage of the crack propagation of the "target system" are randomly chosen to represent the additional response measures. They are $(11.0,\ 50731)$ and $(12.6,\ 81371)$. The standard deviation of the Gaussian likelihood is obtained from the standard error analysis in Fig. 3. For the two measurements, the corresponding standard deviation in the Gaussian likelihood is 0.17mm and 0.32mm, respectively.

Ten million of samples are generated using the trans-dimensional MCMC simulation. To visualize the chain moving across models, a segment of the Markov chain is shown in Fig. 5, where we can see the moves across the three models. The updated model probabilities and model parameter distributions are shown in Table 1, where $\langle\cdot\rangle$ denotes the estimates. The crack size prognosis results are shown in Fig. 6(a) and Fig. 6(b) for the first and second Bayesian updatings, respectively.

4.6 Discussion of Results

The prior deterministic mean predictions of three models are not close to the actual crack growth curve of the "target system", as shown in Fig. 4(b). The prior model probabilities of the three models are equally assigned. After the Bayesian updatings, the model probabilities are revised (given in Table 1). The Bayes factor in favor of one model over another (Eq. (5)) is calculated according to Eq. (10). The results of Bayes factors are shown in Eq. (17).

$$1^{st}\ \text{update}: \begin{cases} B_{p,f} = \langle P(M_p)\rangle / \langle P(M_f)\rangle = 12.046 \\ B_{m,f} = \langle P(M_m)\rangle / \langle P(M_f)\rangle = 23.689 \\ B_{m,p} = \langle P(M_m)\rangle / \langle P(M_p)\rangle = 1.967 \end{cases} \quad (17)$$

$$2^{nd}\ \text{update}: \begin{cases} B_{p,f} = \langle P(M_p)\rangle / \langle P(M_f)\rangle = 40.413 \\ B_{m,f} = \langle P(M_m)\rangle / \langle P(M_f)\rangle = 80.702 \\ B_{m,p} = \langle P(M_m)\rangle / \langle P(M_p)\rangle = 1.997 \end{cases}$$

The Bayes factors can be interpreted as a summary of the evidence provided by the measured data in favor of one model over another. Jeffreys suggested interpreting Bayes factor between 1 and 3.2 as no evidence, 3.2 to 10 as substantial, 10 to 100 as strong, and >100 as decisive evidence (Jeffreys, 1961). As far as the two measured data are concerned, we can suggest leaving out Forman's model in this problem because the data show strong evidence against using it. However, we are unable to determine whether Paris' equation or McEvily's model performs better. Based on this consideration, we keep Paris' equation and McEvily's model. To make further determination, more data are needed.

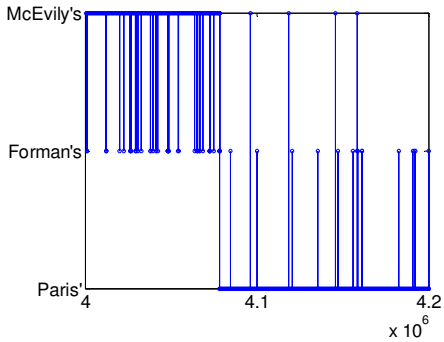

Figure 5: Markov chain (partial segment) moving across models in the general state space

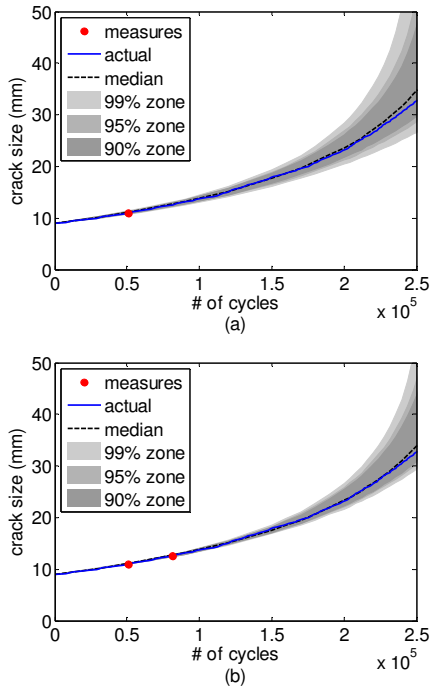

Figure 6: Updated crack size prognosis. (a) first updating; (b) second updating

The fatigue crack growth prognosis results averaged from the three models (Fig. 6) show that the uncertainties associated with the confidence bounds are reduced as more data are used in the Bayesian updating. The median predictions after both updatings are close to the actual crack growth curve as expected. It is worth mentioning that if one particular model is of interest, we can also obtain the prognosis results using the simulation samples associated with that model. As we mentioned earlier, the simulation results are just a reproduction as if we perform a standard MCMC simulation using only one model. For example, the parameter distributions in Paris' equation before and after the first updating are shown in Fig. 7.

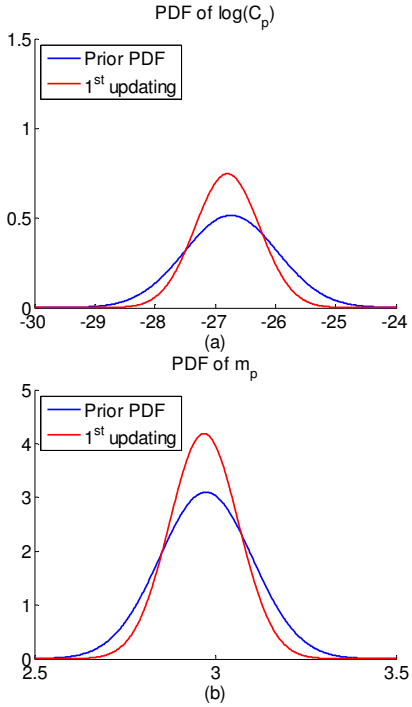

Figure 7: The prior and updated parameter PDFs for Paris' equation. (a) $log(C_p)$ (b) m_p

Observing the mean values of the model parameters before (Eq. (14)) and after the updating (Table 1) shows that these values change very slightly. This is because the $da/dN \sim \Delta K$ based crack growth models are sensitive to its parameters. A relatively small change of its parameters affects the crack growth curve significantly. This property of the crack growth models is another important reason why we need to choose $q(u|i,j)$ and $T_{i\to j}(\cdot)$ carefully. Because the parameters are highly dense (small standard deviations) in the general state space, we have to ensure $T_{i\to j}(\cdot)$ can place the samples in the region with high probabilities. Ignoring this property will lead a simulation chain which is either not fully mixed or has prohibitively high rejection rate. We use three classical fatigue crack growth models that are suitable for constant amplitude cyclic loads in this example. For variable amplitude block loading and non-stationary loadings, appropriate mechanism models should be adopted. The general procedures and algorithms remains the same, only models need change.

5 CONCLUSION

A general Bayesian framework for fatigue model determination, updating and averaging using trans-dimensional MCMC simulations is presented in this paper. Uncertainties associated with model choice, mechanism modeling, model parameters, and response

measures are systematically included. A new algorithm to construct the dimension matching densities and bijection functions is developed for efficient simulations. The simulation results update the model probabilities, the parameter PDFs associated with each of the models, and the Bayes factors. The prognosis averaging is readily evaluated using the simulation samples. The Bayes factors serve as guides for model determinations. A fatigue crack growth prognosis problem with experimental data is presented for methodology demonstration and validation. Several conclusions are drawn based on the current study:

1. The presented Bayesian framework using trans-dimensional MCMC for model determination, updating and averaging is computationally effective and efficient to calculate the model probabilities, parameter distributions, and Bayes factors for Bayesian models where analytical approximation methods and other MC simulations are difficult to achieve the same results simultaneously. More mechanism models can be flexibly included as necessary.

2. The proposed algorithm is effective in constructing the dimension matching densities and bijection functions required for trans-dimensional MCMC simulations. This algorithm is independent of the actual simulation problems thus it is also applicable to more general problems.

3. Using the results of Bayes factors, model determinations can be carried out according to Jeffreys' criterion.

4. Model averaging is more appropriate when the Bayes factors do not show a strong evidence for model determinations. The prognosis result based on model averaging is likely to be more conservative.

ACKNOWLEDGMENT

The research reported in this paper was supported in part by the NASA ARMD/AvSP IVHM project under NRA NNX09AY54A. The support is gratefully acknowledged.

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