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A SIMPLIFIED BAYESIAN APPROACH FOR THE CALIBRATION OF DISTRICT-BUILDING ENERGY MODELS

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Abstract

Bayesian optimization with surrogate modeling is widely used to calibrate building energy models. However, complexities arise in surrogate modeling due to the variability in building morphology at the urban scale. Thus, maintaining dynamic simulation accuracy is crucial. This study presents a novel optimization framework for calibrating district-building energy models using Bayesian decision theory. Once tested on a case study district, the approach reduces monthly calibration error by approximately 45%. Future works could be employing more robust classifiers and handling imbalanced target variables. The proposed approach can minimize computational demands for optimizing dynamic models while ensuring reliability.

Introduction

Building energy use contributed to 60 million tons of increase in greenhouse gas (GHG) emissions globally in 2022, comprising over 19% of the total rise in GHG emissions from the world's overall energy consumption (OECD, 2023). The construction industry should be investigated thoroughly to understand and reduce such a vast energy use. The occupant-related uncertainties (Santin et al., 2009) and the diversity in the characteristics of the urban building stocks (Oraiopoulos and Howard, 2022) complicate the analysis of the building energy demand with reliable assumptions. Similarly, the construction industry's partial failure in digitization and the resulting lack of comprehensive data hinder studies examining the energy consumption of urban building stocks (Reinhart and Davila, 2016) (Ferrando et al., 2020). However, well-equipped building energy models can provide sustainable solutions to monitor and control urban building energy use (Wang et al., 2018) (Buckley et al., 2021). Dynamic models in building energy modeling (BEM) and urban building energy modeling (UBEM) involve creating computer models that simulate the energy performance of buildings. During simulation, these models evaluate many factors, such as building materials, HVAC systems, occupancy patterns, and weather conditions. Unlike statistical models that analyze the correlation between the building energy-related parameters and the resulting energy consumption and provide predictions usually at lower temporal resolutions (e.g., annual predictions), dynamic models track how energy usage fluctuates throughout the day, week, month, or even year by considering the variations in the building operational schedules and the climate conditions (Pan et al., 2023).

The parameters of dynamic models often need calibration due to insufficient data to characterize buildings accurately, especially at urban level analysis, where diverse building stocks complicate calibration against metered consumption data (Chong et al., 2021). However, calibration is an iterative process that hinders the parametric optimization of dynamic models, which are computationally expensive due to exhaustive simulations covering the thermal interaction between building components. In this sense, Bayesian Optimization stands out as a powerful technique for calibrating simulation parameters (Hou et al., 2021). Traditionally, Bayesian Optimization employs surrogate models, such as regression models or Gaussian processes, to approximate the complex relationships within the dynamic simulation framework (Hou et al., 2021). These surrogate models replace the actual dynamic models and significantly reduce the computational time. They facilitate assessing various scenarios and obtaining optimal parameter combinations efficiently.

For instance, Markov chain Monte Carlo (MCMC) algorithms are prevalent optimization methods that employ surrogate modeling to estimate the posterior distribution of unknown parameters in Bayesian calibration. MCMC algorithms iteratively determine optimization directions by assessing parameter combination errors. In this regard, it resembles the online learning concept adopted in Artificial Neural Network (ANN) models (Rumelhart et al., 1986). Dynamic models are black box models whose simulation output depends on various complex assumptions and factors. Therefore, surrogate modeling approaches are valuable in BEM or UBEM when the dynamic models offer no analytical solution that refers to a direct mathematical method for determining the likelihood of parameter values and, consequently, the posterior probabilities (Hou et al., 2021). Surrogate models are effective when there is little or no knowledge about the possible values of the parameters and their prior probabilities.

However, replacing the dynamic models with surrogate models might yield a loss of accuracy in modeling complex patterns in building morphology at the district and urban scales. When the objective function is spoiled due to the high uncertainty raised by urban building stocks, the optimization process can be faulty. Therefore, the precision of models defining the optimization function becomes crucial even though utilizing an actual model instead of a surrogate model in the likelihood creation process can be exhaustive. Hence, this study proposes a simplified Bayesian optimization method to overcome the limitations arising from the computational requirements and reliability of surrogate modeling. Here, the primary aim is to filter and reduce the size of the parameter space. The proposed approach defines a simplified version of the Bayesian likelihood by assessing the probability of success in scenarios. This approach can be utilized for optimization problems that involve complex computational models (dynamic models) where the actual objective function is not easily accessible. It can be precious when uncertainty regarding the possible value ranges for simulation parameters can be significantly reduced through knowledge acquired from buildings' energy-related records or thorough research. Therefore, it can potentially enhance the optimization process without relying on surrogate modeling techniques.

Methodology

The methodology consists of five sequential steps. First, a dynamic model of the buildings in a selected district is constructed. Next, energy simulations are conducted for various scenarios, each comprising different combinations of simulation parameters, through the dynamic model. These scenarios are then compared with the measured data and labeled as desired and undesirable according to their monthly simulation errors. Subsequently, a Gaussian Naive Bayes Classifier is developed to classify scenarios as either desired or undesired. This classifier enabled the optimal parameter combination to be derived from the posterior distributions of the simulation parameters. Ultimately, a Bayesian Model is created using the optimal parameter combination, and a final energy simulation is performed to evaluate the proposed calibration of the dynamic model. The methodology workflow is demonstrated in Figure 1.

1. Building A Dynamic Model

The proposed calibration approach begins by creating a dynamic energy model for a sample district. Choosing a modeling tool with a user-friendly interface is crucial for easy adjustments to input data to optimize the dynamic model. Furthermore, the performance of the selected modeling tool must be validated, particularly in urban-level building energy assessment, to ensure its robustness and reliability. Therefore, the Urban Modeling Interface (UMI), a widely used tool in urban planning studies worldwide (Ang et al., 2022), is selected to assess the building energy consumption of the sample district. UMI is developed by MIT Sustainable Design Lab (Reinhart et al., 2013). UMI is integrated into a computer-aided design (CAD) program called Rhinoceros 3D (Rhino) that provides a user-friendly environment for the modeling and simulation steps (McNeel and Associates, 2008). UMI requires three main types of input data to create a 3D dynamic model. These are building templates, building geometries, and weather data. A building template is text-based data that includes various categories with the essential characteristics of the buildings, such as the building envelope properties, zone conditioning details, HVAC details, domestic hot water (DHW) details, and building operational schedules. Each category requires a detailed description of the mechanical systems, building parts, or operations. A building template should adequately represent the selected buildings in a district to ensure the accuracy of the energy simulation. Buildings are represented within archetypes of building energy models since modeling each building with its specific characteristics is time-consuming at the district and urban scales. The following input of the dynamic model is the building geometries. Building geometries are attained from existing building footprints or newly created ones in GEOJSON format. These footprints, along with building heights and glazing ratio of building surfaces, are processed in the UBEM.io tool (Ang et al., 2022) to create the building geometries. The final input of the dynamic model is weather data in EnergyPlus Weather (EPW) format. Typical EPW weather data includes comprehensive meteorological information such as temperature, humidity, wind speed and direction, solar radiation, and precipitation recorded at regular intervals. Once these three components of the dynamic model are gathered, the 3D UMI model is ready for the energy simulations.

2. Performing Energy Simulations

The dynamic model consists of various inputs (simulation parameters) that represent the energy consumption characteristics of buildings. These parameters need optimization to minimize simulation errors. Once the simulation parameters are identified for optimization, scenarios are crafted by combining them, and these scenarios are integrated into the 3D UMI Model as building templates. Monthly energy simulations are subsequently conducted for each scenario.

3. Labeling Scenarios

Monthly simulation errors of the scenarios against metered data are calculated using the Coefficient of Variation of the Root Mean Square Error (CV-RMSE) (Equation 1).

$$CV - RMSE = \frac{1}{\bar{r}} \sqrt{\frac{\sum_{t=1}^{N} (r^t - y^t)^2}{N}} \quad (1)$$

In Equation 1, $\bar{r}$ is the average of the monthly target consumption obtained from metered data, r^t represents the monthly cumulative target consumption, y^t is the monthly cumulative simulation result, and N is the total number of monthly simulation outputs, which is twelve. As seen from Equation 1, CV-RMSE decreases as the monthly simulation errors get smaller and more consistent. Hence, it simultaneously evaluates the stability and accuracy of the dynamic model. Additionally, an error metric named MAPE, which calculates the average percentage difference between simulation results and metered data, is utilized to measure the scenario errors (Equation 2).

$$MAPE = \frac{1}{N} \sum_{t=1}^{N} \left| \frac{r^t - y^t}{r^t} \right| \quad (2)$$

The main idea of the proposed approach is to label scenar-

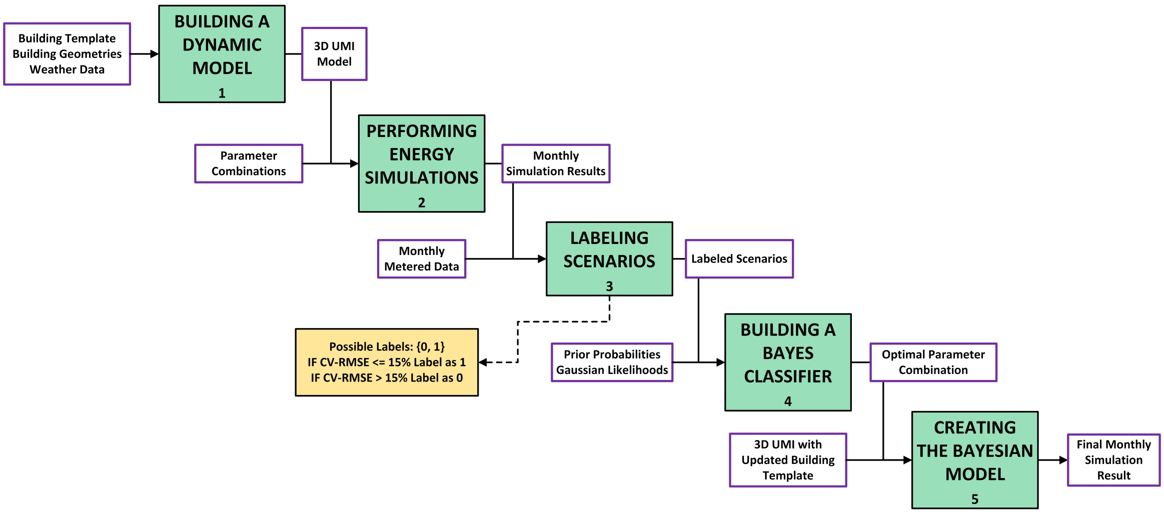

Figure 1: Methodology workflow

ios according to their simulation errors and subsequently perform classification to derive the optimal parameter values. To achieve this, a maximum allowable error limit for CV-RMSE is defined. ASHRAE suggests that the simulation (or prediction) error should not exceed 15% at the monthly resolution based on the evaluation metric CV-RMSE (ASHRAE, 2002). Thus, the maximum allowable error is set to 15% of CV-RMSE, and each scenario is labeled according to the total operational energy use intensity. For example, if a scenario's error is less than or equal to the maximum allowable error, the scenario is labeled one, and zero otherwise. The scenarios with label one are considered as desired scenarios.

4. Building A Bayes Classifier

The optimization becomes a binary classification task after labeling scenarios. Here, the goal is to derive the posterior probability distributions for the scenario labels (zero and one) using the Bayes formula in Equation 3:

$$P(L_i \mid X) = \frac{P(X \mid L_i)P(L_i)}{P(X)} \tag{3}$$

In Equation 3, X denotes the parameter combination, and L_i represents the scenario label. There are two possible labels for each scenario: $L_i = \{0, 1\}$. The posterior distributions for the labels zero and one are determined using the likelihood function $P(x \mid L_i)$ and prior probabilities $P(L_i)$ since the denominator $P(X)$ is the same for both labels. The term $P(X)$ in the denominator is called evidence, which is the probability of observing a certain parameter regardless of a condition. The prior probability $P(L_i)$ is the ratio of the number of scenarios with label i (zero or one) to the total number of scenarios. The likelihood function is the joint probability distribution of the simulation parameter combinations for each label. Here, the simulation parameters are assumed to be conditionally independent for simplicity of the optimization (Equation 4. This transforms the model into a Naive Bayes classifier.

$$P(X \mid L_i) = \prod_{m=1}^{n} P(x_m \mid L_i) \tag{4}$$

The likelihood function is the multiplication of the conditional probability of each simulation parameter over a given label. In Equation Equation 4, m is five since there are five parameters in scenarios. Each conditional probability $P(x_m \mid L_i)$ is assumed to have a Gaussian (normal) distribution with the parameters μ_m (mean) and σ_m (standard deviation) as shown in Equation 5.

$$P(x_m \mid L_i) = \frac{1}{\sigma_m\sqrt{2\pi}} \exp\left(-\frac{(x_m - \mu_m)^2}{2\sigma_m^2}\right) \tag{5}$$

Here, the objective is to find the optimal normal distribution parameters for each conditional probability $P(x_m \mid L_i)$. This is achieved by using the maximum likelihood estimation, wherein the gradient of the likelihood function is taken with respect to the distribution parameters (mean and standard deviation) to derive the optimal distribution parameters. These means and standard deviations are chosen to maximize the likelihood of the observed data given each label. Consequently, there are two posterior distributions with optimal mean and standard deviation corresponding to the labels zero and one. The expected value of a simulation parameter x_m, representing the average outcome expected to occur over many repetitions of the random event, can be calculated from its posterior probability distribution conditioned on a specific label L_i. Therefore, the expected values of the simulation parameters are the means of their posterior distributions based on labels one and zero, Here, it is essential to differentiate between simulation and distribution parameters to avoid confusion. Once the classification over the labeled scenarios using a Gaussian Naive Bayes classifier is implemented, each simulation parameter gets posterior distributions for the labels zero and one. The expected values of the simulation parameters are then derived from the means of these posterior distributions. As the optimal values of the simulation parameters should fall within the desired label distributions, the optimal parameter combination is obtained using the expected values of the distributions conditioned over label one.

5. Creating The Bayesian Model

The optimal values of the simulation parameters are integrated into the 3D UMI Model as an updated building template. This updated model forms the Bayesian model. Subsequently, the Bayesian model is simulated, and the monthly simulation results are compared to metered data to evaluate the optimization performance.

Case Study

The dormitory area of Özyeğin University campus in Istanbul was selected as the sample district. There are six dormitory buildings in this area Figure 2. Two energy audit reports from 2014 and 2020, which contain essential information about the energy performance of the dormitory buildings, were used to identify and characterize buildings in the building template. The dormitory buildings have similar building properties and energy consumption patterns. Therefore, a single archetype, named Dormitory, was created to represent all the buildings in the dynamic model. To create building geometries, polygons representing the building footprints in the district on the map were initially drawn in Yandex Map Constructor. These footprints were then saved as a map layer and exported as a GEOJSON file. Subsequently, this file was processed in the UBEM.io tool, in which a GIS interface ensured that the buildings were located in valid coordinates and that the footprints were not overlapping. Building heights were incorporated into UBEM.io to finalize the geometric model. There are multiple weather stations near campus. The hourly weather data between September 2018 and September 2023 were obtained from the Turkish State Meteorological Service (TSMS) from the nearest station to the campus. This data includes temperature, relative humidity, dew point temperature, wind direction and speed, sun exposure intensity, global solar radiation, and total precipitation at the hourly resolution within the given years. After obtaining three major components of UMI, a dynamic model of the district was established.

The metered data obtained from the campus energy management department includes natural gas and electricity consumption. This data forms the study's validation data. The dynamic model created via UMI considers several end-uses when determining the operational energy consumption of the dormitory buildings. Among these end-uses, cooling, equipment use, and lighting energy are set to be provided with electricity, whereas heating and DHW are supplied by natural gas. The electricity and natural gas consumption are recorded for each building at the monthly resolution. Even if small air conditioners cool the offices of the authorized dormitory personnel, it is assumed that the dormitory buildings do not have a cooling system. The validation data was derived from the average monthly metered consumption data between September 2018 and September 2023. Notably, the time intervals overlapping with the COVID-19 pandemic significantly impacted the energy consumption patterns of the dormitory buildings due to the absence of occupancy. Thus, the period spanning March 2020 to October 2021 was excluded from the weather and validation data.

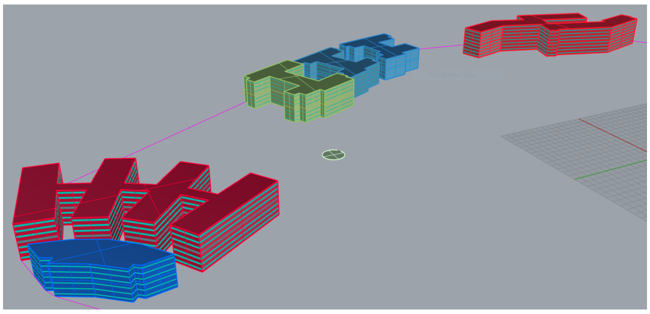

Figure 2: 3D dormitory model in Rhino

The building properties in the energy audit reports were processed, and the average values of the available parameters were used to characterize the archetype in the dynamic model. Table 1 shows the details of the essential parameters of the dynamic model. The dormitory buildings on the campus have similar characteristics. Y1, Y2, Y3, and Y4/5 buildings were built in 2012, whereas Y6 and GH were built in 2019. Hence, there is a small variation in the envelope properties of the dormitory buildings. Some parameters could not be obtained from the energy audit reports, such as infiltration rate, equipment power density (EPD), lighting power density (LPD), and DHW flow rate. There needs to be prior knowledge about the possible value ranges for these parameters. Thus, these parameters were assumed to hold the most uncertainty among the parameter space of the dynamic model and were selected for optimization. In addition, the heating set point was manually selected for optimization since this parameter can drastically affect the intensity of the zone conditioning and the resulting energy consumption.

The unit of the infiltration rate is the air change per hour (ACH), which denotes the ratio of the inside air volume replaced by the outside air due to the natural leakages on the building surface. The air leakage from the building surfaces is expected to be low in the campus buildings since dormitory buildings are constructed after 2012. Therefore, the upper limit of the infiltration rate was set to 0.5, where the minimum was 0.1. Similarly, an upper and lower limits were determined for EPD (Deru et al., 2011) (Mahajan et al., 2017) (Chang and Crawley, 2018), LPD (Deru et al., 2011) (ASHRAE., 2020), and DHW flow rate (Deru et al., 2011) (Murakawa et al., 2005) (Pérez-Lombard et al., 2008) using the literature. Overall, five parameters were chosen for optimization. The average values detected from the literature and the energy audit reports formed the input of the Baseline Model. The possible value ranges for these simulation parameters are outlined in Table 2. Five distinct values were generated for each

Table 1: Simulation parameters of the dynamic model

Parameter Name	Unit	Prior Knowledge
Wall U-Value	$W/m^2/K$	Available
Roof U-Value	$W/m^2/K$	Available
Ground U-Value	$W/m^2/K$	Available
Window U-Value	$W/m^2/K$	Available
Occupant Density	$people/m^2$	Available
Heating and Cooling Set Points	Degree Celsius	Available
Heating COP	%	Available
Infiltration	ACH	Not Available
EPD	W/m^2	Not Available
LPD	W/m^2	Not Available
DHW Flow Rate	$m^3/h/m^2$	Not Available

simulation parameter within the minimum and maximum bounds from Table 2 with equal intervals. This resulted in a total of 3125 parameter combinations. These diverse combinations were simulated in UMI. Monthly simulation errors against the metered data were then calculated using CV-RMSE (Equation 1) and MAPE (Equation 2) metrics. The metered data for monthly natural gas and electricity consumption are available for the dormitory buildings. However, for the sake of simplicity in the calibration process, the total operational energy (TOE) use intensities in kWh/m^2, representing the TOE over the gross floor area of the dormitory buildings, were utilized to compute scenario errors against the metered data. These scenarios were categorized according to their error, with those exhibiting an error smaller than 15% of CV-RMSE labeled as one, and zero otherwise.

Lastly, a simplified Bayesian optimization approach classified these scenarios by employing a Gaussian Naive Bayes classifier. The classifier determined posterior probability distributions for scenario labels based on a likelihood function derived from the simulation parameter combinations. Maximum likelihood estimation determined optimal distribution parameters (mean and standard deviation) for each conditional probability distribution. The expected values of simulation parameters were then obtained from the mean of the posterior distributions. The combination of these simulation parameters formed the Bayesian Model. Subsequently, UMI simulations were performed once more for the Bayesian Model.

Table 2: Optimization ranges for the selected parameters

Parameter	Baseline Value	Min. Value	Max. Value
Infiltration	0.30	0.10	0.50
Heating Set Point	21.50	20.00	23.00
EPD	7.50	5.00	10.00
LPD	6.00	3.00	9.00
DHW Flow Rate	2.55E-04	7.09E-05	7.09E-04

Results and Discussion

The optimal values for the simulation parameter were determined as the means of the posterior distributions for label one (Table 3). The new scenario with the optimal simulation parameters formed the Bayesian Model. A fundamental way to detect the optimal scenario combination is to select the scenario with the least CV-RMSE manually. The manually selected parameter combination with the least CV-RMSE was named the Deterministic Model. According to Table 4, the Deterministic Model decreased the simulation CV-RMSE of the Baseline Model by nearly 60%, whereas the Bayesian Model decreased the baseline error by around 45%. Even though the deterministic calibration seems to provide the optimal parameter combination with the least simulation error, this can be deceptive.

Table 3: Parameter combinations of different models

Parameter	Baseline	Deterministic	Bayesian
DHW Flow Rate	3.90E-04	5.49E-04	6.11E-04
EPD	7.50	5.00	7.41
Heating Set Point	21.50	21.50	20.93
Infiltration	0.30	0.40	0.39
LPD	6.00	3.00	5.77

Let us recall that the simulation parameters were calibrated based on a single target end-use, TOE use intensity. TOE provides an aggregated energy use as it is the summation of electricity and natural gas consumption values. Table 5 and Table 6 demonstrate detailed error comparisons of the calibrated model based on the monthly CV-RMSE and MAPE values. According to Table 5 and Table 6, it is evident that the Bayesian Model achieved a more balanced error distribution between electricity and natural gas. Specifically, the combined average CV-RMSE for electricity and natural gas is 0.267 for the Bayesian Model, compared to 0.318 for the Deterministic Model. This superior performance of the Bayesian Model can be attributed to its detailed parameter combination. As illustrated in Table 3, the simulation parameters of the Bayesian model exhibit distinct values, unlike the predetermined values within optimization ranges provided in Table 2. The likelihoods in the Gaussian Naive Bayes classifier enabled the determination of more precise parameter values. Consequently, these refined values contributed to a more stable and accurate electricity and natural gas consumption simulation at the monthly resolution. Therefore, the proposed Bayesian calibration is more robust than the deterministic calibration.

Table 4: Monthly simulation errors of different models

Model	CV-RMSE	MAPE
Baseline	0.196	0.149
Deterministic	0.080	0.069
Bayesian	0.107	0.101

The efficiency of the proposed Bayesian calibration can be further enhanced when considering the limitations of the Gaussian Naive Bayes classifier. This classifier relies on the naive assumption that simulation parameters are conditionally independent, which may not be entirely true in all cases. The correlation between these parameters can significantly impact the resultant energy consumption. Therefore, modeling the Bayesian likelihood in Equation 4 as a multivariate probability distribution, where the simulation parameters are considered conditionally dependent, could yield more reliable calibration results.

Table 5: Monthly CV-RMSE comparison of the calibrated models based on different end-uses

Model	TOE	Electricity	Natural Gas
Deterministic	0.080	0.478	0.159
Bayesian	0.107	0.277	0.257

The Gaussian Naive Bayes classifier also assumes that simulation parameters follow a Gaussian distribution with a single mean and variance. However, in reality, nonlinear relationships may exist between between the simulation parameters and the resultant energy consumption. Utilizing non-parametric models would enable the detection of these nonlinear patterns in the actual probability distributions of the simulation parameters.

Table 6: Monthly MAPE comparison of the calibrated models based on different end-uses

Model	TOE	Electricity	Natural Gas
Deterministic	0.069	0.466	0.260
Bayesian	0.101	0.156	0.295

Most parameter combinations were considered undesirable scenarios based on their simulation results. Figure 4 shows that almost 90% of the scenarios have more than 15% of CV-RMSE. This caused an imbalanced distribution in the target variable with 2774 zeros and only 351 ones. When the model was trained using these observations, the learning process predominantly focused on the majority class (zeros) rather than the minority class (ones). Therefore, the model tended to classify scenarios as belonging to the majority class. According to Figure 3, the Gaussian Naive Bayes classifier accurately predicted 94% of the zero-labeled, while it only correctly predicted 71% of the one-labeled observations. The imbalanced distribution of the zeros and ones in the target variable induced the classifier to struggle to identify which simulation parameter influences the scenario result and to what extent. Handling such imbalanced data can drastically improve the classification performance and the calibration results.

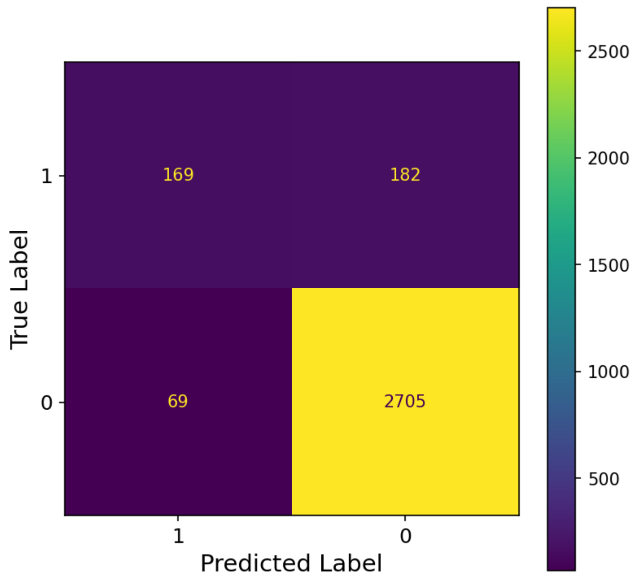

Figure 3: Confusion Matrix for Gaussian Naive Bayes Classifier

Conclusions

Bayesian optimization is widely used to calibrate building energy models. It involves surrogate modeling to reduce computational complexity since the dynamic models

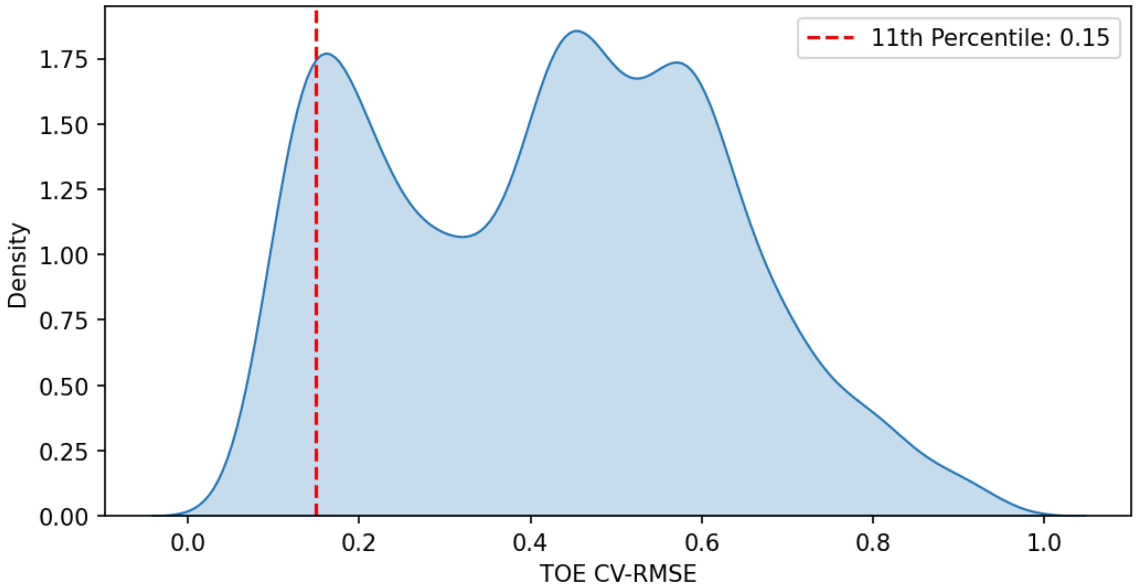

Figure 4: Probability Density Function for the CV-RMSE of the TOE

require extensive simulation time. However, the variability in building morphology and energy consumption patterns complicates surrogate modeling at the urban scale. This study proposes a simplified Bayesian optimization approach to calibrating building energy models at the district and urban scales while retaining dynamic modeling. The proposed approach introduces a novel framework for the parametric optimization of district-building energy models by filtering and reducing the parameter space to enhance the efficiency of the optimization process.

The proposed approach minimizes computational demands for optimizing dynamic models while ensuring reliability by leveraging Bayesian decision theory. Based on the monthly simulation errors, the methodology starts by labeling scenarios with varying combinations of the simulation parameters as either desired or undesired. Subsequently, a binary classifier is employed to categorize these scenarios. To achieve this, the Bayesian likelihoods are modeled as Gaussian probability distribution, with the simulation parameters being conditionally independent. Once the optimal distribution parameters (mean and standard deviation) are determined using the maximum likelihood estimation based on the scenario errors, the expected values of the simulation parameters obtained from the probability distributions constitute the Bayesian Model. This allows for acquiring more detailed and reasonable values of the simulation parameters without the need for exhaustive dynamic simulations. A case study implemented over a dormitory area on a university campus demonstrated the proposed approach's effectiveness. Here, the Bayesian Model significantly reduced the monthly simulation CV-RMSE of TOE for the Baseline Model by around 45% while also delivering balanced and accurate monthly simulation results for the dormitory buildings' electricity and natural gas consumption.

The approach's ability to derive optimal parameter combinations from labeled scenarios offers a practical solution for optimizing dynamic energy models. Urban planners can utilize it to enhance the accuracy of the district building energy models and reduce the energy consumption of the building stocks after testing various energy-efficiency scenarios. A possible future work of this study is to focus on integrating more robust classification models that involve correlations between the simulation parameters and the non-linear patterns in their probability distributions. Another future work can be overcoming the imbalanced label distribution in the target variable to improve the classification performance and the probabilistic calibration. Moreover, classifying scenarios based on natural gas and electricity consumption rather than TOE can help detect seasonal variations in building energy consumption patterns and identify essential parameters affecting seasonal building energy demand.

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