Intelligent Simulation: Fast Deep Multi-fidelity Surrogate Models to Assess Building Green Performances at the Early Design Stage

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Abstract
Surrogate modelling makes it possible to replace expensive simulations in green building designs. However, the commonly used surrogate models still rely on large volume data sets to reach acceptable accuracy. Therefore, this paper proposes the deep multi-fidelity surrogate modelling method. The proposed method is utilized in a practical case for validation by comparing with commonly used surrogate modelling methods. Results show that the proposed method performs better in data feature extraction and is able to eliminate the prediction error with fewer training samples needed. The method is applicable at the early design stage to improve green building design efficiency.

Highlights
• A new surrogate modelling method is proposed to assist green building design.
• Fewer training samples are needed with the help of deep learning.
• Prediction uncertainties are eliminated by means of Gaussian Process.
• Data feature extraction ability and prediction error of the model are validated in a practical case.

Introduction
In the big data era, simulation data have become quantitative sources for green building design. Although simulations assist architects a lot to evaluate green performances at the early design stage, the whole process is still time consuming [1], which impedes the enhancement of automation level in green building design. For instance, setting up a simulation for a design alternative normally involves many manual definitions like adjustments of design variables, parameter settings of simulation software etc. Meanwhile, the calculation time of green performances using simulation tools is too long for an architect to make creative decisions. According to a study in 1968, the desired feedback time of human-computer interaction should be less than ten seconds to bring architects’ initiative into full play [2]. It is obvious that the current simulation method hinders the improvement of green building design. With the development of computational techniques, machine learning models are utilized as surrogates to predict building green performances and the prediction results can be trustworthy compared with the real simulation results when the models are well trained. The purpose of surrogate modelling is to replace expensive high-fidelity simulations using training samples with certain quantity of physical knowledge and make fast assessment on basis of prediction results [3]. The method of surrogate modelling to assist architects at the early design stage advances in two aspects. Firstly, rapid feedback can be achieved by architects with less than 0.1 seconds [4], which guarantees the creativity of architects in conceptual design. Secondly, the surrogate model is able to provide continuous results compared with traditional simulation methods and the design space can be better explored.

The improvement degree of surrogate modelling methods compared with the traditional simulation methods is closely related to the prediction ability of the surrogates. Surrogate models like artificial neural network, random forest, support vector regression etc. are widely used for building green performances prediction. Although the commonly used surrogate models improve the efficiency of evaluation to a certain extent, the accuracy relies on large volume data sets and it is difficult to deal with sophisticated prediction problems. Uncertainties in prediction is another problem of surrogate modelling. Figure 1 shows the prediction results of the surrogate model in theory, the model with plenty of data samples and the model with shortage of data samples. The ideal goal of surrogate modelling is to approximate the real simulation model. However, the accuracy of the prediction results will not exceed the real simulation results in theory [5]. When the volume of training samples reaches a certain level, the accuracy of the surrogate model stops increasing. As the data volume gradually become smaller, large uncertainties will occur in the prediction of the model constructed by shortage of training samples [6]. Therefore, the increasing of training samples will not help much in the accuracy amelioration and cause expensive simulation costs. Meanwhile, the prediction uncertainties are difficult to eliminate with shortage of training samples. On this condition, an improved surrogate modelling method with higher prediction ability needs to be proposed, which is able to achieve acceptable prediction accuracy with fewer training samples and reduce the prediction uncertainties.
The rapid development of artificial intelligence propels the improvement of traditional simulation methods [7]. Deep learning model shows advantages in data feature extraction and is more likely to achieve higher prediction accuracy compared with traditional machine learning models [8]. On this basis, deep learning model can be utilized to obtain acceptable prediction accuracy with fewer samples. Besides, multi-fidelity modelling has been widely used in uncertainties elimination and time-consuming simulation problems. The method of multi-fidelity modelling is able to integrate limited high-fidelity time-consuming samples as well as large volume easily obtained un-accurate low-fidelity data sets [9], which reduces the uncertainties of surrogates constructed by fewer samples. Considering the existing problems of the commonly used surrogate modelling method as well as the technical advantages of deep learning and multi-fidelity modelling, this paper proposes an intelligent simulation method to realize fast assessment of green performances at the early design stage. A deep belief network is utilized as the low-fidelity model while Gaussian process is adopted to establish the multi-fidelity model. The number of samples for model establishment is reduced with acceptable prediction accuracy obtained using the two techniques compared with commonly used surrogates, which manifests in that the proposed surrogate modelling method is promising in the improvement of green building design efficiency with design accuracy that meets decision-making achievement.

Figure 2 compares the modelling approaches of deep multi-fidelity models, multi-fidelity models and commonly used surrogate models to demonstrate the advantages of the deep multi-fidelity modelling method in theory. As for commonly used surrogate models, large number of training samples are needed to achieve acceptable accuracy for green building design decision-making. Multi-fidelity models adopt the high accuracy of the high-fidelity data and the high efficiency of the low-fidelity data simultaneously. The high-fidelity data are used to set up the low-fidelity model and the prediction results are regarded as the low-fidelity data. The uncertainties of the low-fidelity data can be eliminated by the high-fidelity data with the help of proper machine learning algorithms. On this occasion, the number of training samples can be reduced and acceptable accuracy can be obtained compared with commonly used surrogate models.
models. Deep multi-fidelity models adopt the technique of deep learning and improves the data feature extraction ability. Fewer training samples are needed for deep multi-fidelity models to achieve acceptable accuracy compared with multi-fidelity models. In this way, the prediction uncertainties can be effectively reduced even with fewer training data with the help of deep learning and multi-fidelity modelling techniques. The design efficiency will be enhanced with design accuracy guaranteed. Based on the above analysis, a practical case of 17 design variables and 5 design objectives is selected to build a deep multi-fidelity model for validation sequentially, assessing the performances of 500 design alternatives. The results are evaluated from data feature extraction ability and prediction error compared with the commonly used surrogate models to demonstrate the technical advantages of the proposed method.

Methods

Workflow of Deep Multi-fidelity Modelling

The workflow of the deep multi-fidelity model establishment is presented in Figure 3. Firstly, the input variables and constraints are determined and the samples for model establishment are generated by means of Latin Hypercube Sampling (LHS). Secondly, the generated samples are exported to the building information model for parametric modelling to create design alternatives and the alternatives are simulated respectively to achieve the values of the output objectives. Consequently, the samples are utilized to build the low-fidelity DBN model where the model structure is determined. After the low-fidelity model is well trained, the data set for prediction is introduced to get the low-fidelity data. Eventually, the samples and the low-fidelity data are integrated to establish the multi-fidelity model with an appropriate structure. The data set for prediction is used by the multi-fidelity model to obtain the final results eventually. The parametric building information modelling is based on Revit software and Dynamo plug-in while the calculation of the output objectives is completed with simulation tools of green performances. The training of the low-fidelity DBN model and the establishment of multi-fidelity model are finished by Pycharm using Python coding. The procedure of training data preparation is completed with both architects and computers, which takes advantages of the architects’ creativity and the automation potential of computers. The establishment of the deep multi-fidelity model is done by computer programs totally, which helps architects to make up for the lack of machine learning knowledge.

Training Data Preparation

In the training data preparation procedure, an initial model of the design problem is set up in modelling tools like Revit, Rhino and Sketchup. Taking Revit as an example, the BIM model is made parametric with the help of Dynamo visual programming. The nodes in Dynamo make it possible to realize the controlling of design variables like building width, building height, window width and insulation width etc. Thus, a parametric model is established and series of design alternatives can be generated. The alternatives are consequently processed to form simulation files and imported into simulation tools for calculation. The simulation of diversified green performances can be completed in the Revit environment. For instance, an LCA tool named Tally is embedded in Revit as a plug-in and the gradually expanded open source packages enable the simulation of other green performances like daylighting, energy and carbon etc. The values of design variables and the corresponding simulation results are recorded in an Excel file to construct the high-fidelity data set for the establishment of the multi-fidelity model.
and window dimensions of four directions. The material construction of enclosure structure is taken into account by extracting the parameters of insulation type and insulation thickness. The constraints of the input variables are listed in Table 1.

Table 1: Input variables and constraints.

<table>
<thead>
<tr>
<th>Variable ID</th>
<th>Variable Names</th>
<th>Variable Types</th>
<th>Variable Constraints</th>
<th>Steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Building Width</td>
<td>Form</td>
<td>7800 mm – 8400 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>2</td>
<td>Building Depth</td>
<td>Form</td>
<td>15000 mm – 16800 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>3</td>
<td>Floor Number</td>
<td>Form</td>
<td>5 - 7</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>Building Height</td>
<td>Form</td>
<td>3600 mm - 4200 mm</td>
<td>100 mm</td>
</tr>
<tr>
<td>5</td>
<td>Number of Building Width</td>
<td>Form</td>
<td>3 - 5</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>South Window Width</td>
<td>Form</td>
<td>1800 mm – 2400 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>7</td>
<td>South Window Height</td>
<td>Form</td>
<td>1500 mm – 2400 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>8</td>
<td>North Window Width</td>
<td>Form</td>
<td>1500 mm – 1800 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>9</td>
<td>North Window Height</td>
<td>Form</td>
<td>1500 mm – 2400 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>10</td>
<td>East Window Width</td>
<td>Form</td>
<td>1200 mm – 1500 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>11</td>
<td>East Window Height</td>
<td>Form</td>
<td>1500 mm – 2400 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>12</td>
<td>West Window Width</td>
<td>Form</td>
<td>1200 mm – 1500 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>13</td>
<td>West Window Height</td>
<td>Form</td>
<td>1500 mm – 2400 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>14</td>
<td>Wall Insulation Thickness</td>
<td>Construction</td>
<td>50 mm – 100 mm</td>
<td>10mm</td>
</tr>
<tr>
<td>15</td>
<td>Roof Insulation Thickness</td>
<td>Construction</td>
<td>50 mm – 100 mm</td>
<td>10mm</td>
</tr>
<tr>
<td>16</td>
<td>Wall Insulation Types</td>
<td>Construction</td>
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<td>17</td>
<td>Roof Insulation Types</td>
<td>Construction</td>
<td>0, 1, 2, 3, 4, 5</td>
<td>—</td>
</tr>
</tbody>
</table>

* 0: EPS board. 1: XPS board. 2: Mineral wool board. 3: Glass fiber board. 4: PIR board. 5: PUR board.

Low-fidelity Model Establishment

The procedure of low-fidelity model establishment is completed in Pycharm. The model can be trained automatically when the Python code starts running with a simple click after the basic structure of the model is determined by the user. The deep belief network (DBN) is utilized as the low-fidelity model, which is a widely used deep learning probability generation model proposed by Geoffrey Hinton in 2006 [111]. The DBN model consists of multiple restricted Boltzmann machine (RBM) models and one back propagation (BP) neural network, as shown in Figure 5. The training of the model adopts the method of greedy learning. First of all, the RBM models of each layer are trained by means of un-supervised learning to finish the process of pre-training. Then comes the fine tuning process, where a BP neural network is set up between the last two layers to fine-tune the weights between each layer through back propagation utilizing the supervised learning method. The DBN model is thus well trained repeating the two procedures through iterations.

![Figure 5: Structure of the DBN model.](image-url)
Multi-fidelity Model Establishment

The Python code of multi-fidelity modelling runs automatically after the low-fidelity model is well trained. A type of liner multi-fidelity model proposed by Kennedy and O’Hagan in 2000 [12] is utilized in this study, as shown in equation (1). In the equation, \( f_{\text{high}}(x) \) and \( f_{\text{low}}(x) \) stand for the outputs of the high-fidelity and low-fidelity model, while \( \rho \) is a scaling factor symbolizing for the correlation between the high-fidelity data and the low-fidelity data. Meanwhile, \( f_{\text{err}}(x) \) denotes the bias term for the high-fidelity data.

\[
  f_{\text{high}}(x) = f_{\text{err}}(x) + \rho f_{\text{low}}(x)
\]

(1)

Gaussian process (GP) is adopted to build the multi-fidelity model. A GP model can be expressed as equation (2). In this equation, \( f(x) \) stands for the multi-fidelity model, \( m(x) \) symbolizes for the mean function and \( k(x,x') \) is the covariance function between the values of \( f(x) \) at point \( x \) and \( x' \). Radical basis function (RBF) kernel, also known as square exponential kernel, is utilized to make the model smooth for the reason that the kernel is infinitely differentiable [13]. On this condition, the covariance function \( k(x,x') \) can also be expressed as equation (3). \( \delta^2 \) is a coefficient which stands for the variance that determines the average distance from the mean value. \( l_1,\ldots,l_k \) is the length scale that adjusts the width of the kernel. Both \( \delta^2 \) and \( l \) are regarded as hyper-parameters and can be obtained by means of maximum likelihood estimate (MLE) [14].

\[
  f(x) \sim \text{GP}(m(\cdot), k(\cdot, \cdot))
\]

(2)

\[
  k(x,x') = \delta^2 \exp\left(-\frac{1}{2} \sum_{i=1}^{k} \frac{(x_i-x'_i)^2}{l_i^2}\right)
\]

(3)

Effectiveness Validation

The effectiveness of the proposed deep multi-fidelity modelling method is evaluated by comparing the prediction result and the simulation data with two indices of R-square (\( R^2 \)) as well as the difference of Root Mean Square Error (\( \Delta \text{RMSE} \)) between the low-fidelity DBN model and the multi-fidelity model, as shown in equation (4) to equation (6). The value of \( \Delta \text{RMSE} \) above zero demonstrates that the uncertainties caused by the low-fidelity model are eliminated effectively while the value minus zero stands for failures.

\[
  R^2 = 1 - \frac{\sum_{i=1}^{N} (\text{predict}_i - \text{true}_i)^2}{\sum_{i=1}^{N} (\text{predict}_i - \text{true}_i)^2}
\]

(4)

\[
  \text{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} (\text{predict}_i - \text{true}_i)^2}{N}}
\]

(5)

\[
  \Delta \text{RMSE} = \frac{(\text{RMSE}_{LF} - \text{RMSE}_{MF})}{\text{RMSE}_{LF}}
\]

(6)

In order to further validate the technical advantages of the proposed deep multi-fidelity (MF) modelling method, the method is compared with low-fidelity deep belief network (DBN), artificial neural network (ANN), radical basis function (RBF) and support vector machine (SVM) as benchmarks. Three groups of large (450 samples), medium (270 samples) and small (90 samples) volume data sets are provided to build the surrogate models. Since the design problem in this study is to assess 500 design alternatives, the three scenarios stand for the replacement of simulations with different extents. The large, medium and small volume groups reduce the times of simulations by 10%, 46% and 82%, corresponding to the data volume from plenty, slight shortage to serious shortage.

In the technical advantages validation section, the \( R^2 \) and \( \text{RMSE} \) of each surrogate is calculated and compared. Besides, a method based on Self Organized Map (SOM) to evaluate data feature extraction abilities quantitatively is proposed, which directly expresses the relationship between data and data feature in the form of topology figures. SOM is an un-supervised machine learning method, which is able to map high dimensional feature into low dimensions [15]. SOM firstly extracts the feature of the real simulation data and flattens it into a two-dimensional space with certain number of neurons. Then the real simulation data are mapped to the neurons and a type of topological relationship is formed. The relationship can be expressed as a topology figure of hexagonal mesh with black dots. An individual hexagonal grid symbolizes for a neuron in the data feature space and the black dots reflect the number of data samples mapped into the grids. The figure demonstrates the topological relationship between the real simulation data and the data feature, which acts as a reference for technical advantages validation. The topology figure of other prediction data can be completed in a similar way by mapping the data into the neurons of the original SOM. The topology figures are compared with the reference and the figures similar to the reference can be regarded as surrogates with strong data feature extraction abilities.

Results

Model Validation Results

The validation results using the large volume data set are shown in Figure 6. According to the validation results, the prediction \( R^2 \) of the five objectives all reach 99% and the \( \text{RMSE} \) are limited to a negligible extent. Besides, the \( \text{RMSE} \) of the model is reduced by 2% compared with the low-fidelity DBN model after calculation. Therefore, the established deep multi-fidelity model is capable of assessing building green performances with acceptable accuracy at the early design stage and the model is able to eliminate the uncertainties of the low-fidelity model, which testifies the effectiveness of the model.
Data Feature Extraction Ability Comparison

The topology figures of MF, DBN, ANN, RBF and SVM are shown in Figure 7. As for large volume data set, the topology figures of MF, DBN and ANN are most similar to the reference topology figure of the simulation results. Big differences occur for the topology figure of the RBF and SVM model compared with the simulation results. As for medium volume data set, the topology figures of MF and DBN are similar to the topology figure of the simulation results. Differences begin to appear as the decrease of samples for the ANN model. Big differences remain for the RBF and SVM model. As for small volume data set, big differences exist in all the topology figures compared with models trained by large and medium volume data sets. Therefore, MF and DBN are capable of extracting data feature with large and medium volume data sets while the ability is weak with severe shortage of samples. ANN performs well in data feature extraction with large volume data set but the ability becomes weaker as the number of samples reduce. The data feature extraction ability of the RBF and SVM model are the weakest among the compared models.

Prediction Error Comparison

The prediction evaluation indices of MF, DBN, ANN, RBF and SVM trained by large, medium and small volume data sets are presented in Figure 8. The $R^2$ of the five objectives trained by MF, DBN and ANN all reach 99% for the large volume data set. As for RBF model, the $R^2$ of the first three objectives are difficult to improve. The
The R² of the five objectives trained by SVM model is even lower than the RBF model. The R² of the five objectives trained by MF and DBN all reach 99% for the medium volume data set. The R² of the five objectives trained by ANN begin to decrease because of the reduction of samples. It is also difficult for RBF and SVM to achieve acceptable prediction R² but the performance of RBF is slightly better than SVM. The R² of the five objectives cannot all reach an acceptable level for small volume data set. The R² of models trained by MF, DBN and RBF are the highest compared with ANN and SVM. The prediction R² of three objectives for ANN are higher while the other two are lower than SVM. The RMSE of the five objectives for MF and DBN trained by large and medium volume data sets are relatively low but the RMSE for small volume data set are much higher. Meanwhile, the RMSE of the five objectives for MF are lower than DBN with the help of Gaussian processes, which demonstrates that the uncertainties are eliminated effectively. The RMSE of the objectives for ANN are the lowest with large volume data set but the RMSE become higher as the reduction of samples. The RMSE of the objectives become the highest in the small volume scenario among all the compared models. The RMSE of the objectives for RBF and SVM remain a relatively high level in regardless of data volume.

**Figure 8:** Prediction error of the five compared surrogates.

**Discussions and Future Work**

The aim of the proposed method is to reduce the expensive simulations in green building design, which can be regarded as a universal approach dealing with diversified design problems. In this study, a design problem of LCA assessment is set up to validate the effectiveness and technical advantages. The design variables that influence the objectives are not totally introduced into the model and the accuracy of the simulation tool Tally is not fully validated, which shows certain limitations. However, the study mainly focuses on the innovation of artificial intelligence techniques that improve the performances of surrogates. Hence, any practical case can be utilized for validation. As for the accuracy validation of the simulation tool Tally, architects are more interested in the improvement degree among the alternatives rather than...
the absolute value of the objectives. Thus, the simulation tool accuracy validation problem is not of vital importance in this study.

The program of the method is able to run automatically without human interventions and thus makes up for architects’ lack of machine learning knowledge. The deep multi-fidelity model can be constructed with a simple click, which is promising to assist architects in their green building designs. In the future work, the deep multi-fidelity models will be integrated with multi-objective optimization algorithms as surrogates to cope with more complicated problems and helps to reduce the time-consuming simulations in the optimization process. In this way, the proposed method will be more widely used by architects and dedicates to improve the design efficiency continually.

**Conclusion**

Simulation data are widely used for green building design at the early design stage. However, the traditional simulation method is time-consuming and is difficult to provide rapid feedback, which impedes the creativity of architects into full play. Surrogate modelling is able to realize fast evaluation of green performances and thus becomes a promising method to replace expensive simulations. The commonly used surrogate modelling methods are able to obtain acceptable accuracy but the prediction ability still needs improving. The development of artificial intelligence techniques provide opportunities to ameliorate the performances of surrogates by reducing the training samples needed, which improves the efficiency with acceptable accuracy achieved. On this condition, the intelligent method based on deep multi-fidelity modelling is proposed to realize fast assessment of building green performances.

A practical case of an office building is utilized for validation to demonstrate the effectiveness of the proposed method. The deep multi-fidelity model built by plenty of samples is able to make $R^2$ of all the objectives above 99% and eliminate the prediction uncertainties by 2%, which demonstrates the effectiveness as a type of surrogate modelling method preliminarily. Meanwhile, the method is also validated to reach acceptable accuracy with samples of slightly shortage. As for the commonly used surrogate modelling methods, only plenty of training samples are able to achieve equivalent accuracy. Therefore, the proposed method is testified to reach acceptable accuracy with fewer samples compared with other commonly used surrogate modelling methods.

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