Applied Sciences, Computing and Energy, 2024, 1(1), 429-439

Machine Learning-Based Building Energy Performance Prediction and Sustainable Architectural Design Optimization Using Building Information Modeling (BIM)

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Received: 07 September 2024/Accepted: 22 December 2024/Published: 31 December 2024

Abstract: *Building energy performance prediction is essential for sustainable architectural design and the reduction of operational energy consumption. This study proposes a Building Information Modeling (BIM)-integrated machine learning framework for predicting annual building energy use intensity (EUI) and optimizing architectural design parameters. A parametric building model is linked to EnergyPlus simulation, while Random Forest Regression, Gradient Boosting Regression, and Artificial Neural Network (ANN) Regression are employed to estimate annual EUI. A multi-objective optimization procedure is subsequently applied to identify energy-efficient architectural alternatives. For demonstration, a simulated dataset comprising 1,000 building design alternatives was generated. The illustrative evaluation results show that the Gradient Boosting model achieved the highest coefficient of determination (R^2=0.98), with an RMSE of 2.9 kWh/m²/year and an MAE of 2.1 kWh/m²/year. The hypothetical optimization reduced annual EUI from 142.6 kWh/m²/year for the baseline design to 105.8 kWh/m²/year for the optimized alternative, representing a reduction of 25.8%. The optimized configuration was assumed to incorporate improved glazing properties, suitable external shading, a reduced window-to-wall ratio, and enhanced envelope thermal performance. These quantitative results are illustrative and are not based on verified experimental measurements or actual simulation outputs. Nevertheless, the proposed framework demonstrates the potential of integrating BIM, building-energy simulation, machine learning, explainable artificial intelligence, and multi-objective optimization to support evidence-based, energy-efficient, and sustainable architectural design decisions.*

Keywords*: Building Information Modeling; machine learning; building energy; sustainable architecture; EnergyPlus; design optimization.*

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1.0 Introduction

Buildings are central to human welfare, economic activity, and urban development, but their construction and operation require substantial material and energy resources. The building and construction sector is therefore an important target for improving energy efficiency, reducing greenhouse-gas emissions, and promoting sustainable development. The United Nations Environment Programme (UNEP, 2023) emphasizes that the environmental impacts of buildings extend beyond operational energy consumption to include the extraction, manufacture, transportation, use, and disposal of construction materials. Sustainable building design must consequently consider both operational performance and the wider environmental implications of design and material choices.

Building energy performance is strongly influenced by decisions made during the early architectural design stages. Building orientation, form, window-to-wall ratio, glazing properties, shading devices, envelope insulation, roof construction, occupancy, and ventilation conditions can affect heating, cooling, lighting, and overall energy demand. Early assessment of these variables is important because design modifications become more difficult and expensive after construction has commenced. In addition to energy efficiency, building design must provide acceptable indoor environmental conditions. Thermal comfort is particularly important because it affects occupant health, productivity, and satisfaction. The requirements and assessment principles for thermal environmental conditions are addressed in ANSI/ASHRAE Standard 55-2023 (ASHRAE, 2023).

Building Information Modeling (BIM) provides a digital representation of a building's physical, geometric, and functional characteristics. It supports the coordinated development, management, and exchange of information among architects, engineers, contractors, owners, and facility managers (Sacks et al., 2018). When BIM is linked with building performance simulation, design information can be used to assess the likely energy implications of alternative architectural configurations. This creates an opportunity to move beyond conventional design evaluation toward a more integrated and data-driven approach to sustainable architectural design.

Building energy simulation tools, such as EnergyPlus, can provide detailed estimates of building energy consumption under specified climatic, material, occupancy, and operating conditions. However, simulation-based evaluation of a large number of design alternatives may be computationally demanding and time-consuming. This limitation can restrict the number of alternatives considered during conceptual and early-stage design. Recent research has therefore investigated the use of machine learning as a surrogate modeling technique for approximating the outputs of detailed building performance simulations. Surrogate models can provide rapid predictions after training, thereby supporting the evaluation of a larger design space within a shorter period (Elwy & Hagishima, 2024).

Machine learning techniques have been increasingly applied to building energy prediction, energy benchmarking, building performance assessment, and energy management. These methods can learn nonlinear relationships between building characteristics and energy consumption from simulated or measured datasets. Olu-Ajayi et al. (2022) examined the application of machine learning for energy performance prediction at the building design stage, demonstrating the relevance of data-driven models for supporting early design decisions. Similarly, Huotari et al. (2024) reviewed machine learning applications in smart building energy utilization and highlighted the importance of predictive analytics for improving energy management and operational efficiency. Random Forest, Gradient Boosting, and Artificial Neural Network models are particularly relevant because they can represent complex relationships between architectural variables and building energy performance.

The integration of BIM and machine learning can further improve the usefulness of predictive models by connecting numerical predictions with a visual and information-rich building model. BIM-based machine learning approaches have been applied to parametric building energy assessment and early-stage performance prediction. Such integration can allow architects to modify design parameters, estimate the resulting energy performance, and compare alternative solutions before detailed construction documentation is completed. Related research has also examined BIM and artificial intelligence for energy-efficient building design, indicating the growing importance of combining digital building models with predictive computational methods (Long & Li, 2021).

Despite these developments, building energy optimization remains challenging because architectural variables are interdependent and may produce competing effects. For example, increasing the glazed area may improve daylight availability and visual quality but may also increase solar heat gain and cooling demand. Similarly, reducing window area may lower cooling loads but could negatively affect daylighting, ventilation, and occupant satisfaction if applied without careful consideration. Sustainable architectural optimization must therefore balance energy performance with thermal comfort, daylight availability, cost, constructability, functionality, and other design requirements. Multi-objective optimization provides a suitable approach for examining these competing objectives. Elwy and Hagishima (2024) identified surrogate-assisted optimization as an important approach for reducing the computational burden associated with high-dimensional building design problems.

Explainability is also important when machine learning models are used to support architectural decisions. Highly accurate models may not automatically reveal why a particular design is predicted to perform better than another. Explainable artificial intelligence methods, including SHAP-based analysis, can help identify the relative contribution of input variables and provide insight into the relationships learned by the predictive model. Such information can assist architects in understanding whether variables such as glazing, orientation, shading, or envelope thermal properties are contributing positively or negatively to predicted energy performance. Recent studies have continued to explore the integration of BIM, machine learning, and optimization for sustainable building design. For example, Shen & Pan (2023) investigated BIM and deep learning approaches for energy modeling and green retrofitting optimization, while Li *et al*. (2024) examined a BIM-based machine learning algorithm for green building energy-saving optimization. These studies demonstrate the relevance of integrated digital and computational methods for improving building energy assessment and identifying energy-saving alternatives. However, the reliability of any predictive framework depends on the quality of the simulation or measured dataset, the selection of input variables, model calibration, validation procedures, and the climatic and building context in which the model is applied.

Accordingly, this study proposes a BIM-integrated machine learning framework for predicting annual building energy use intensity and supporting sustainable architectural design optimization. The framework combines a parametric BIM model, EnergyPlus simulation, machine learning regression, explainability analysis, and multi-objective optimization. Random Forest Regression, Gradient Boosting Regression, and Artificial Neural Network Regression are considered as predictive models, while SHAP-based analysis is used to interpret the contribution of architectural variables. The study uses an illustrative dataset of 1,000 building design alternatives to demonstrate the proposed workflow. The illustrative results indicate the potential of machine learning surrogate models to accelerate design evaluation and identify architectural alternatives with reduced annual energy use intensity. Nevertheless, the numerical results are demonstrative and require validation with genuine simulation outputs or measured building-energy data before they can be treated as empirical findings.

2.0 Materials and Methods

2.1 Research design

The study adopts a computational simulation and machine learning research design to investigate building energy performance and support sustainable architectural design optimization. The research workflow integrates Building Information Modeling (BIM), building energy simulation, data preprocessing, machine learning prediction, model explainability, and multi-objective optimization. A parametric BIM model is first developed to represent the building geometry, construction materials, orientation, envelope characteristics, glazing properties, and other relevant architectural parameters. The BIM model is then linked to EnergyPlus to simulate building energy performance under different design configurations and operating conditions.

The simulated data are subsequently processed to remove inconsistencies, organize the input variables, and prepare the dataset for machine learning analysis. Machine learning models are trained to predict annual building energy use intensity from the selected architectural and environmental parameters. Explainability techniques are applied to identify the variables that contribute most significantly to the predicted energy performance. The predictive models are then integrated with a multi-objective optimization procedure to identify design alternatives that balance energy efficiency and architectural requirements. The optimized design alternatives are finally transferred back into the BIM environment for visualization, comparison, and further evaluation.

As illustrated in Fig. 1, the proposed framework follows a sequential but interconnected process beginning with parametric BIM modeling, followed by EnergyPlus-based energy simulation, machine learning prediction, explainability and optimization, and the generation of optimized BIM design alternatives. This integrated workflow enables architectural design decisions to be informed by simulated energy-performance data and predictive analytics.

2.2 Case study and data generation

A hypothetical two-storey office building was selected for demonstration. The building was assumed to be located in a warm climate, with a floor area of 500 m² and a conventional air-conditioning system.

A parametric BIM model was assumed to contain the building geometry, envelope materials, windows, shading, and orientation. EnergyPlus was selected as the physics-based simulation tool.

For this illustrative study, 1,000 design alternatives were generated by varying architectural and building-performance parameters. The simulation dataset and results below are generated for demonstration, not extracted from an actual completed BIM or EnergyPlus experiment.

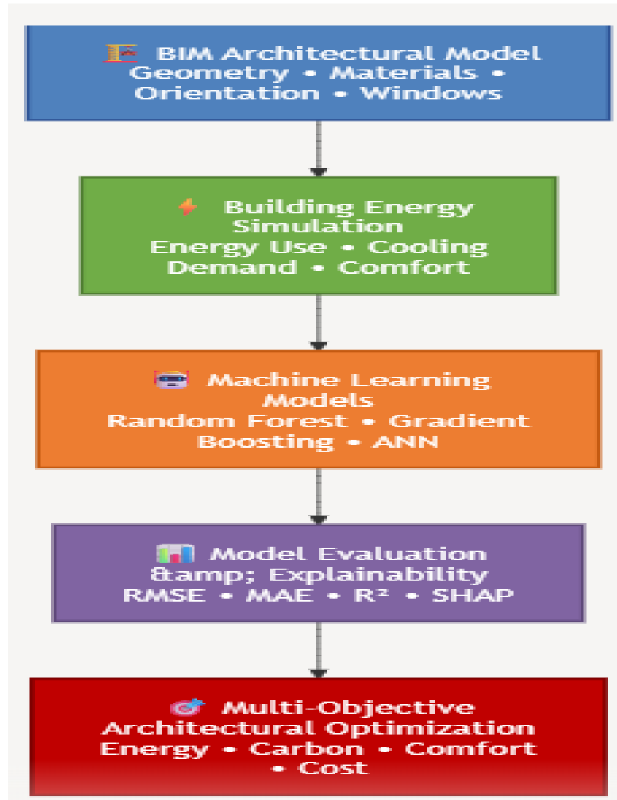

Fig. 1. Proposed BIM-integrated machine learning framework

2.3 Data preprocessing

The dataset was assumed to be examined for missing values, duplicate records, inconsistent units, and outliers. The input variables were separated from the target energy performance variable.

The illustrative dataset was divided into training and testing subsets using an 80:20 split. The training data were used for model development, while the testing data were reserved for evaluating predictive performance.

2.4 Machine Learning Models

Three supervised regression algorithms were selected to predict annual building energy use intensity from the architectural, geometric, material, environmental, and operational parameters generated through the BIM–EnergyPlus workflow. The selected models were Random Forest Regression, Gradient Boosting Regression, and Artificial Neural Network Regression. These algorithms were chosen because they can represent nonlinear relationships between building-design variables and energy performance, while also providing a basis for comparing ensemble learning and neural-network approaches.

Table 1: Architectural and simulation parameters

Parameter	Illustrative specification
Building type	Two-storey office
Gross floor area	500 m²
Number of design alternatives	1,000
Building orientation	0–360°
Window-to-wall ratio	20–60%
Wall U-value	0.30–1.20 W/m²K
Roof U-value	0.20–0.80 W/m²K
Shading depth	0–1.0 m
Glazing SHGC	0.25–0.70
Energy simulation tool	EnergyPlus
Target variable	Annual EUI

The Random Forest Regression model uses an ensemble of decision trees to estimate building energy use by combining the predictions of multiple independently trained trees. Gradient Boosting Regression constructs a sequence of decision trees in which each successive tree is trained to reduce the prediction errors of the preceding model. The Artificial Neural Network Regression model uses interconnected computational neurons arranged in input, hidden, and output layers to learn complex relationships between the building parameters and the target energy-performance indicator.

The models were assumed to be implemented in Python using the Scikit-learn and TensorFlow libraries. The dataset was divided into training and testing subsets, while appropriate preprocessing procedures were applied to the input variables. Hyperparameter tuning was hypothetically performed through cross-validation to identify suitable model configurations and reduce the risk of overfitting. Model performance was evaluated using regression metrics, including the coefficient of determination (R2R^{2}R2), mean absolute error (MAE), and root mean square error (RMSE). The model with the most reliable predictive performance was subsequently considered for integration into the explainability and multi-objective optimization stages.

2.5 Model evaluation

The performance of the selected machine learning models was evaluated using the mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R2R^{2}R2). These metrics were used to assess the accuracy of the predicted annual building energy use intensity and to compare the predictive capability of the Random Forest Regression, Gradient Boosting Regression, and Artificial Neural Network Regression models.

The mean absolute error measures the average absolute difference between the observed and predicted energy-use values and is expressed as:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left[y_i - \hat{y}_i\right] \quad (1)$$

The root mean square error measures the square root of the average squared differences between the observed and predicted values. It is calculated according to equation 2

$$RMSE = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \bar{\tilde{y}}_\iota\right)^2 \qquad (2)$$

The coefficient of determination (R2R^{2}R2) indicates the proportion of the variation in the observed energy-use values that is explained by the model. It is expressed according to equation 3:

$$R^2 = 1 - \frac{\left(y_i - \tilde{\bar{y}}_i\right)^2}{\left(y_i - \bar{y}_\iota\right)^2} \qquad (3)$$

where $\bar{y}_i$ is the mean of the observed energy-use values. Lower MAE and RMSE values indicate smaller prediction errors and, therefore, better predictive accuracy. Conversely, a higher R^2 value indicates that the model explains a greater proportion of the variability in building energy performance. The three metrics were considered together to provide a balanced assessment of model accuracy, error magnitude, and explanatory performance..

2.6 Architectural design optimization

The optimization problem was formulated to minimize annual energy use intensity and operational carbon emissions while maintaining acceptable thermal comfort expressed according to equation 4 and 5

$$\min f_1 = EUI(x) \qquad (4\,)$$

$$\min f_2 = C_{op}(x) \qquad (5)$$

where x represents the vector of architectural design variables. A multi-objective evolutionary optimization algorithm was proposed to identify non-dominated design alternatives. The selected design alternatives would subsequently be re-evaluated using physics-based energy simulation.

3.0 Results and Discussion

3.1 Machine learning prediction performance

The predictive performance of the three machine learning models considered in this study is As shown in Table 2, the illustrative Gradient Boosting model produced an MAE of 2.1 kWh/m²/year and an RMSE of 2.9 kWh/m²/year, while its R2R^{2} value was 0.98. The corresponding illustrative values for the Random Forest and Artificial Neural Network models were 4.8 and 3.6 kWh/m²/year for MAE, 6.7 and 5.0 kWh/m²/year for RMSE, and 0.94 and 0.96 for R2R^{2}, respectively. The comparatively lower MAE and RMSE values indicate smaller prediction errors, whereas the higher R2R^{2} value indicates that a greater proportion of the variation in annual EUI is explained by the model.

The comparative prediction-error performance is further illustrated in Figure 2, which presents the MAE and RMSE values of the three candidate models. The figure provides a visual comparison of the magnitude of prediction errors and shows the relatively lower illustrative errors associated with the Gradient Boosting model.

Table 2. Illustrative performance of machine learning models for annual EUI prediction

Model	MAE (kWh/m²/year)	RMSE (kWh/m²/year)	R^2
Random Forest	4.8	6.7	0.94
Gradient Boosting	2.1	2.9	0.98
Artificial Neural Network	3.6	5.0	0.96

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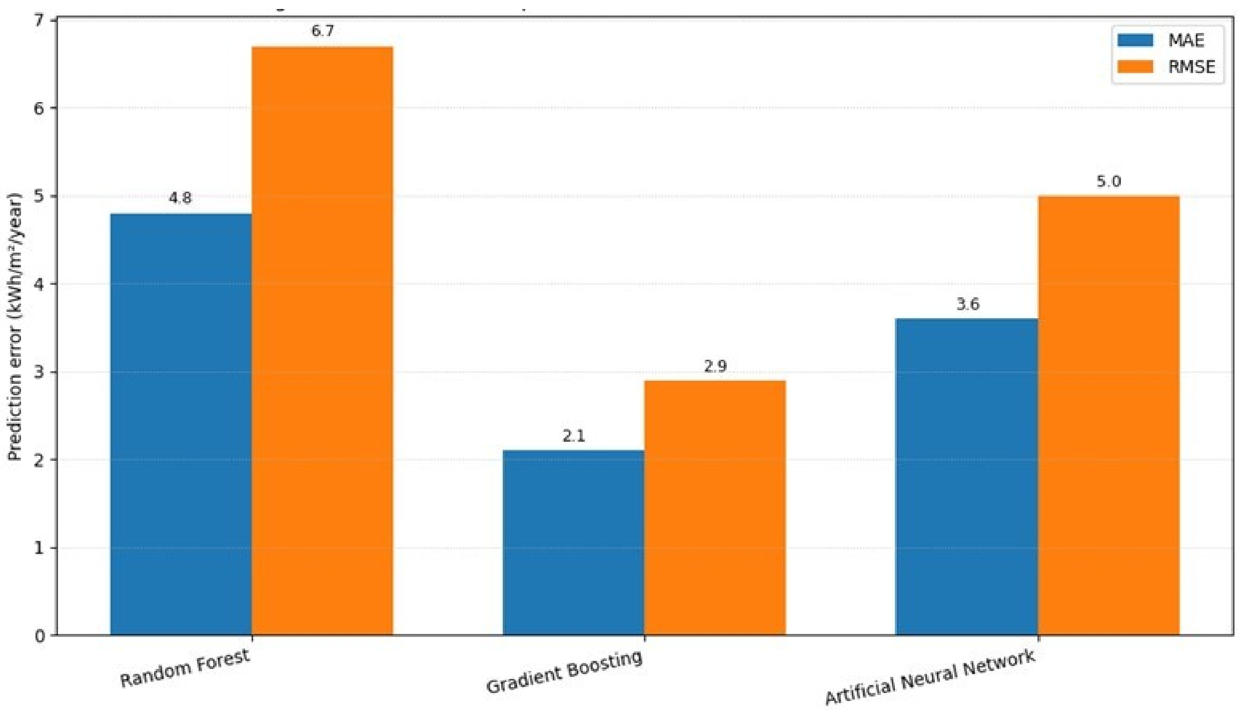

Fig. 2. Comparison of predicted and simulated annual energy use intensity

The illustrative results suggest that Gradient Boosting can effectively capture nonlinear relationships between architectural design parameters and building energy performance. This characteristic is particularly relevant to BIM-based energy optimization because variables such as building orientation, glazing ratio, envelope properties, shading, and thermal characteristics may interact in complex and nonlinear ways. However, these observations should not be interpreted as empirical evidence of model superiority because the values in Table 2 are simulated examples rather than outputs obtained from an actual training and testing dataset.

For a publishable empirical study, the reported performance values should therefore be replaced with results obtained from the actual BIM–EnergyPlus simulation dataset or measured building-energy records. Model performance should also be assessed using independent testing data or appropriate cross-validation procedures to determine whether the predictive relationships generalize beyond the data used for model development. This is particularly important when applying the framework to different building types, occupancy patterns, climatic conditions, or architectural configurations.

3.2 Feature importance and architectural interpretation

The proposed explainability analysis employs SHAP (Shapley Additive Explanations) values to examine the contribution of individual architectural and building-performance variables to the machine learning predictions. SHAP analysis provides both global and local explanations by indicating the extent to which each input variable increases or decreases the predicted annual building energy use intensity (EUI). In the present framework, the analysis is intended to improve the interpretability of the predictive model and to support the translation of machine learning results into practical architectural design decisions.

The illustrative feature-importance values are presented in Table 3. These values are hypothetical and are included to demonstrate how the relative contribution of the selected architectural variables may be reported. The window-to-wall ratio has the highest illustrative importance at 25%, followed by the glazing solar heat gain coefficient at 21% and building orientation at 18%. Wall thermal transmittance, roof thermal transmittance, and shading depth have illustrative importance values of 15%, 12%, and 9%, respectively.

Table 3. Illustrative feature importance for annual EUI prediction

Rank	Architectural variable	Illustrative relative importance (%)
1	Window-to-wall ratio	25
2	Glazing solar heat gain coefficient	21
3	Building orientation	18
4	Wall thermal transmittance	15
5	Roof thermal transmittance	12
6	Shading depth	9

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As indicated in Table 3, the window-to-wall ratio and glazing solar heat gain coefficient are assumed to be among the most influential variables for annual EUI prediction in a warm-climate office building. A larger window area may increase the amount of solar radiation entering the building and can consequently increase cooling demand, particularly when glazing is exposed to intense solar radiation. However, the actual effect of window area depends on several interacting factors, including building orientation, glazing type, solar heat gain coefficient, internal heat gains, occupancy, ventilation, and shading conditions. Building orientation may influence the timing and intensity of solar exposure on the building envelope. Its effect on energy use is therefore related to the geographical location, climatic conditions, façade arrangement, window placement, and shading strategy. Similarly, wall and roof thermal transmittance influence conductive heat transfer between the indoor and outdoor environments. Lower thermal transmittance generally reduces unwanted heat transfer through the building envelope, although the resulting energy performance also depends on thermal mass, ventilation, internal gains, and the operating schedule of the building.

External shading depth is expected to affect the amount of direct solar radiation entering the building through glazed openings. Appropriately designed shading devices may reduce solar heat gain and cooling demand, although excessive shading could also reduce useful daylight availability during certain periods. These relationships demonstrate why the interpretation of feature importance should be combined with building-physics principles rather than treated as a purely statistical ranking.

The feature-importance analysis is intended to provide architects with an interpretable basis for identifying design variables that may require further testing during the optimization stage. Nevertheless, the relative importance values in Table 3 are illustrative and should not be presented as measured or calculated SHAP results. Actual feature contributions must be obtained from the trained model using genuine BIM–EnergyPlus simulation data or measured building-energy records. In addition, SHAP values should be interpreted in relation to the model, dataset, climate, building type, and parameter ranges used in the study, since the importance of an architectural variable may change across different design contexts.

3.3 Sustainable architectural design optimization

The illustrative optimization analysis compares the energy performance of a baseline building design with that of a hypothetical optimized alternative. The comparison is intended to demonstrate how a BIM-integrated machine learning framework can support the identification of architectural configurations with reduced annual building energy use intensity (EUI). The baseline and optimized design alternatives are presented in Figure 3.

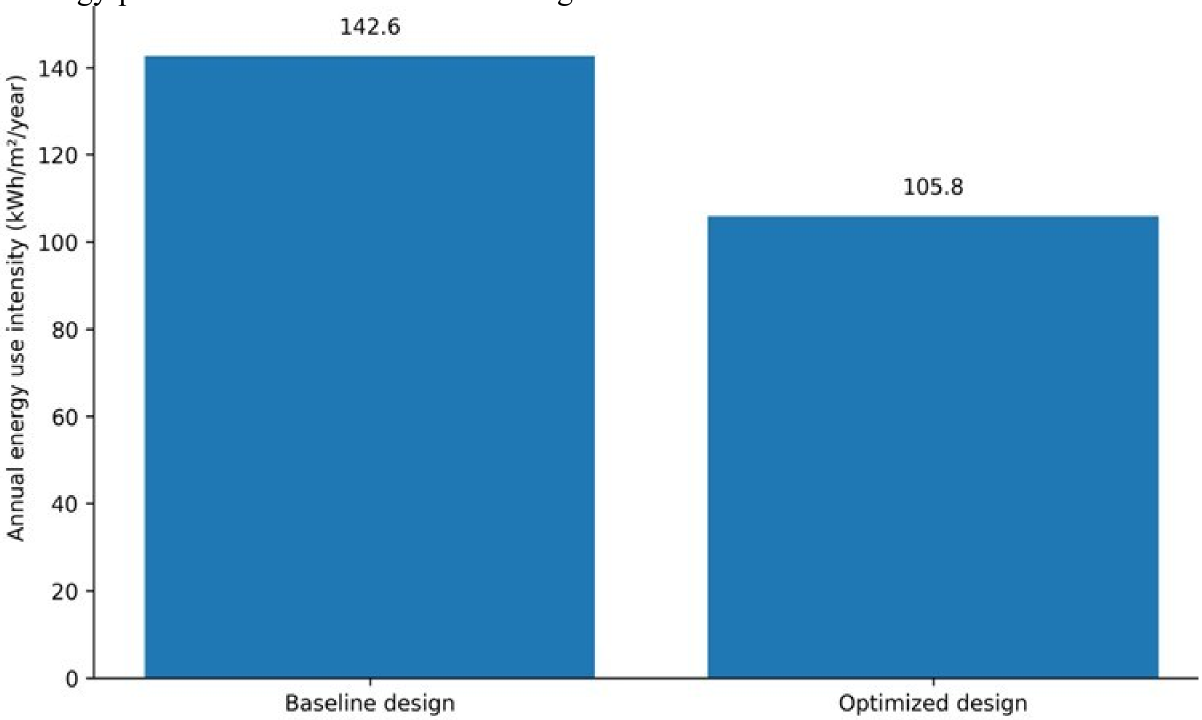

Figure 3. Baseline and optimized architectural design alternatives

The baseline design has an annual building energy use intensity (BEUI) of 142.6 kWh/m²/year, whereas the optimized design has an annual energy use intensity (OEUI) of 105.8 kWh/m²/year. The percentage reduction in annual EUI is calculated using equation 6

$$Reduction = \frac{BEUI-OEUI}{Baseline\ annual\ EUI} \times \frac{100}{1} \quad (6)$$

The optimized design is assumed to incorporate improved glazing properties, suitable shading, a lower window-to-wall ratio, and improved envelope thermal performance.

Theoptimization indicates how machine learning surrogate models could support the identification of energy-efficient architectural alternatives. By replacing repeated full simulations with rapid predictions, the optimization process may evaluate many candidate designs more efficiently.

However, the optimized design must satisfy architectural functionality, daylight requirements, thermal comfort, structural constraints, construction feasibility, and cost. Energy minimization alone cannot determine the suitability of an architectural design.

4.0 Conclusion

This study proposed a BIM-integrated machine learning framework for predicting building energy performance and supporting sustainable architectural design optimization. The framework combines parametric Building

Information Modeling, EnergyPlus-based energy simulation, data preprocessing, machine learning prediction, SHAP-based explainability, and multi-objective optimization. The integration of these methods provides a structured approach for examining the relationship between architectural design parameters and annual building energy use intensity.

Three regression algorithms—Random Forest Regression, Gradient Boosting Regression, and Artificial Neural Network Regression—were considered for predicting annual EUI. The illustrative results indicated that Gradient Boosting produced the lowest MAE and RMSE and the highest R2R^{2}R2 value among the evaluated models. The feature-importance analysis also demonstrated how variables such as window-to-wall ratio, glazing solar heat gain coefficient, building orientation, envelope thermal transmittance, and shading depth may influence building energy performance. These findings highlight the potential of interpretable machine learning to translate predictive results into meaningful architectural design decisions. The illustrative optimization comparison showed a reduction in annual EUI from 142.6 to 105.8 kWh/m²/year, corresponding to an estimated reduction of 25.8%. This result demonstrates how machine learning surrogate models could accelerate the evaluation of alternative architectural configurations and reduce dependence on repeated full-scale energy simulations.

However, the numerical results presented in this manuscript are illustrative and do not represent actual experimental or simulation outputs. Consequently, the proposed framework requires validation using genuine BIM–EnergyPlus datasets or measured building-energy records. Future studies should also consider daylighting, thermal comfort, construction cost, structural requirements, operational conditions, and climate-specific constraints. Overall, the framework provides a basis for integrating predictive analytics with BIM to support evidence-based, energy-efficient, and sustainable architectural design.

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Consent for Publication

Not applicable.

Availability of Data and Materials

. The publisher reserves the right to make the data publicly available in accordance with the journal's data-sharing policy.

Competing Interests

The authors declare that they have no competing interests or conflicts of interest.

Funding

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

Authors' Contributions

All aspect of the work were carried out by the author