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A Hellinger distance-based stochastic model updating framework for the accreditation validation of a material thermal property under limited data

Adolphus Lye

Singapore Nuclear Research and Safety Institute, National University of Singapore, Singapore.
E-mail: snrltsa@nus.edu.sg

Scott Ferson

Institute for Risk and Uncertainty, Department of Civil and Environmental Engineering, University of Liverpool, United Kingdom.
E-mail: ferson@liverpool.com

Sicong Xiao

Singapore Nuclear Research and Safety Institute, National University of Singapore, Singapore.
E-mail: snrxs@nus.edu.sg

The paper presents a distance-based Approximate Bayesian Computation framework involving the use of the Hellinger distance to perform stochastic model updating, and to subsequently perform an accreditation validation procedure based on the 2008 Sandia thermal problem. In computing the Hellinger distance, the adaptive-binning algorithm is implemented to adaptively select an appropriate bin number to approximate the probability density of the experimental data and the model prediction. The distance function subsequently quantifies the difference in the distribution between the two statistical objects. To verify the proposed stochastic model updating framework, the approach is implemented to perform a model calibration on the aleatory input variables of a dynamic temperature model of a slab material based on limited experimental data. This involves the use of the Staircase Density Function to calibrate and characterise the distribution over the input variables based on limited data, thereby providing for a distribution-free approach and eliminating the element of model uncertainty. A stochastic validation of the calibrated model is then performed against a set of accreditation validation experiment data. The results showed that using the mean estimates on the inferred shape parameters of the Staircase Density Function yields a better validation performance by the resulting calibrated model, in contrast to the case where the Maximum A-posteriori estimate on the inferred parameters is used.

Keywords: Stochastic model updating, Approximate Bayesian computation, Hellinger distance, Transitional Ensemble Markov Chain Monte Carlo, Area metric, Model validation, Solid mechanics, Physics-guided machine-learning.

1. Introduction

When addressing engineering problems, a key aspect is the need for well-calibrated and validated models which are representative of a physical system. This is often achieved via stochastic model updating, especially in instances where data is limited and uncertainties are present. Generally speaking, such uncertainties can be categorised into two types: 1) Aleatory uncertainty which is an irreducible uncertainty due to the inherent variability of a given random variable; and 2) Epistemic uncertainty which is a reducible uncertainty due to a lack of knowledge. However, there exists scenarios where both types of uncertainties exist simultaneously. Such is often referred to as polymorphic uncertainty (Lye et al. (2024)) which is the interest of the work presented in the paper.

The objectives of the paper are three-fold: 1) to proposed the use of the Hellinger distance to perform the distance-based Approximate Bayesian Computation for stochastic model updating. To the best of the authors' knowledge, the proposed approach is yet to be investigated or discussed in the existing literature; 2) to demonstrate its feasibility via a model validation problem based on a real-world set-up involving physical experiment data; and 3) to provide a tutorial on the proposed approach and enhance the understanding among the readers.

To realize such objectives, the paper is structured as follows: Section 2 reviews the concept of the distance-based Approximate Bayesian Computation framework for stochastic model updating, as well as the mathematical formalism of the Hellinger distance; Section 3 introduces the case study problem statement which is based on the Sandia thermal problem originally presented by Dowding et al. (2008); Section 4 presents and discusses the results from the stochastic model updating and the subsequent model validation results; and Section 5 summarises the key take-aways from the presented work, before drawing the paper to a close.

2. Bayesian Model Updating

A standard stochastic model updating approach is the Bayesian model updating technique to which its mathematical framework is defined as (Lye et al. (2023); Lye (2023)):

$$P(\boldsymbol{\theta}|\boldsymbol{D}, M) = \frac{P(\boldsymbol{D}|\boldsymbol{\theta}, M) \cdot P(\boldsymbol{\theta}|M)}{P(\boldsymbol{D}|M)} \quad (1)$$

whereby $\boldsymbol{\theta}$ represents the vector of inferred parameter(s), $\boldsymbol{D}$ represents the vector of observed data, M represents the model that is being considered for updating, $P(\boldsymbol{\theta}|M)$ represents the prior, $P(\boldsymbol{D}|\boldsymbol{\theta}, M)$ represents the likelihood function, $P(\boldsymbol{\theta}|\boldsymbol{D}, M)$ represents the posterior, and $P(\boldsymbol{D}|M)$ is the model evidence term or the normalising constant to ensure that $P(\boldsymbol{\theta}|\boldsymbol{D}, M)$ integrates to 1. Detailed reviews on each of the above terms are found in Lye and Marino (2023); Lye et al. (2020, 2023).

The term $P(\boldsymbol{D}|M)$ is often neglected as it is a numerical constant and is independent of $\boldsymbol{\theta}$. Hence, $P(\boldsymbol{\theta}|\boldsymbol{D}, M)$ can be re-expressed in its un-normalised form following:

$$P(\boldsymbol{\theta}|\boldsymbol{D}, M) \propto P(\boldsymbol{\theta}|M) \cdot P(\boldsymbol{D}|\boldsymbol{\theta}, M) \quad (2)$$

To sample from the un-normalised $P(\boldsymbol{\theta}|\boldsymbol{D}, M)$, direct Monte Carlo sampling becomes inapplicable and advanced sampling approaches are to be implemented. One such approach is the Transitional Ensemble Markov Chain Monte Carlo (TEMCMC) sampler, proposed by Lye et al. (2022), to which its description is outlined in Section 2.1.

2.1. *Transitional Ensemble Markov Chain Monte Carlo*

The TEMCMC sampler is a state-of-the-art variant of the Transitional Markov Chain Monte Carlo (TMCMC) sampler, where the Metropolis-Hastings sampler is replaced with the Affine-invariant Ensemble sampler as the MCMC kernel to improve the mixing performance of the sampler and to overcome the computational challenge of sampling from a highly skewed and anisotropic posterior. Like the TMCMC sampler, the TEMCMC sampler generates samples from $P(\boldsymbol{\theta}|\boldsymbol{D}, M)$ through a series of intermediate distributions known as “transitional” distributions P^j defined as (Ching and Chen (2007)):

$$P^j \propto P(\boldsymbol{\theta}|M) \cdot P(\boldsymbol{D}|\boldsymbol{\theta}, M)^{\beta_j} \quad (3)$$

where $j = 0, 1, \ldots, m$ is the iteration number, and β_j is the tempering parameter such that $\beta_0 = 0 < \beta_1 < \cdots < \beta_m = 1$.

In the interest of the length of the paper, the readers are referred to Lye et al. (2022) for full details on the TEMCMC algorithm and its implementations.

2.2. *Approximate Bayesian Computation*

An essential component of the Bayesian model updating procedure is the definition of the likelihood function $P(\boldsymbol{D}|\boldsymbol{\theta}, M)$ as shown in Eq. (1). Under the independence assumption between N_{obs} observations, the analytical likelihood function is defined as:

$$P(\boldsymbol{D}|\boldsymbol{\theta}, M) = \prod_{k=1}^{N_{\text{obs}}} P(\boldsymbol{D}_k|\boldsymbol{\theta}, M) \quad (4)$$

where N_{obs} denotes the total number of observations.

The evaluation of Eq. (4) can be a computationally demanding endeavour when: 1) the model M becomes computationally expensive; and 2) a large number of model evaluations is required (Lye et al. (2024)). To address the above issues, Bi et al. (2019) proposed the use of the approximate Gaussian likelihood function defined as:

$$P(\boldsymbol{D}|\boldsymbol{\theta}, M) = \exp\left[-\left(\frac{d(\boldsymbol{D}, \boldsymbol{D}^{\text{sim}})}{\varepsilon}\right)^2\right] \quad (5)$$

where $d(\bullet)$ is the distance function serving to quantify the statistical difference between the distribution of the data $\boldsymbol{D}$ and $\boldsymbol{D}^{\text{sim}} = M(\boldsymbol{\theta})$, while ε is the width-factor which controls the centralization degree of the resulting posterior. For the work presented in the paper, the Hellinger distance serves as the distance function to which its mathematical formalism is reviewed in Section 2.3.

In the interest of the length of the paper, the readers may refer to the tutorial paper on Approximate Bayesian Computation by Lye et al. (2024).

2.3. *Hellinger Distance*

The Hellinger distance d_H is defined mathematically as (Hellinger (1909)):

$$d_H(\boldsymbol{D}, \boldsymbol{D}^{\text{sim}}) = \sqrt{\frac{\sum_{x_{n_d}=1}^{N_{\text{bin}}} \cdots \sum_{x_1=1}^{N_{\text{bin}}} \left(\sqrt{p_{\boldsymbol{D}}(\boldsymbol{x})} - \sqrt{p_{\boldsymbol{D}^{\text{sim}}}(\boldsymbol{x})}\right)^2}{2}} \quad (6)$$

where $\boldsymbol{x} = (x_1, \ldots, x_{n_d})$ denotes the input bin vector, n_d denotes the total number of data components, and N_{bin} is the total number of bins used to approximate the probability density functions of $\boldsymbol{D}$ and $\boldsymbol{D}^{\text{sim}}$ which are denoted respectively as $p_{\boldsymbol{D}}(\bullet)$ and $p_{\boldsymbol{D}^{\text{sim}}}(\bullet)$ respectively. It is observed from Eq. (6) that $d_H \in [0, 1]$.

To compute N_{bin}, the adaptive-binning approach proposed by Zhao et al. (2022) is implemented:

(1) Compute $\Delta^{\text{sim}} = \max\left(\max|\boldsymbol{D}_{i,m}^{\text{sim}} - \boldsymbol{D}_{j,m}^{\text{sim}}|\right)$; where $i, j = 1, \ldots, N$, $m = 1, \ldots, n_d$, and N denotes the total samples obtained from the posterior.
(2) Compute the Euclidean distance between the data set $\boldsymbol{D}$ and $\boldsymbol{D}^{\text{sim}}$: $d_E(\boldsymbol{D}, \boldsymbol{D}^{\text{sim}}) = \sqrt{(\overline{\boldsymbol{D}^{\text{sim}}} - \overline{\boldsymbol{D}}) \cdot (\overline{\boldsymbol{D}^{\text{sim}}} - \overline{\boldsymbol{D}})^{\text{T}}}$; where $\overline{\boldsymbol{D}^{\text{sim}}}$ and $\overline{\boldsymbol{D}}$ are the respective means of $\boldsymbol{D}^{\text{sim}}$ and $\boldsymbol{D}$.
(3) Compute $w = \frac{\log\left(\Delta^{\text{sim}}+1\right)}{\max\left(N^{1/3}, {N_{\text{obs}}}^{1/3}\right)} \times \exp\left(d_E\right)$
(4) Compute $N_{\text{bin}} = \frac{\Delta^{\text{sim}}}{w}$, and ensure that $N_{\text{bin}} \in \left[2, \frac{\max(N, N_{\text{obs}})}{10}\right]$.

3. Case Study: Sandia Thermal Problem

3.1. *Problem description*

The set-up is based on the challenge problem published by Dowding et al. (2008) involving a slab material which can be used in the construction of the nuclear reactor components (e.g., reactor vessel containment structure). The temperature response model M_T of the slab material under the different heating conditions is defined according to the following physics equation such that (Dowding et al. (2008)):

$$M_T(x, t) = T_i \quad \text{, for } t = 0s \quad (7)$$

$$M_T(x,t) = T_i + \frac{qL}{k} \cdot \left[\frac{(k/\rho C_p)t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2}\left(\frac{x}{L}\right)^2 - \frac{2}{\pi^2}\sum_{n=1}^{6}\frac{1}{n^2}\exp\left(-n^2\pi^2\frac{(k/\rho C_p)t}{L^2}\right)\cos\left(n\pi\frac{x}{L}\right)\right] \quad \text{, for } t > 0s \quad (8)$$

where $T_i = 25.0^oC$ denotes the initial ambient temperature, $L = 0.0190\ m$ denotes the slab's thickness, x denotes the location variable along the slab's thickness, t denotes the time elapsed since the start of the heating process, $q = 3000\ W/m^2$ denotes the heat flux, k denotes the slab's thermal conductivity $[W/m^oC]$, and ρC_p denotes the heat capacity of the slab material $[J/m^{3o}C]$.

For the problem, the material properties k and ρC_p are aleatory variables whose respective distributions are to be determined based on a set of data illustrated as a scatter plot in Figure 1, whose numerical values are presented in Table 4 of the literature by Dowding et al. (2008) (i.e., see case $N_c = 20$). As such, there are two objectives to the problem:

(1) to characterise the variability of k and ρC_p under limited data; and
(2) to validate M_T over a set of accreditation validation data, given the calibrated distribution over k and ρC_p.

3.2. *Methodology*

The initial analysis of the scatter plot in Figure 1 indicate a significant statistical correlation between k and temperature T, with a Pearson correlation coefficient of 0.870. In contrast, the statistical correlation between ρC_p and temperature T yielded a Pearson correlation coefficient of 0.127. For this reason, the variable ρC_p is assumed to be temperature-independent, while the dependence of k on T is modelled via a linear regression procedure which yielded:

$$k(T) = (2.25 \times 10^{-5}) \cdot T + 0.05 + \epsilon_k \quad (9)$$

where ϵ_k is the residual term, which is also an aleatory variable. Such observation is also consistent with the physics of the system where the thermal conductivity of the material can be temperature-dependent. Using Eq. (9), the data for ϵ_k is computed from that of k presented in Figure 1 to which its resulting histogram representation is presented in Figure 1.

Given no information on the distribution class of the aleatory variables, to eliminate the element of model uncertainty, a distribution-free approach involving the Staircase Density Function (SDF) is implemented to characterise the variability of ϵ_k and ρC_p. The SDF is a moment-matching meta-model that models a given data distribution based on its r^{th} central moment m_r defined as (Crespo et al. (2018)):

$$m_r = \int_{\underline{z}}^{\overline{z}} (z-\mu)^r \cdot f_z(z) \cdot dz; \quad \text{for } r = 0, 1, 2, \ldots \quad (10)$$

where the integration limits $\Delta_z = [\underline{z}, \overline{z}]$ is the bounded support set over the staircase random variable z, the function f_z is the probability density function, and μ is the expected value of the data variable z.

The probability density function f_z of the SDF is defined as (Crespo et al. (2018)):

$$f_z = \begin{cases} h_{i_b} \; \forall \; z \in ((i_b - 1) \cdot \kappa, i_b \cdot \kappa] & \text{, for } 1 \leq i_b \\ 0 & \text{, otherwise} \end{cases} \quad (11)$$

where $n_b = 25$ is the number of bins, $h_{i_b} \geq 0$ is the height of the SDF in the ${i_b}^{th}$ bin, and $\kappa = 2/n_b$ is the length of each sub-interval.

Based on Eq. (10), it is to be noted that the moments $m_0 = 1$, $m_1 = 0$, m_2 is the variance, m_3 is the third-order central moment, and m_4 is the fourth-order central moment. The constraints on the moments are such that: $\mu \in [\underline{z}, \overline{z}]$, $m_2 \in \left[0, \frac{(\overline{z}-\underline{z})^2}{4}\right]$, $m_3 \in \left[-\frac{(\overline{z}-\underline{z})^3}{6\sqrt{3}}, \frac{(\overline{z}-\underline{z})^3}{6\sqrt{3}}\right]$, and $m_4 \in \left[0, \frac{(\overline{z}-\underline{z})^4}{12}\right]$. Details on the SDF and the derivation of the aforementioned constraints are found in the literature by Crespo et al. (2018).

The SDF is calibrated on the data set of ϵ_k and ρC_p via the Hellinger-based stochastic model updating framework described in Section 2. The bounds Δ_z on the SDF for the respective variables are defined in Table 1 to ensure sufficient degree of freedom in the variability characterisation. The inferred parameters of the SDF are μ, m_2, m_3, and m_4 for which each of them is assigned a Uniform prior with bounds defined in Table 1.

For the approximate Gaussian likelihood function, the width parameter ε is decided to provided for 5 to 6 sampling iterations by the TEMCMC sampler, which ensures sufficient convergence of the sample distribution to the posterior. The values of ε used in calibrating the SDF of ϵ_k and ρC_p are defined in Table 1.

4. Results and Discussions

The resulting posteriors on the inferred parameters are illustrated in Figure 2. As seen in the figure, the parameter m_3 is normalized to $m_3/{m_2}^{3/2}$ which denotes the skewness term, while the parameter m_4 is normalized to $m_4/{m_2}^2$ which denotes the kurtosis term. As part of the challenge, the analyst is to provide a distribution over the data set of k and ρC_p. There are two ways to construct the distribution using the SDF: 1) using the Maximum A-posteriori (MAP); or 2) the mean estimates from the posterior. The numerical results to the respective type of estimates are presented in

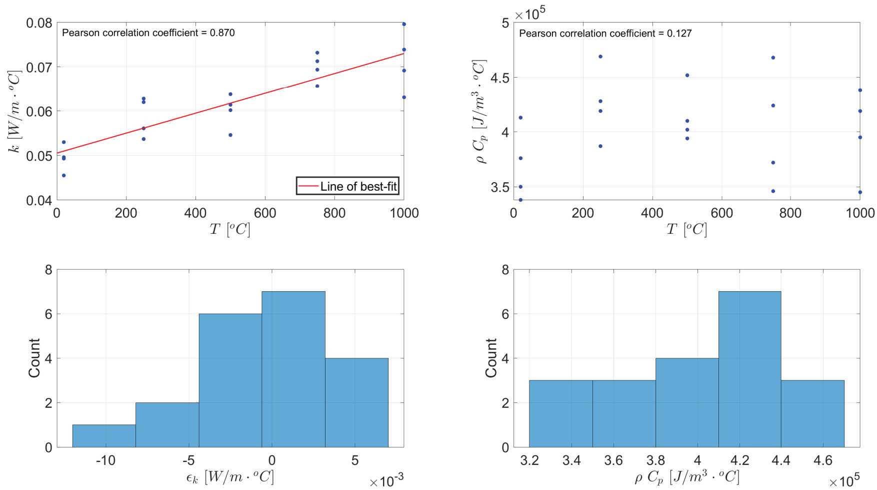

Fig. 1. Scatter plot and histogram representation of the data for k, ϵ_k, and ρC_p obtained from Dowding et al. (2008).

Table 1. Details on the SDF parameters for ϵ_k and ρC_p.

Parameter	Description	ϵ_k	ρC_p
ε	Width factor	0.10	0.05
Δ_z	SDF bounds	$[-2, 2] \times 10^{-2}\ W/m^oC$	$[3, 5] \times 10^5\ J/m^{3o}C$
μ	Mean	$[-2, 2] \times 10^{-2}\ W/m^oC$	$[3, 5] \times 10^5\ J/m^{3o}C$
m_2	Variance	$[0, 16] \times 10^{-4}\ (W/m^oC)^2$	$[0, 1] \times 10^{10}\ (J/m^{3o}C)^2$
m_3	Third central moment	$\left[-\frac{32}{3\sqrt{3}}, \frac{32}{3\sqrt{3}}\right] \times 10^{-6}\ (W/m^oC)^3$	$\left[-\frac{4}{3\sqrt{3}}, \frac{4}{3\sqrt{3}}\right] \times 10^{15}\ (J/m^{3o}C)^3$
m_4	Fourth central moment	$\left[0, \frac{64}{3}\right] \times 10^{-8}\ (W/m^oC)^4$	$\left[0, \frac{4}{3}\right] \times 10^{20}\ (J/m^{3o}C)^4$

Table 2, while the resulting calibrated distribution of k and ρC_p given the respective estimates are illustrated in Figure 3.

Subsequent analysis seeks to quantify and compare the validation performance of the temperature response model M_T given the calibrated SDF of k and ρC_p when the MAP estimates of the inferred parameters are used versus that when the mean estimates are used. To do so, a series of accreditation heating experiment has been conducted on the slab material for which 3 sets of 21 data points of the material response temperature T are obtained across time $t \in [0, 1000]\ s$ at $x = \{0, L/2, L\}$ respectively. The numerical data values are provided in Table 8 of the literature by Dowding et al. (2008) (i.e., see Exp 1).

The model validation procedure, based on a previous work by Ferson et al. (2008), is performed for a given value of x and time $t \in [0, 1000]\ s$ at time-step $\Delta t = 1\ s$ to which the procedure follows:

(1) For $t \geq 1\ s$, generate a sample of ϵ_k and ρC_p from their respective calibrated SDF. From which, compute the value of k via Eq. (9) using the sample realization of ϵ_k, and the output temperature T_1 computed from model M_T at time $t - 1$;

(2) Compute the temperature T_2 via model M_T. After which, compute the term $\delta = |T_2 - T_1|$. If $\delta > 0.005^oC$, proceed to Step (3). Otherwise, proceed directly to Step (4);

(3) Set $T_1 = T_2$ and compute the new value of T_2 via model M_T with the same seed value of k

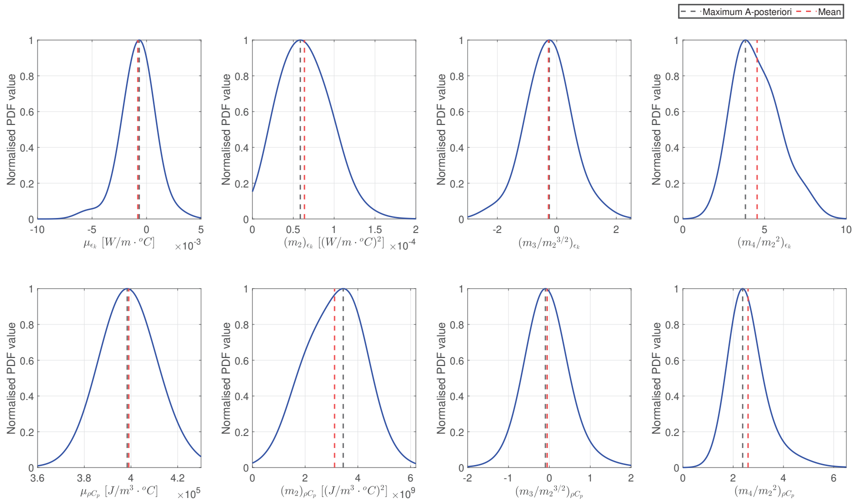

Fig. 2. The posterior distribution on the inferred parameters obtained via the Hellinger distance-based stochastic model updating framework.

Table 2. Posterior estimates on the SDF parameters for ϵ_k and ρC_p.

Parameter	Description	Estimate	ϵ_k	ρC_p
μ	Mean	Mean MAP	$-8.00 \times 10^{-4}\ W/m^oC$ $-6.71 \times 10^{-4}\ W/m^oC$	$3.99 \times 10^5\ J/m^{3o}C$ $3.98 \times 10^5\ J/m^{3o}C$
m_2	Variance	Mean MAP	$6.37 \times 10^{-5}\ (W/m^oC)^2$ $5.86 \times 10^{-5}\ (W/m^oC)^2$	$3.12 \times 10^9\ (J/m^{3o}C)^2$ $3.45 \times 10^9\ (J/m^{3o}C)^2$
$m_3/{m_2}^{3/2}$	Skewness	Mean MAP	-2.80×10^{-1} -2.52×10^{-1}	-5.38×10^{-2} -9.66×10^{-2}
$m_4/{m_2}^2$	Kurtosis	Mean MAP	4.54 3.83	2.59 2.38

and ρC_p obtained in Step (2). Compute δ and repeat this step until $\delta < 0.005^oC$;

(4) Set $t = t + \Delta t$, and repeat Steps (1) to (3) until the termination time $t = 1000\ s$.

The above procedure yields one set of outputs from M_T across all t, and a particular x given one stochastic realization of k and ρC_p from their respective calibrated SDF. To account for the variability, the above procedure is repeated $N_a = 1000$ times from the N_a realizations of k and ρC_p. The N_a ECDF representation of the temperature output from M_T across the time t obtained at each x are presented in Figure 4. As seen in the figure, the probability-box encloses the ECDF of the validation data which provides a first indication that the temperature model M_T given the corresponding calibrated SDF of k and ρC_p is sufficiently validated against the accreditation validation data.

The area metric d_A is computed to quantify the model validation performance by reflecting the degree of agreement of each model output ECDF against a given set of accreditation validation data. The area metric d_A is defined mathematically as:

$$d_A = \int_{-\infty}^{\infty} |F_{M_T}(y) - F_{\text{data}}| \cdot dy \qquad (12)$$

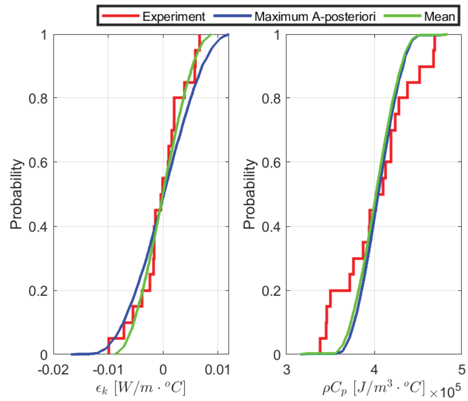

Fig. 3. The resulting calibrated SDF on ϵ_k and ρC_p.

where F_{M_T} is the ECDF of the model output, and F_{data} is the ECDF of the given accreditation validation data. From which, the mean and standard deviation values of d_A is obtained for which the results are represented as bar-charts in Figure 5. Based on the results, it is observed that the resulting calibrated SDF on k and ρC_p using the posterior mean on the inferred parameters results in a significantly better model validation performance against that when the posterior MAP on the inferred parameters are used.

5. Conclusion

The paper proposed a Hellinger distance-based stochastic model updating framework which contributes to the existing literature on the distance-based Approximate Bayesian Computation. From there, the proposed framework is implemented to perform an accreditation validation procedure based on the Sandia thermal problem by Dowding et al. (2008) where the shape parameters of the Staircase Density Function is inferred to characterise the variability of the aleatory model inputs, thereby providing a distribution-free approach to the problem. The results showed that the use of the posterior mean estimate values as input to the Staircase Density Function results in a better model validation performance than the posterior Maximum A-posteriori estimates.

Future research works may consider the following:

- implementing the proposed framework in updating models with a larger number of inferred parameters (e.g., >10 parameters) to assess its robustness; and
- to further improve the adaptive-binning algorithm towards improving the distribution approximation in cases where the data set is scarce (e.g. 6 data-points).

To provide a better understanding of the proposed framework and reproduce the results presented in the paper, the MATLAB codes used in the analysis are accessible on GitHub via: `https://github.com/Adolphus8/stochastic-model-updating.git`

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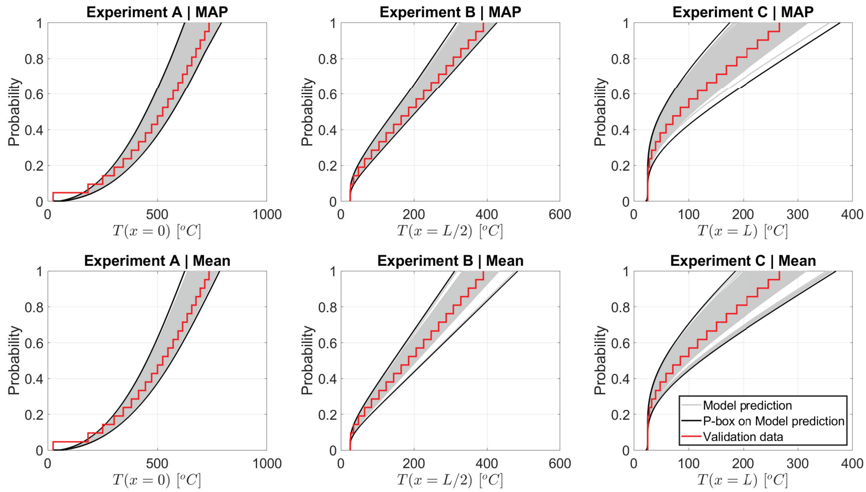

Fig. 4. The resulting prediction by the temperature response model M_T given the calibrated distribution of k and ρC_p against the accreditation validation data.

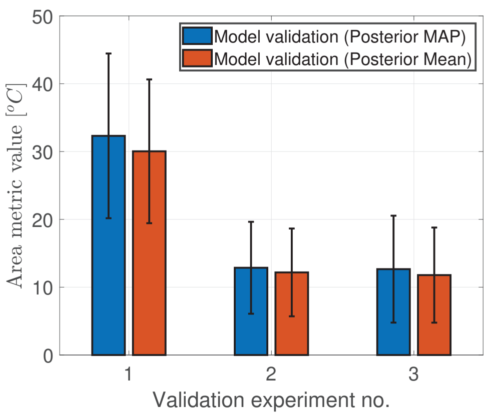

Fig. 5. The statistics to the validation performance by the temperature response model M_T. Note: The error bars denote the one standard deviation error.

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