A Novel Framework for Bayesian Calibration of Building Energy Models with Sub-hourly Building Operational Data
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Abstract
Building energy simulation models are useful for optimizing building systems, detecting and diagnosing faults, and making retrofit decisions. However, these models need to be calibrated with building data to accurately represent building systems. Bayesian calibration approaches have been developed to address the uncertainties in building behavior, but most of them are designed for monthly or yearly operational data. In this study, we propose a novel framework for Bayesian calibration of building energy models using sub-hourly building operational data. The framework employs parametric modeling methods for surrogate modeling and model inadequacy representation to improve computational efficiency and enable calibration with large time series datasets. In addition, it uses variational inference for the estimation of the posterior distribution over uncertain parameters. Our simulation study shows that the proposed Bayesian calibration framework provides reliable and cost-effective calibration of a building energy simulation model with a large time series dataset. With the proposed framework, it is expected that users can have well-calibrated detailed building models that can be used for whole building level problems (e.g., measurement and verification, retrofit) as well as subsystem level control and maintenance with a proper level of risk assessment.

Highlights
• A novel Bayesian framework is proposed, which allows the calibration of building energy simulation (BES) models with sub-hourly building operational data.
• To improve computational efficiency and enable calibration with a large time series dataset, the framework employs parametric modelling methods for both surrogate modelling and model inadequacy representation.
• This framework uses variational inference to further improve its computational efficiency.
• The performance of the proposed Bayesian calibration framework was evaluated through a simulation study.

Introduction
A detailed and accurate BES model can be used to (i) optimize the operation of building systems, (ii) detect and diagnose various faults, and (iii) make optimal decisions in building retrofit processes. However, previous literature has shown that a significant performance gap often exists between BES models created during the design phase and the actual target buildings (de Wilde, 2014). One of the major causes of such a gap is various assumptions made by modellers creating BES models. Making assumptions is unavoidable because accurate information about model input parameters is often not available (e.g., ground truth material properties, infiltration rates). Therefore, calibration of a model based on historical operational data from the target building is crucial before using the model in the operation phase. By improving the accuracy of a BES model through calibration, it becomes a valuable tool for improving building performance.

Generally, BES calibration approaches can generally be categorized as manual and automatic (Coakley, Raftery, and Keane 2014). Manual calibration approaches are typically labour-intensive, and the quality of the calibration is dependent on each modeller’s skills and experience (Coakley, Raftery, and Keane 2014). In recent decades, various automatic calibration approaches have been developed to address the limitations of manual calibration (Chong, Gu, and Jia, 2021). However, the majority of the automatic approaches aim to find deterministic point estimates of model parameters, which fit the data best (Chaudhary et al., 2016). This can result in estimates that are far from the true values, especially when the effect of varying one parameter is similar to that of another (e.g., window and wall R-values) (Heo, Choudhary, and Augenbroe, 2012). Additionally, the inherent imperfection of BES tools, rooted in assumptions and simplifications they are based upon (e.g., 1-D analysis for convective heat transfer), can lead to model inadequacy which can further exacerbate the potential for inaccurate calibration. Therefore, models calibrated using such automatic approaches may not be suitable for decision-making during the operation phase.

To address these issues, Heo (2012) first employed a Bayesian approach to calibrate normative energy models given monthly aggregated energy consumption data. Instead of seeking point estimates, Bayesian calibration considers uncertain model inputs as random variables. To proceed, a prior probability distribution over the inputs is first assigned. The distribution represents our current state of knowledge on the inputs, which is usually weak at the beginning, i.e., a high uncertainty. Given building operational data, Bayesian calibration returns the posterior probability distribution over the uncertain inputs.
which represents our updated knowledge after observing the data. In addition, the uncertainty due to model inadequacy is explicitly modelled and quantified simultaneously. The explicit consideration of model inadequacy helps decreasing unwanted biases in calibration. Based on the posterior distribution over inputs and model inadequacy, one can make reliable decisions considering the quantified uncertainty. To reduce computational load, Bayesian calibration often employs a surrogate model of the original BES model. Heo (2012) used two Gaussian process (GP) models for surrogate modelling and model inadequacy, which shows the potential of the Bayesian approach in BES calibration. However, the two GP models required a large amount of computation especially with bigger building operational datasets.

There have been various efforts to improve the computational efficiency in Bayesian calibration. Chong (2017) used the No-U-Turn Sampler, a Markov chain Monte Carlo (MCMC) sampling algorithm more efficient than the Metropolis-Hastings algorithm which Heo used, and reported improved efficiency. Li (2016) used a linear model for surrogate modelling, while modelling inadequacy as a GP. This method significantly improved the computational efficiency of both calibration and prediction. Lim (2017) compared five different surrogate modelling techniques, including multiple linear regression, neural network, supported vector machine, multivariate adaptive regression splines, and GP regression. Lim (2017) found that linear regression is the computationally most efficient approach while exhibiting the worst performance in estimating the posterior distribution. In reverse, GP regression is the most demanding computationally while showing the best performance. Zhang et al. (2019) used GP regression for surrogate modelling but ignored model inadequacy assuming that their building model can adequately represent the building. The assumption reduced computational load significantly and enabled BES calibration with one month data of five-minute interval. However, it remains unclear to what extent such an assumption can influence the accuracy of calibration in different scenarios. Rysanek (2019) proposed to use a pre-trained GP regression model as part of Bayesian calibration to improve its computational efficiency. The GP model is pre-trained to predict the root mean squared error (RMSE) between building model outputs and sub-hourly real-world data as a function of uncertain model inputs. They claimed that the most-likely values of uncertain parameters should minimize the RMSE and make RMSE converge to the sum of building model inadequacy and observational errors. However, according to the code released with this paper, it was assumed that there was no model inadequacy. Again, this assumption, ignoring model inadequacy, may degrade the accuracy of the calibration. Zhu et al. (2020) used approximate Bayesian computation (ABC) algorithms to avoid the expensive computation of likelihood. The ABC algorithms sample from the prior distributions randomly, conduct simulations under the surrogate model, and retain relevant samples as the posterior, based on the model bias with some predefined acceptance rate. Such method can be rather ineffective. To improve the sampling efficiency, this research adjusts the samples by applying a linear or non-linear regression model mapping model bias to uncertain inputs. But this research merely makes use of monthly energy consumption data. Similarly, Cant and Evins (2022) implemented an ABC method for model calibration, and this method incorporated Sequential Monte Carlo to increase the sampling efficiency. Still this research is also limited to calibration with monthly energy consumption data. The literature indicates that it remains a challenge to perform Bayesian BES model calibration with a large time series dataset not ignoring potential model inadequacy.

This study presents a novel Bayesian framework for the calibration of BES models with sub-hourly building operational data. To reduce online computational cost while addressing model inadequacy, the framework is equipped with parametric approaches for both surrogate modelling and model inadequacy representation.

**Methodology**

**Bayesian calibration**

Similar to previous research, the proposed framework employs the approach in Kennedy and O’Hagan (2001) to calibrate uncertain inputs, $\zeta$, in a BES model. This approach presents the relationship between observed data, $y$, and BES model output, $\eta(x, \zeta)$, as:

$$y(x) = \eta(x, \zeta) + \delta(x) + \epsilon$$

(1)

There are two model inputs: known inputs $x$ and uncertain model parameters $\zeta$. $\delta(x)$ denotes model inadequacy, which is the bias of the model from the true building behaviour. $\epsilon$ is observational error, which is assumed here to follow a zero-mean normal distribution, $\mathcal{N}(0, \sigma^2)$, where $\sigma$ is the standard deviation. The objective of the calibration problem is to estimate the posterior probability distribution over $\zeta$, $\delta$, and $\sigma$ given data, $x$ and $y$, as:

$$p(\zeta, \delta, \sigma | y, x) \propto p(y | x, \zeta, \delta, \sigma) \cdot p(\zeta, \delta, \sigma)$$

(2)

where $p(y | x, \zeta, \delta, \sigma)$ is data likelihood, and $p(\zeta, \delta, \sigma)$ is the prior probability distribution over the estimands, which represents the state of one’s knowledge before observing any data. With data, the state of one’s

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**Figure 1: Proposed Bayesian calibration framework**

- Select parameters $\zeta$ to calibrate
- Train RNN model as the surrogate
- Collect building operational data
- Determine priors for $\zeta$ and observational error $\epsilon$
- Apply pre-trained NP model to deal with model inadequacy
- Bayesian inference with variational inference
knowledge on the estimands is updated from the prior to the posterior. The posterior distribution is proportional to the product of prior distribution and likelihood function. In another word, both our belief and data of observation influence the posterior distribution. If the size of dataset is large, or the prior encodes relatively little information, then information from the data will overwhelm that of the prior, and vice versa (Pathak et al. 2019). If we have little knowledge about the parameter, an uninformative prior should be used.

Figure 1 shows the proposed framework. The following sections explain three key elements in the framework: (i) a recurrent neural network (RNN) for surrogate modelling; (ii) a neural process (NP) model for the representation of model inadequacy; and (iii) variational inference (VI), to reduce the online computational load for Bayesian calibration.

**RNN for surrogate modelling of BES model**

While the computational cost of a BES model such as EnergyPlus model may not be significant in a prediction task. It becomes a computational bottleneck in Bayesian calibration as it requires a huge number of simulation runs. To resolve this issue, surrogate modelling techniques are often used in Bayesian calibration. Many previous studies proposed to use a GP for surrogate modelling because of its flexibility. However, using a GP is computationally expensive, especially with a large amount of data, as the computational cost scales cubically with respect to the number of data points (Garnelo et al. 2018).

This study proposes to employ a recurrent neural network (RNN) for the surrogate modelling of a BES model. RNN is a parametric model and is specialized for processing a sequence of values, with the idea of sharing parameters across different parts of the model (Goodfellow, Bengio, and Courville 2016). Such sharing feature is very effective for time series data because it uses the same group of parameters for each timestep. Its high scalability and computational efficiency, compared to GP models, as well as its excellence in dealing with complex time series problems make it suitable for surrogate modelling.

Figure 2 shows a typical RNN which maps an input sequence to an output sequence of the same length. In this study, the RNN predicts room temperatures at time $t$ ($y^t$) with the hidden-state at time $t$ ($z^t$). The hidden-state is predicted with the inputs (including time-invariant building model parameters) at time $t$ ($x^t$) and the hidden-state at time $t-1$ ($z^{t-1}$). Since RNN has this recurrent structure, the inputs of previous time ($x^1$, ..., $x^t$) are used to predict the room temperatures at time $t$ ($y^t$). In this research, we use a multi-hidden-layer structure to increase the RNN expressive power.

To develop a surrogate model, the uncertain parameters should be first determined, followed by a number of simulations with the BES model varying these uncertain input parameters within a reasonable range. A Latin hypercube sampling can be used to generate samples over the input space effectively. Finally, a surrogate can be developed with these input and output data. The surrogate training can be done offline using high performance computing resources. Once trained, the parameters (e.g., weights) of the RNN model are frozen to be used as a replacement for the BES model in Bayesian calibration.

**NP for model inadequacy**

The model inadequacy term, $\delta(x)$, is essential for accurate estimation of the posterior probability distribution. The term is often modelled as a function of inputs, $x$. Existing approaches mostly use a GP to model the inadequacy term (Kennedy and O’Hagan, 2001). Modelling the inadequacy term as a GP has a couple of benefits. It has a high level of flexibility and expressive power. More importantly, unlike traditional parametric modelling methods, it allows for assigning a prior distribution over functions rather than parameters (Rasmussen and Williams, 2006). This is particularly useful when one has prior knowledge about how the function would look like, as is the case in BES model calibration. Performing model calibration, one expects that a well calibrated BES model would be good enough to mimic the true building behaviour even though there will be a certain level of discrepancy due to model inadequacy. In other words, it is a fair assumption that the inadequacy term, $\delta(x)$, is a smooth function close to zero over a reasonable range of inputs, $x$. With a typical parametric modelling method, it is difficult to encode such a function in a probabilistic way, especially if the degree of freedom in the model is high. GP as a distribution of functions is a perfect solution to capture the probabilistic behaviours of model inadequacy. However, the prohibitively high computational cost of modelling the inadequacy term with a GP overburdens the entire Bayesian calibration process and the use of the calibrated model especially when the dataset size is large.

The proposed framework employs a technique called neural process (NP) for modelling the inadequacy term, which combines the advantages of both GPs and neural networks (NNs) (Garnelo et al. 2018). NP is a neural network approximating a distribution over functions and can estimate the uncertainty in its predictions as a GP does. In addition, NP is computationally efficient in evaluation as a NN. Once trained, NPs generate predictions via forward-pass, the computational cost of NP is $O(n + m)$, much lower than that of GPs, $O(n + m)^3$, where $n$ and $m$ denote the numbers of testing data points and training data points, respectively. In this study, a NP model is trained with samples from a GP prior with a radial basis function.
kernel (Garnelo et al. 2018). As the behaviour of the trained NP model resembles that of a GP model, the NP model is used to model the inadequacy term instead of a GP model.

Variational inference

Most of the previous Bayesian calibration studies use MCMC sampling algorithms to acquire a set of samples that approximate the posterior probability distribution over the estimands (Heo, 2012; Chong, 2017; Li, 2016; Lim & Zhai, 2017; Rysanek, 2019; Hou, 2021). However, sampling methods are computationally intensive, especially for high-dimensional problems (Bishop 2006). To overcome this, variational inference (VI) methods (a.k.a. variational Bayesian methods) have been used. VI methods approximate the posterior distribution with a variational distribution by minimizing the difference between the posterior and variational distributions. Although there always exists an approximation error, solving an optimization problem is computationally considerably cheaper than sampling. Recent studies in the field of building science have demonstrated the efficacy of VI methods in tackling complex Bayesian modeling problems (Lee et al. 2019; Sadeghi et al. 2018). In terms of the quality of the inference result, Pathak et al. (2019) found that the mean field variational approximation approach achieved a similar level of accuracy as the more computationally intensive sampling approach. Another benefit of using VI is that it allows seamless integration of a Bayesian model with non-Bayesian components. Based on these benefits, this study uses VI for BES model calibration. In this study, Pyro, a probabilistic programming language written in Python and supported by PyTorch on the backend (Bingham et al. 2019), is used for Bayesian calibration with VI.

Simulation study

Previous studies have shown that a small discrepancy between the calibrated model outputs and real building data, as measured by metrics such as low normalized mean bias error (NMBE) or coefficient of variation of the root mean squared error (CVRMSE), does not necessarily indicate that the estimated parameters are close to the true values (Heo, 2012). Therefore, evaluating the goodness of a calibration method based solely on predictive performance metrics computed over a certain dataset may not be sufficient. To address this limitation and examine the quality of the posterior distributions estimated by the proposed Bayesian calibration framework, a simulation study is designed and conducted. Since all ground truth mechanisms are known in a simulation study, by comparing the calibrated model with the ground truth, the strengths and limitations of the framework can be investigated, and opportunities for improvement can be identified.

For the simulation study, the ASHRAE standard 90.1 prototype small office building model for Climate Zone 6A (PNNL, 2018) is utilized assuming it is a real building. This building model (Figure 3) includes five conditioned thermal zones and one un-conditioned zone (attic). To generate building operational data with the model, a simulation is conducted using Toronto weather data in the Canadian Weather Year for Energy Calculation (CWEC) library (Government of Canada, 2018). The simulation period is set to January 2nd to January 15th, and 10-minute timestep is used, i.e., 2016 timesteps in total. During this period, indoor temperature setpoints are randomly changed every two hours to generate data under system excitation. The indoor air temperatures and sensible cooling and heating rates are used for calibration. To simulate sensor errors, random numbers generated from a zero-mean Normal distribution with a variance of 0.5°C are added to the air temperature data. To test the proposed calibration framework, first, it is necessary to choose a set of parameters and treat them as unknowns. Through sensitivity analysis, previous studies have shown that material thermal properties, internal loads, setpoint temperatures, ventilation and infiltration rates, and HVAC system efficiencies are important parameters affecting building thermal behaviour (Heo 2012; Chong 2017). In this study, the seven parameters listed in Table 1 are selected and assumed to be uncertain. Some of the parameters, such as SHGC, infiltration rate, and appliance/lighting power density are likely to vary with time. However, they are treated as time-invariant parameters in this study for simplicity. In addition, it is assumed that all the other inputs including weather are known.

To calibrate the uncertain parameters, a model for the target building is necessary. In this study, the EnergyPlus model used for data generation is utilized. This means that there is no model inadequacy, and if the ground truth parameters are provided, the model will perfectly replicate the behaviour of the true building. But please

<table>
<thead>
<tr>
<th>Table 1: Selected uncertain parameters</th>
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<tr>
<td>Category</td>
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<td>--------------------------</td>
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<tr>
<td><strong>Thermal property</strong></td>
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<tr>
<td>Glass U-factor</td>
</tr>
<tr>
<td>Glass SHGC</td>
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<tr>
<td>Attic roof deck conductivity</td>
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<tr>
<td>Exterior wall insulation layer thermal resistance</td>
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<tr>
<td><strong>Infiltration</strong></td>
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<tr>
<td>Flow rate per exterior surface area</td>
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<tr>
<td><strong>Internal load</strong></td>
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<tr>
<td>Appliance power density</td>
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<tr>
<td>Lighting power density</td>
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note that the use of a surrogate model (described in the subsequent section) adds model inadequacy into this calibration problem.

**Surrogate modelling**

With the building model, a synthetic dataset, which consists of 1000 simulation cases, is first generated by varying the seven uncertain parameters in Table 1. Every simulation case produces sequential data of 2016 timesteps. Since training an RNN model for 2016 timesteps is computationally expensive, each set of 2016 sequential data points is subdivided into 56 sequences (36 timesteps for 6 hours in each sequence). 80% of the 56000 sequences (1000 simulation cases × 56 sequences), are used to train an RNN, and the rest (20%) is used for testing. Table 2 shows the inputs and outputs for surrogate modelling. For the evaluation of the posterior distributions, an RNN model showing a test dataset RMSE of 0.2821°C is used.

**Model inadequacy**

Because of the discrepancy between the EnergyPlus model and its surrogate (i.e., RMSE of 0.2821°C), model inadequacy is introduced in this calibration problem. The model inadequacy term is modelled with a pre-trained NP model which emulates the behaviour of a GP model. The training of the NP model makes use of data sampled from a GP prior and is independent of this simulation study.

The input dimension of the NP model is one, while that of the surrogate model excluding the seven uncertain parameters is 25 (i.e., dimension of \( x \) in Eq. (1) is 25). For dimensionality reduction, a NN is connected to the input side of the NP model. The training of the NN is performed concurrently with Bayesian calibration.

**Bayesian calibration**

A prior distribution is assigned for each of the uncertain parameters. In this simulation study, we refer to ASHRAE Handbook (2009) and construct priors of a wide range. Since all the uncertain parameters should be positive, a Gamma distribution is chosen for each of them. The standard deviations for the observation error terms, an exponential distribution is assigned to each. All the prior distributions are visualized in Figure 4.

<table>
<thead>
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<th>Table 2: Inputs and outputs for surrogate modelling</th>
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<tr>
<td>Inputs</td>
</tr>
<tr>
<td>- Sensible cooling and heating rates in 6 zones</td>
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<tr>
<td>- 11 weather parameters in the weather data</td>
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<tr>
<td>- Day of week</td>
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<tr>
<td>- Time of day</td>
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<tr>
<td>- The 7 uncertain parameters</td>
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<tr>
<td>Outputs</td>
</tr>
<tr>
<td>- Indoor air temperatures in 6 zones</td>
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</table>
Results
Posterior distribution of uncertain input parameters

Figure 4 shows the marginal distributions of samples from the prior distribution (blue histogram) and fitted variational distribution (orange histogram) for the uncertainty model input parameters, $\zeta$, and the standard deviations for the observational error terms, $\epsilon$. The orange histograms are much narrower than the blue ones. This means the state of knowledge on these estimands was improved by observing the data, and the level of uncertainty decreased. In other words, it implies that the data contained sufficient information to update our knowledge. For all the uncertain model input parameters, $\zeta$, the ground truth parameter values (black vertical lines) lie within the orange histograms. Regarding the standard deviations, although there are some discrepancies, but in general, the histograms are close to the ground truth values. This provides evidence that the proposed framework is effective in calibrating a BES model with a time series dataset in a Bayesian way, i.e., estimating the posterior distribution. However, it also suggests that the framework needs improvements. There are three potential causes that resulted in the discrepancies between the ground truth values and the histograms. First, the expressive power of the NP model, which was used to model the inadequacy term, $\delta(x)$, might not be sufficient to fully capture the model inadequacy. In this simulation study, the inadequacy term is solely attributed to the discrepancy between the original EnergyPlus model and its RNN surrogate. It was found that there was an autocorrelation in the error between the original and surrogate models, shown in Figure 5. Since a GP model without information from previous time steps usually show limited performance in dealing with autocorrelated time series data, it is natural that the NP model trained with data from a GP prior cannot perfectly model the inadequacy term. Second, the variational distribution used in this study, which is a normal distribution with a diagonal covariance matrix in a transformed space, might not be suitable to approximate the true posterior. Third, the optimization for VI might be converged at a local minimum, not the global.

The marginal distributions for Insulation, Appliance power density, and Light power density show high variation while the marginal distributions for the other parameters are narrower. This suggests that while the data was effective in significantly reducing uncertainty for the other parameters, it was not as effective as for these three parameters. As the amount of data increases, the uncertainty for these parameters is expected to decrease. However, it is worth noting that the quality of a dataset also affects how effective the dataset is in reducing the uncertainty for specific parameters. In addition, the way the inadequacy term is modelled also influences the estimated posterior distribution given a certain dataset.

Figure 5: Posterior predictive distributions for the indoor air temperatures of the six zones over a 6-hour period. The blue solid lines are the mean of the distributions. The blue shaded areas represent the model uncertainty. The yellow shaded areas show the full uncertainty including both the model uncertainty and observation errors. The orange lines denote the ground truth, and the blue dots denote the observation data.

Figure 6: Error between EnergyPlus model and its surrogate given ground truth of uncertain input parameters. $\epsilon \sim \epsilon_x$, denote the prediction discrepancies of indoor temperature in 6 zones.
Posterior predictive distribution

Figure 6 illustrates the posterior predictive distributions for the indoor air temperatures of the six zones over a 6-hour period. The blue shaded areas represent the model uncertainty attributed to the uncertain model inputs and model inadequacy. The blue solid lines are the mean of the distributions. The yellow shaded areas show the full uncertainty including both the model uncertainty and observation errors. The shaded areas are the 90% credible intervals (i.e., 5- and 95-quantiles) of the predictive distributions. The ground truth temperatures (orange solid lines) are within the blue shaded areas, and most of the observations (blue dots) are within the yellow shaded areas. This suggests that the combination of the surrogate model (RNN) and the model for the inadequacy term (NP) with the posterior distribution over the uncertain input parameters can find reliable predictions.

Conclusion and discussion

This paper proposes a novel framework for Bayesian calibration of BES models with sub-hourly building operational data. This framework employs parametric modelling techniques to improve computational efficiency. For surrogate modelling, a recurrent neural network (RNN) is used to deal with time series data. For modelling of the model inadequacy term, a neural process (NP) model, which emulates the behaviour of a GP model, is used.

To evaluate the performance of the proposed framework, a simulation study was performed. The marginal posterior distributions for the estimands were coinciding with or close to the ground truth values. In addition, the surrogate model and model for the inadequacy term returned reliable posterior predictive distributions for the zone air temperatures, which cover the ground truth air temperatures. These results provide evidence that the proposed Bayesian calibration framework enables reliable and cost-effective calibration of a building energy simulation (BES) model with a fairly large time series dataset. Since a reliable building model is one of the major hurdles in developing advanced solutions for buildings, the proposed framework will contribute significantly to advancing our buildings.

However, the results also revealed that further research is required to improve the proposed framework. Since there is a high chance that autocorrelation exists in model inadequacy, the method for modelling the inadequacy term needs to be improved to reduce potential bias. In addition, using a richer family of distributions for variational inference (VI) will significantly improve the quality of the estimated posterior distribution.

In this study, the uncertainty in weather, occupancy, HVAC operational data were ignored, i.e., it was assumed that they were all known. In our future study, the framework will be tested under more realistic scenarios with diverse sources of uncertainty. In addition, the impact of the quality and quantity of a dataset on updating one’s state of knowledge will be investigated as Lee et al. (2020) did. There have been extensive efforts to develop better deep learning methods for sequential data. The surrogate modelling part would benefit from adopting such new time series modelling methods.

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