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Approximate Bayesian Computation for Parameter Identification in Computational Mechanics

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ABSTRACT: This paper explores the application of Approximate Bayesian Computation for efficient parameter identification in problems of computational stochastic mechanics. ABC is implemented based on informative summary statistics that contrast measured and simulated data. These summary statistics are estimated efficiently by means of a perturbation approach, which is advantageous from a numerical viewpoint. To update the simulation process, so-called subset simulation combined with a Markov Chain Monte Carlo approach is used. An illustrative example leverages the potential of our methodological proposal for parameter identification in computational mechanics.

1. INTRODUCTION

Computational mechanics offers the possibility to construct numerical models that simulate the behaviour of real-world engineering systems (Bathe, 1996). These numerical models usually depend on a set of parameters such as material properties and boundary conditions, whose precise characteristics may be unknown due to lack of knowledge. It is of interest to infer such characteristics using, e.g. Bayesian approaches (Sivia, 1996), since they allow to account for potential prior knowledge and direct risk assessment through posterior distributions. To this end, responses measured on the real system are contrasted with those coming from the numerical model, allowing the identification of the unknown parameters.

Bayesian approaches for identification are widely accepted by the engineering community

(Papadimitriou et al., 2001; Kerschen et al., 2006; Straub and Papaioannou, 2015; Jensen and Jerez, 2019; Faes et al., 2019). A key issue for its practical application is the evaluation of the likelihood function, which expresses the probability of observing the measured responses given the parameters that are being identified and the numerical model at hand. However, for many practical cases, the likelihood is unavailable analytically, numerically unstable or costly to evaluate. To overcome these issues, Approximate Bayesian Computation (ABC; Sisson et al., 2018) is a likelihood-free method that has been shown to be a feasible way to address these challenges (see e.g. Blum and François, 2010; Fan et al., 2013; Chiachio et al., 2014). In particular, ABC does not require explicit knowledge on the likelihood, but only requires the ability to simulate from the system whose parameters are being updated (Marin et al., 2012; Nott et al., 2018; Klein et al., 2021). In this work, we explore the potential of ABC in the context of mechanical engineering. To this end, summary statistics such as means and covariances are considered to compare the measured and simulated responses. These summary statistics are calculated using a perturbation approach (Yamazaki et al., 1988) to speed up numerical computations. Bayesian updating is carried out resorting to Subset Simulation (Au and Beck, 2001), which is a simulation method that has shown excellent performance for performing ABC, as shown in Chiachio et al. (2014).

2. PROBLEM SETTING

2.1. *Definition of the Model*

Assume we have an engineering system of interest. To study this system, we develop a model composed of two parts. The first part consists of a numerical model $\mathscr{M}$, that can be implemented resorting to, e.g.the finite element method (Bathe, 1996). The role of this numerical model is to describe the relationship $\mathbf{y} = \mathscr{M}(\boldsymbol{x})$, where $\boldsymbol{x}$ is a vector that collects a series of input parameters of the model, such as material properties, loading, boundary conditions, etc.; and $\boldsymbol{y}$ is another vector that collects responses of interest of the model, such as displacements, strains, stresses, etc. It is assumed that these responses $\boldsymbol{y}$ can be observed (measured) from the engineering system experimentally. The second part of the model concerns the characterization of the input parameters $\boldsymbol{x}$. Describing these input parameters in a deterministic fashion may be challenging due to inherent uncertainties. A feasible strategy for describing these uncertainties is resorting to probability theory (Ang and Tang, 2007). Thus, a probability distribution $p_{\boldsymbol{X}}(\boldsymbol{x}|\boldsymbol{\theta})$ is associated with the input parameters, where $\boldsymbol{\theta}$ denotes a vector of model parameters that characterize this probability distribution. For practical applications, the selection of a crisp value for $\boldsymbol{\theta}$ may be far from trivial due to issues such as lack of knowledge, imprecise measurements, etc. In other words, $\boldsymbol{\theta}$ can be subject to epistemic uncertainty. We are thus interested in reducing its uncertainty to improve the characterization of the engineering system of interest.

2.2. *Bayesian Updating*

Assume that $\mathscr{D}_{\boldsymbol{y}}$ represents a data set containing measurements of the actual response of the engineering system under study. This data set $\mathscr{D}_{\boldsymbol{y}}$ can be used in order to improve our knowledge on the unknown model parameter $\boldsymbol{\theta}$ by invoking Bayes' theorem (see e.g. Sivia, 1996):

$$p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}|\mathscr{D}_{\boldsymbol{y}}) = \frac{p\left(\mathscr{D}_{\boldsymbol{y}}|\boldsymbol{\theta}\right) p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})}{p\left(\mathscr{D}_{\boldsymbol{y}}\right)}. \tag{1}$$

In (1), $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$ represents the prior probability distribution which reflects our knowledge on $\boldsymbol{\theta}$ before any measurement is available; $p\left(\mathscr{D}_{\boldsymbol{y}}|\boldsymbol{\theta}\right)$ denotes the likelihood, which expresses how likely it is to observe $\mathscr{D}_{\boldsymbol{y}}$ given a particular value $\boldsymbol{\theta}$; $p(\mathscr{D}_{\boldsymbol{y}})$ is the probability of the evidence; and $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}|\mathscr{D}_{\boldsymbol{y}})$ is the posterior probability distribution, which reflects our knowledge on $\boldsymbol{\theta}$ after taking into account the prior and data measurements.

The Bayes' theorem in Equation (1) provides a systematic way to improve our knowledge on $\boldsymbol{\theta}$. That is, starting from existing (and possibly subjective) information contained in the prior distribution, it is possible to consider data measurements that lead to a posterior distribution. Undoubtedly, the challenge lies on the practical application of the Bayes' theorem. For example, the likelihood function, which plays a central role for the updating procedure, may not be available in closed form. The latter may occur as the relation between inputs and outputs $\mathbf{y} = \mathscr{M}(\boldsymbol{x})$ is usually only available as the result of a numerical scheme such as the finite element method (FEM; Bathe, 1996). That is, values of the response $\boldsymbol{y}$ must be calculated numerically for specific realizations of the uncertain input parameter vector $\boldsymbol{x}$.

3. STRATEGY FOR PARAMETER IDENTIFICATION

3.1. Approximate Bayesian Computation

ABC allows estimating the posterior distribution of model parameters whenever the likelihood function is not known explicitly (Rubin, 1984). In fact, ABC provides a way for (approximately) sampling from the posterior distribution $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}|\mathscr{D}_{\boldsymbol{y}})$ by means of the following procedure.

1. Generate $\boldsymbol{\theta}^*$ from its prior distribution $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$.

2. Simulate a sample of the uncertain input parameters $\boldsymbol{x}$ from the probability distribution $p_{\boldsymbol{X}}\left(\boldsymbol{x}|\boldsymbol{\theta}^*\right)$.

3. Calculate the responses of the numerical model for each observation in the sample generated in the previous step, that is, $\boldsymbol{y} = \mathscr{M}(\boldsymbol{x})$. These responses are collected in the set of simulated data $\tilde{\mathscr{D}}_{\boldsymbol{y}}$.

4. Compare the simulated data set $\tilde{\mathscr{D}}_{\boldsymbol{y}}$ with the measured data set $\mathscr{D}_{\boldsymbol{y}}$ through a distance measure ρ based on summary statistics of the data responses. In case that the distance measure is below a certain threshold ε:

$$\rho\left(\mathscr{D}_{\boldsymbol{y}}, \tilde{\mathscr{D}}_{\boldsymbol{y}}\right) \leq \varepsilon, \tag{2}$$

   it is assumed that $\boldsymbol{\theta}^*$ is distributed according to the target posterior distribution. Otherwise, $\boldsymbol{\theta}^*$ is simply discarded.

The procedure described above can be repeated a number of times until a sufficiently large sample of the model parameters $\boldsymbol{\theta}$ becomes available. Then, these samples which are (approximately) distributed according to the posterior distribution can be employed for, e.g. determining confidence bounds on the values of $\boldsymbol{\theta}$. The above discussion highlights the fact that ABC relies purely on the ability to simulate the response of the system of interest, without the need to evaluate or know the likelihood function analytically but only a summary of the data trough summary statistics. Hence, its implementation is straightforward from a numerical viewpoint. However, it requires the careful selection of summary statistics and an appropriate distance measure. Examples of such distance measure comprise the Bhattacharyya (Bi et al., 2019) or the Bray-Curtis (Zhao et al., 2022) distance. For this work, a very catchy distance measure based on summary statistics is considered:

$$\rho\left(\mathscr{D}_{\boldsymbol{y}}, \tilde{\mathscr{D}}_{\boldsymbol{y}}\right) = \max\left(\mu, \sigma\right), \tag{3}$$

where μ and σ are defined as

$$\mu = \left\|\left(\boldsymbol{\mu}_{\boldsymbol{y}} - \tilde{\boldsymbol{\mu}}_{\boldsymbol{y}}\right) \oslash \boldsymbol{\mu}_{\boldsymbol{y}}\right\|_{\infty}, \tag{4}$$

$$\sigma = \left\|\left(\boldsymbol{\Sigma}_{\boldsymbol{y}} - \tilde{\boldsymbol{\Sigma}}_{\boldsymbol{y}}\right) \oslash \boldsymbol{\Sigma}_{\boldsymbol{y}}\right\|_{\max}. \tag{5}$$

In the above equations, $\boldsymbol{\mu}_{\boldsymbol{y}}$ and $\tilde{\boldsymbol{\mu}}_{\boldsymbol{y}}$ represent the (estimated) mean vector of the data contained in $\mathscr{D}_{\boldsymbol{y}}$ and $\tilde{\mathscr{D}}_{\boldsymbol{y}}$, respectively; while $\boldsymbol{\Sigma}_{\boldsymbol{y}}$ and $\tilde{\boldsymbol{\Sigma}}_{\boldsymbol{y}}$ represent the (estimated) covariance matrices of the data contained in $\mathscr{D}_{\boldsymbol{y}}$ and $\tilde{\mathscr{D}}_{\boldsymbol{y}}$, respectively. Furthermore, $\oslash$ represents the Hadamard division (that is, element-wise division between entries of a vector or matrix), while $\|\cdot\|_{\infty}$ and $\|\cdot\|_{\max}$ denote the infinity and maximum norm, respectively.

A key aspect for the practical implementation of ABC is the selection of an appropriate threshold level ε.

3.2. Subset Simulation

The threshold level ε contained in (2) plays a central role for the practical implementation of ABC. In principle, a small value of ε ensures that the simulated data set $\tilde{\mathscr{D}}_{\boldsymbol{y}}$ and the measured data set $\mathscr{D}_{\boldsymbol{y}}$ are sufficiently *close* to each other, which is a desirable feature. However, selecting a value of ε which is too small may lead to frequent rejections of sampled model parameters, as the inequality in (2) would be difficult to fulfil. The latter can be particularly disadvantageous, as it is usually numerically demanding to evaluate the model $\mathscr{M}$. A possible workaround consists of performing ABC by means of Subset Simulation, which is an advanced variant of the Monte Carlo method.

Subset Simulation was originally conceived as a means for estimating small failure probabilities (Au and Beck, 2001). Its potential for performing ABC has been explored in (Chiachio et al., 2014; Barros et al., 2022) and hence, it is employed in this contribution.

In essence, Subset Simulation for ABC involves generating samples of model parameters which, starting from the prior distribution, gradually approach the (approximate) target posterior distribution. The following steps are involved in the implementation of Subset Simulation for ABC.

1. Set a sample size N and a parameter $p_0 \in (0,1)$ such that $p_0 N$ is an integer number.

2. Set $i = 1$. Note that i denotes the current subset under consideration.

3. Sample N model parameters $\boldsymbol{\theta}_i^{(j)},\ j = 1,\ldots,N$ from the prior $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$. For each, compute the distance measure $\rho_i^{(j)},\ j = 1,\ldots,N$.

4. Arrange the samples $\left(\boldsymbol{\theta}_i^{(j)}, \rho_i^{(j)}\right)$ such that the distance measures are sorted from the smallest to the largest, that is, $\rho_i^{(1)} \leq \rho_i^{(2)} \leq \ldots \rho_i^{(N)}$.

5. Set the intermediate threshold ε_i such that:
$$\varepsilon_i = \rho_i^{(p_0 N)} \tag{6}$$

6. Simulate N model parameters $\boldsymbol{\theta}_{i+1}^{(j)},\ j = 1,\ldots,N$ such that they are distributed according to $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$ and fulfil the condition $\rho \leq \varepsilon_i$. To this end, employ an appropriate Markov Chain Monte Carlo method and use as sample seeds those from the previous level and whose distance is equal or smaller than ε_i. Calculate the resulting distance measures $\rho_{i+1}^{(j)},\ j = 1,\ldots,N$.

7. Repeat steps 4. to 6. until
$$\rho_{i+1}^{(p_0 N)} \leq \varepsilon \tag{7}$$
holds.

The final samples of $\boldsymbol{\theta}$ for which the distance measure ρ is equal or smaller than the threshold ε are (approximately) distributed according to the target posterior distribution. As noted from the above description, Subset Simulation allows generating sets of model parameters whose distance measures become smaller as the simulation process progresses across subsets.

For the practical implementation of Subset Simulation, one must choose the hyperparameters N and p_0. N should be sufficiently large such that it is representative of the underlying probability distribution associated to the corresponding subset. Numerical experience indicates that $N \geq 500$ (Au and Beck, 2001). The parameter p_0 controls the speed with which the subsets converge to the sought probability distribution. While in principle small values of p_0 may be desirable, a value of p_0 which is too small may prevent an appropriate exploration of the support associated with $\boldsymbol{\theta}$. Numerical validations as reported in Au and Beck (2001) and Zuev et al. (2012) suggest that $p_0 \in [0.1, 0.3]$.
In addition to selecting N and p_0, there is another issue which is critical for a successful implementation of Subset Simulation: the application of an appropriate Markov Chain Monte Carlo approach for generating model parameters which follow the prior distribution and whose distance value is smaller than a certain threshold. In this contribution, the so-called preconditioned Crank-Nicolson algorithm is implemented. This algorithm has been shown to be a reliable method for sampling from distributions which are known up to an integration constant and is particularly suitable for problems which involve high dimensional spaces (Beskos et al., 2008; Papaioannou et al., 2015; Au and Patelli, 2016).
The preceding paragraphs have discussed the selection of the different parameters associated with the implementation of Subset Simulation for ABC, except for the threshold level ε. Numerical validation indicates that this parameter should be selected between 1% and 5%. These values are appropriate for the class of problems considered in this work, particularly because the chosen distance metric is dimensionless. Admittedly, additional research efforts are required in order to identify a more robust

criterion for selecting ε.

3.3. Estimation of Summary Statistics

The practical implementation of the ABC framework discussed previously demands the calculation of the mean vector $\tilde{\boldsymbol{\mu}}_{\boldsymbol{y}}$ and covariance matrix $\tilde{\boldsymbol{C}}_{\boldsymbol{y}}$ of the response $\boldsymbol{y}$ for specific values of $\boldsymbol{\theta}$, as defined in (4) and (5), respectively. The calculation of these statistics is based on the simulated data set $\tilde{\mathscr{D}}_{\boldsymbol{y}}$, that is constructed based on simulations of the model $\mathscr{M}$. This step can be demanding, as the model $\mathscr{M}$ may be numerically expensive to evaluate. To avoid this demanding step, the mean and covariance can be estimated using a perturbation approach (see e.g. Yamazaki et al., 1988; Matthies et al., 1997). In a perturbation approach, the responses of the system $\boldsymbol{y}$ are approximated as a linear function of the input variables $\boldsymbol{x}$. Thus, both mean and covariance become available in closed form. From a numerical viewpoint, the implementation of a perturbation approach is straightforward, as it demands performing a single deterministic analysis followed by a sensitivity analysis (Haftka and Gürdal, 1992).

4. EXAMPLE

The application of ABC via Subset Simulation considering a perturbation approach as described in the preceding sections is illustrated here with a test example. The system under consideration involves a two-degree-of-freedom system, as illustrated in Figure 1.

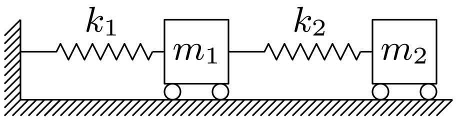

Figure 1: Two-degree-of-freedom system.

The two masses m_1 and m_2 are regarded as deterministic quantities whose magnitude is 1 [kg]. The linear springs connecting these two masses are uncertain and their elastic constants k_1 and k_2 are assumed to follow independent lognormal distributions whose means and standard deviations are unknown and must be identified. That is, $\boldsymbol{\theta} = [\theta_1, \ldots, \theta_4] = [\mu_{k_1}, \sigma_{k_1}, \mu_{k_2}, \sigma_{k_2}]$, where μ_{k_i} and σ_{k_i} denote the mean and standard deviation of the stiffness of the i-th linear spring. The prior knowledge on these unknown model parameters is synthesized into uniform distributions whose support is $[0.1, 2]$ [N/m] for the mean values and $[0.01, 0.5]$ [N/m] for the standard deviation, respectively. To improve our knowledge on the model parameters, the two natural frequencies of the system are measured for 30 different structures. These 30 data measurements are generated synthetically considering nominal values for the model parameters equal to $\boldsymbol{\theta} = [\theta_1, \ldots, \theta_4] = [1, 0.1, 1, 0.1]$.
To implement ABC, the 30 (synthetically generated) measured data are synthesized into the mean $\boldsymbol{\mu}_{\boldsymbol{y}}$ and covariance matrix $\boldsymbol{\Sigma}_{\boldsymbol{y}}$ associated with the natural frequencies. Furthermore, the threshold level associated with ABC is set as $\varepsilon = 0.03$. Subset Simulation is implemented considering $N = 2000$ samples per subset and p_0 is selected as 0.1. These values are selected following recommendations found in the literature, see e.g. Zuev et al. (2012); Chiachio et al. (2014). The results for the Bayesian updating procedure are presented in Figure 2 in terms of histograms. Note that these histograms are normalized such that the area below them is equal to 1 and thus, provide a rough idea of how the different probability distributions look like. The histograms in light blue color illustrate the prior distribution while those in orange color illustrate the posterior distribution. The histograms for the posterior distribution for the cases of θ_2 and θ_4 look black instead of orange because the posterior samples are concentrated in a specific region. In addition, the red line indicates the *true* value of the associated model parameter. The results show that the updating procedure is successful in identifying the neighborhood of the true model parameters. Of course, the identification is not perfect, as there are different sources of error, for example:

- The 30 (synthetically generated) data measurements do not carry all the necessary information associated with the model parameters.
- ABC provides by construction an approximation of the actual problem.
- The summary statistics do not necessarily con-

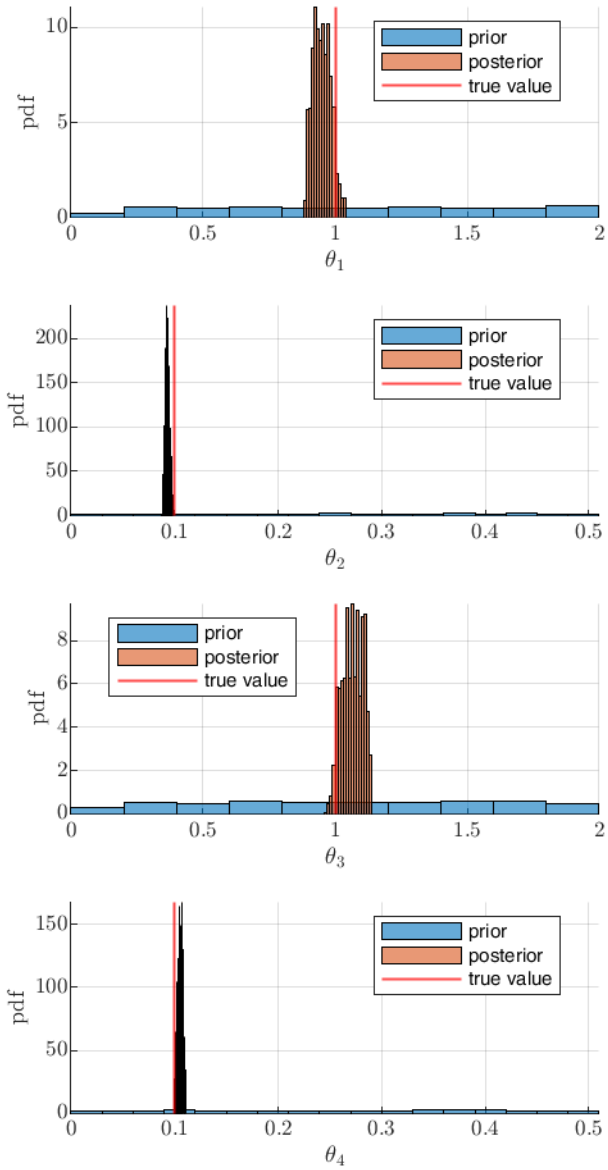

Figure 2: Normalized histograms of prior, posterior and true values for model parameters.

tain all information for performing updating.

- The statistics for a given set of the model parameters are calculated using the perturbation approach, which is approximate only. In fact, it is well known that perturbation may not be applicable when the input parameters $\boldsymbol{x}$ possess a probability distribution with a large variability (Yamazaki et al., 1988; Matthies et al., 1997).

5. CONCLUSIONS

Our results suggest that the combination of ABC, Subset Simulation and perturbation approach provides a valid means for performing parameter identification. Evidently, this approach could be further improved by choosing more sophisticated summary statistics, resort to regression-based ABC (Blum, 2018), or making the perturbation approach more robust. In addition, once the updating procedure has been completed using a perturbation approach, one may consider re-launching the updating procedure with the posterior distributions identified so far, but this time using a better approach to estimate the summary statistics. Another path for further developing our work is considering a more general approach to describe uncertainty. The model considered in this contribution corresponds to a parametric probability box. However, a more general model for describing uncertainty would be a distribution-free probability box (see e.g. Beer et al., 2013). Yet, our work shows that our method has a strong potential to be an effective tool for understanding important problems in computational mechanics. As the method was only demonstrated on a first exemplary feasibility study, limitations of our method will be analyzed in the future.

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