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Article

A Hybrid Machine Learning–Optimization Framework for Energy Demand Forecasting and Decision Support in Smart Infrastructure

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Abstract: This study addresses the growing need for accurate and actionable energy demand forecasting in smart infrastructure systems, where data-driven decision-making is essential for efficiency, sustainability, and system reliability. Despite advances in machine learning-based forecasting, most approaches remain prediction-centric and are rarely integrated with operational optimization and decision-support mechanisms, limiting their real-world applicability. To address this gap, this study proposes a sequentially integrated hybrid machine learning–optimization framework that combines ensemble-based forecasting, optimization-driven energy allocation, and explainable artificial intelligence (XAI) within a unified architecture. The term hybrid denotes the integration of heterogeneous methodological components, while the framework is implemented as a pipeline in which forecasting outputs inform downstream optimization. The predictive module incorporates XGBoost and Long Short-Term Memory (LSTM) models, alongside an ensemble approach that operates within the forecasting stage to enhance robustness and generalization. The optimization component utilizes forecasted demand to minimize energy cost under demand and capacity constraints, while SHAP-based analysis im-proves interpretability and transparency. Empirical evaluation using the UCI Building Energy Efficiency dataset shows that XGBoost achieves the highest predictive accuracy (MAE = 0.429, RMSE = 0.613, R^2 = 0.996), while the ensemble model provides strong robustness (R^2 = 0.994). The integrated framework effectively smooths demand fluctuations, improves allocation efficiency, and identifies relative compactness and glazing area as dominant features. The results demonstrate that sequential integration of forecasting, optimization, and interpretability enhances predictive reliability, operational efficiency, and decision transparency.

Keywords: Hybrid Machine Learning, Energy Demand Forecasting, Smart Infrastructure Systems, Optimization-Based Decision Support, Explainable Artificial Intelligence (XAI).

1. Introduction

The transformation of contemporary energy systems into data-intensive smart infrastructures has fundamentally redefined the paradigms of energy planning, forecasting, and operational control [1]. Smart infrastructure systems encompassing smart grids, intelligent buildings, distributed energy resources, and cyber–physical urban environments are increasingly governed by complex interactions between physical assets, digital platforms, and data-driven intelligence [1]. Within this context, accurate energy demand forecasting has become a foundational component of system stability, economic efficiency, and sustainability planning. The proliferation of high-resolution sensing technologies, smart meters, and Internet of Things (IoT) devices has enabled unprecedented access to real-time energy data, thereby creating new opportunities for advanced predictive modeling and algorithmic decision-making [2]. Machine learning techniques, particularly deep learning architectures such as long short-term memory networks (LSTM) and ensemble methods such as XGBoost, have demonstrated significant potential in capturing nonlinear relationships and complex correlations in energy consumption data [3]. However, despite these advances, the dominant research paradigm remains largely prediction-centric, as also highlighted in recent studies on hybrid energy forecasting frameworks [4], where models are primarily evaluated based on predictive accuracy without systematic integration into operational decision-making structures.

This separation between predictive intelligence and operational optimization represents a fundamental methodological limitation in current smart infrastructure research. Forecasting systems are frequently deployed as standalone analytical tools, disconnected from the control, scheduling, and resource allocation mechanisms that govern real-world infrastructure operations, as reported in prior hybrid and energy management studies [4]. As a result, high-accuracy predictions often fail to translate into meaningful operational improvements, creating a gap between algorithmic performance and system-level impact. Traditional optimization frameworks, on the other hand, typically rely on static assumptions or simplified demand representations that do not reflect the dynamic and uncertain nature of real-world energy systems [5]. The absence of adaptive, data-driven forecasting inputs within optimization processes leads to suboptimal scheduling decisions, inefficient resource allocation, and limited responsiveness to demand variability, ultimately constraining the scalability and resilience of smart infrastructure systems [6].

In parallel, the growing reliance on black-box machine learning models introduces challenges related to transparency and trust. Many high-performance forecasting models operate as opaque systems, making it difficult for system operators and stakeholders to understand the basis of predictions and the rationale behind automated decisions [7]. In safety-critical infrastructure contexts, such lack of interpretability can hinder adoption and limit effective human–AI collaboration [8]. These challenges highlight the need for unified approaches that integrate predictive modeling, optimization, and interpretability, as explored in emerging integrated energy intelligence frameworks [9].

To address these limitations, this study proposes a hybrid machine learning–optimization framework for energy demand forecasting and decision support in smart infrastructure systems, in line with recent developments in hybrid modeling approaches. The term hybrid is used in a systems-integration sense to denote the combination of machine learning–based forecasting, optimization-based decision-making, and explainable artificial intelligence within a unified architecture. The interaction between these components is implemented in a sequential pipeline, where forecasting outputs serve as inputs to the optimization module. This design enables predictive models to directly inform energy scheduling, load balancing, and resource allocation, thereby aligning data-driven intelligence with infrastructural control processes while maintaining modularity and computational flexibility, consistent with prior system integration studies [10], [11].

By embedding forecasting outputs within optimization formulations, decision-making becomes adaptive and data-responsive, allowing infrastructure systems to dynamically adjust to demand fluctuations and system constraints. At the same time, the incorporation of explainable artificial intelligence mechanisms, such as SHAP-based attribution, enhances interpretability and supports transparent decision-making [12]. Within this framework, the integration of forecasting and optimization components has been widely investigated in the literature [13], while recent studies emphasize the importance of bridging the gap between prediction and operational decision-making in energy systems [14]. Building upon these directions, the present study integrates machine learning models, specifically XGBoost and LSTM, with an optimization module for energy allocation under operational constraints, forming a unified decision-support system that links predictive intelligence with operational control while maintaining interpretability and practical applicability.

The primary objective of this study is to develop an integrated architecture that not only achieves high forecasting accuracy but also translates predictive outputs into optimized, actionable energy allocation strategies while ensuring model transparency. Methodologically, the study follows established hybrid modeling and evaluation practices in intelligent energy systems [15], combining machine learning-based forecasting, optimization-driven decision-making, and SHAP-based explainability within a single coherent framework. The key contribution lies in the structured integration of these components, enabling a direct linkage between prediction, optimization, and interpretability in intelligent energy management systems.

The remainder of the paper is organized as follows.

Section 2 reviews related literature on energy demand forecasting, optimization-based energy management, and explainable artificial intelligence. Section 3 presents the proposed methodology and framework. Section 4 reports the experimental results, Section 5 discusses the findings, and Section 6 presents the conclusions of the study, followed by Section 7 which discusses the limitations and outlines directions for future research.

2. Literature Review

The literature on energy demand forecasting and intelligent energy management has expanded substantially over the past two decades, driven by the convergence of smart grid technologies, digital infrastructure, and data-driven analytics. Early research in energy demand modeling was dominated by statistical and econometric approaches, including autoregressive integrated moving average (ARIMA), seasonal ARIMA (SARIMA), regression-based models, and stochastic time-series formulations. These methods provided foundational insights into temporal patterns, seasonality, and trend components in energy consumption data, offering interpretability and mathematical tractability [16]. However, their reliance on linear assumptions, stationarity constraints, and predefined functional forms limited their ability to capture the nonlinear, high-dimensional, and dynamic behaviors characteristic of modern smart infrastructure systems, particularly in environments with distributed generation, renewable energy integration, and heterogeneous consumption patterns.

With the advancement of machine learning, data-driven forecasting models increasingly replaced traditional statistical approaches, enabling more flexible representation of complex temporal and contextual relationships. Shallow learning models, including support vector machines, k-nearest neighbors, decision trees, and random forests, demonstrated improved predictive performance by learning nonlinear mappings between input variables and energy demand [17], [18]. Ensemble learning techniques, particularly gradient boosting frameworks such as XGBoost and LightGBM, further enhanced forecasting accuracy through model aggregation, robustness to noise, and feature interaction modeling. These approaches marked a significant methodological shift from parametric modeling to data-adaptive learning systems. However, while they improved predictive performance, many of these models remained limited in their ability to represent long-term temporal dependencies and sequential dynamics inherent in time-series energy data.

Deep learning architectures addressed these limitations by introducing memory mechanisms and hierarchical feature learning. Long short-term memory networks and gated recurrent units became widely adopted for energy forecasting due to their ability to model long-range temporal dependencies, temporal nonlinearity, and sequential patterns [19]. More recently, Transformer-based architectures and attention mechanisms have been introduced to energy systems research, enabling dynamic weighting of temporal features and improved modeling of complex temporal interactions. These models have demonstrated state-of-the-art performance in multivariate energy forecasting, renewable generation prediction, and load demand estimation. Despite their predictive power, the majority of deep learning studies remain focused on forecasting accuracy as an isolated objective, with limited attention to how predictions are operationalized within infrastructure control and decision-making systems [20].

Parallel to forecasting research, a distinct body of literature has developed around optimization and decision-making in energy systems. Classical optimization approaches, including linear programming, mixed-integer programming, and nonlinear optimization, have been extensively applied to energy scheduling, unit commitment, load dispatch, and resource allocation. Evolutionary algorithms such as genetic algorithms [21], particle swarm optimization, and multi-objective optimization frameworks have been employed to address complex, multi-criteria decision problems involving cost, reliability, emissions, and efficiency trade-offs. These methods provide mathematically rigorous and computationally efficient mechanisms for operational planning. However, they often rely on static demand assumptions, simplified forecasting inputs, or deterministic scenarios, which limit their responsiveness to real-time system dynamics and uncertainty. As a result, optimization frameworks frequently operate independently of advanced predictive intelligence, reinforcing the structural separation between forecasting and decision-making.

Recent studies have begun to explore hybrid and integrated approaches that combine forecasting models with optimization strategies, particularly in smart grid and renewable energy applications. These hybrid systems aim to use predictive outputs as inputs to scheduling and resource management algorithms, thereby improving operational performance. While such studies represent important methodological progress, many existing hybrid frameworks adopt loosely coupled architectures in which forecasting and optimization remain conceptually and structurally distinct modules [22]. The integration is often limited to data flow rather than methodological co-design, resulting in systems that lack unified learning–decision structures, adaptability, and theoretical coherence. Moreover, most hybrid models prioritize operational performance metrics without addressing interpretability, transparency, and human-centered decision support, which are increasingly critical for real-world deployment in regulated infrastructure environments. The issue of model interpretability has emerged as a central concern in the application of artificial intelligence to critical infrastructure systems [23]. Black-box learning models, particularly deep neural networks, offer limited transparency regarding feature influence, decision logic, and causal relationships. Explainable AI (XAI) methods, including SHAP, LIME, and rule-extraction techniques, have been introduced to address this limitation by providing post hoc interpretability and feature attribution [24]. In energy systems research, these methods have primarily been used for model explanation and feature importance analysis rather than integrated decision-support design. As a result, explainability remains peripheral to system architecture rather than embedded as a core methodological component that informs both prediction and optimization processes [25].

Collectively, the existing literature reveals a fragmented methodological landscape in which forecasting, optimization, and interpretability are treated as largely independent research domains. Prediction-focused studies emphasize accuracy without operational integration, optimization-focused studies emphasize efficiency without adaptive intelligence [26], and interpretability-focused studies emphasize transparency without systemic integration. This fragmentation constrains the development of intelligent infrastructure systems that are not only accurate and efficient, but also adaptive, transparent, and operationally meaningful [27]. Consequently, there exists a clear research gap for unified hybrid frameworks that integrate machine learning forecasting, optimization-based decision support, and explainable AI within a single coherent architecture. Addressing this gap requires a systems-oriented methodological paradigm that aligns predictive modeling with operational control and governance requirements, enabling the translation of data-driven intelligence into sustainable, reliable, and trustworthy infrastructure decision-making [28]. The present study contributes to this emerging paradigm by proposing a fully integrated hybrid machine learning–optimization framework that unifies forecasting, decision support, and interpretability within a comprehensive methodological structure for smart infrastructure systems.

The reviewed literature reveals significant advancements in energy demand forecasting, optimization-based energy management, and explainable artificial intelligence within smart infrastructure systems. Statistical models laid the foundational groundwork for time-series analysis, while machine learning and deep learning approaches substantially improved predictive accuracy by capturing nonlinear and high-dimensional relationships [29]. Parallel developments in optimization techniques have enabled efficient resource allocation and operational planning. However, the literature remains fragmented, with forecasting, optimization, and interpretability often treated as independent research streams [30]. Most studies emphasize prediction accuracy without systematic integration into operational control frameworks, while optimization models frequently rely on static or simplified demand assumptions. Furthermore, explainability is typically applied as a post hoc analytical tool rather than embedded within decision-support architectures. These gaps highlight the need for a unified methodological paradigm that integrates predictive intelligence, adaptive optimization, and transparent model interpretation. The present study addresses this gap by proposing a coherent hybrid framework that bridges these domains, thereby contributing to the development of more adaptive, efficient, and trustworthy intelligent energy management systems.

3. Methodology

This study presents a hybrid intelligent framework that integrates machine learning forecasting, optimization-based energy allocation, and Explainable Artificial Intelligence (XAI) to enable efficient and transparent decision-making in smart infrastructure systems. The framework connects predictive modeling with operational energy management, ensuring that forecast outputs are both actionable and interpretable.

An ensemble model combining XGBoost and LSTM is employed to predict building heating load using design and environmental features, leveraging the strengths of both models for improved accuracy and reliability. The predicted outputs are then fed into an optimization module, which determines efficient energy allocation strategies to enhance system performance and reduce energy waste. To ensure transparency, SHAP-based explainability is incorporated to quantify the contribution of individual features to model predictions, thereby improving trust and interpretability. The framework is implemented through sequential stages, including data collection (UCI dataset), preprocessing, predictive modeling, optimization, explainability analysis, and performance evaluation using MAE, RMSE, and R^2 metrics. The proposed approach enables accurate, efficient, and interpretable energy management.

3.1. Dataset Description

The empirical analysis utilizes the Building Energy Efficiency dataset obtained from the UCI Machine Learning Repository [31], which is also publicly available via platforms such as Kaggle. The dataset comprises 768 building configurations generated using Ecotect simulation software, with each sample representing a building structure described by eight input parameters, including relative compactness, surface area, wall area, roof area, overall height, orientation, glazing area, and glazing area distribution. The target variable is heating load, representing the energy required to maintain thermal comfort within buildings.

While this dataset provides realistic and widely used benchmark data with diverse structural variations and energy demand conditions suitable for regression-based forecasting and decision-support modeling, it is inherently static and non-temporal. As such, the proposed framework is evaluated under a static data setting rather than real-time streaming conditions. Consequently, further validation using dynamic or real-time datasets is required to fully assess the framework's applicability to live smart infrastructure systems.

3.2. Data Preprocessing and Exploratory Analysis

Data preprocessing was conducted to enhance model stability and ensure analytical reliability. The dataset was examined for inconsistencies, missing values, and outliers. Feature normalization was applied to standardize variable scales and improve model convergence during training. The dataset was then divided into training and testing subsets to allow unbiased performance evaluation. Exploratory data analysis was performed to examine statistical relationships among building design parameters and heating load demand. Correlation analysis was conducted using Pearson correlation coefficients to identify interdependencies among structural features. Visualization techniques, including correlation heatmaps and distribution plots, were used to analyze feature variability and data clustering patterns. This analysis supports model development by identifying dominant structural influences on heating load demand.

3.3. Machine Learning-Based Forecasting Models

Multiple predictive models were developed to capture nonlinear relationships between building parameters and heating load demand.

3.3.1. XGBoost Model

Extreme Gradient Boosting (XGBoost) was implemented as a tree-based ensemble learning method. The model constructs sequential decision trees that minimize prediction errors through gradient-based optimization. XGBoost was selected due to its ability to capture complex feature interactions, handle structured tabular datasets efficiently, and provide high predictive accuracy with strong generalization performance.

The XGBoost model predicts the output as an additive ensemble of decision trees:

$$\hat{y}_i = \sum_{k=1}^{K} f_k(x_i), \quad f_k \in \mathcal{F} \tag{1}$$

where f_k represents the k-th regression tree and $\mathcal{F}$ is the space of all possible trees.

The objective function is defined as:

$$\mathcal{L} = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k) \tag{2}$$

3.3.2. Long Short-Term Memory Model

A Long Short-Term Memory (LSTM) neural network was implemented as a deep learning baseline to model complex nonlinear relationships between building characteristics and heating load demand. LSTM is a specialized form of recurrent neural network designed to capture dependencies through gated memory mechanisms. While LSTM is primarily developed for sequential data modeling, it is employed in this study as a comparative benchmark to evaluate its capability in learning nonlinear feature interactions within structured tabular data.

The LSTM architecture consists of memory cells and three gating mechanisms, namely the forget gate, input gate, and output gate, which regulate the flow of information. The model is mathematically defined as follows:

$$f_t = \sigma\left(W_f[h_{t-1}, x_t] + b_f\right) \tag{3}$$

$$i_t = \sigma(W_i[h_{t-1}, x_t] + b_i) \tag{4}$$

$$\tilde{C}_t = \tanh(W_c[h_{t-1}, x_t] + b_c) \tag{5}$$

$$C_t = f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t \tag{6}$$

$$f_o = \sigma(W_o[h_{t-1}, x_t] + b_o) \tag{7}$$

$$h_t = o_t \cdot \tanh(C_t) \tag{8}$$

where ft, it, and ot denote the forget, input, and output gates, respectively; Ct represents the cell state; and ht is the hidden state at time step t. The variables W and b correspond to the learnable weight matrices and bias vectors, while σ and tanh denote the sigmoid and hyperbolic tangent activation functions.

Although the dataset used in this study is static and does not explicitly contain temporal sequences, the LSTM model is utilized to investigate whether its internal gating mechanisms can capture implicit nonlinear relationships among features. This allows a direct comparison with tree-based models, particularly in terms of representation capability and predictive performance. The experimental results demonstrate that LSTM provides lower predictive accuracy compared to XGBoost, indicating that sequential deep learning architectures may be less suitable for structured tabular energy datasets.

Table 1 shows the architecture of the implemented LSTM model. The model is constructed using a sequential architecture consisting of a single LSTM layer with 64 hidden units followed by a fully connected dense layer with one neuron for regression output. The LSTM layer serves as the primary feature extractor, capturing complex nonlinear interactions within the input space, while the dense layer maps the learned representation to a scalar prediction value.

Table 1. LSTM model architecture summary (Sequential model).

Layer (Type)	Output Shape	Number of Parameters
LSTM	(None, 64)	18,688
Dense	(None, 1)	65

Total trainable parameters: 18,753.

The total number of trainable parameters in the model is 18,753, with the majority contributed by the LSTM layer due to its recurrent weight matrices and gating structure. This configuration ensures sufficient model capacity while maintaining computational efficiency for training and evaluation.

3.3.3. Ensemble Learning Integration

To improve forecasting robustness and reduce model-specific prediction bias, an ensemble learning strategy was implemented. The ensemble model aggregates outputs from individual predictive models using weighted averaging. By combining tree-based and neural network learning approaches, the ensemble framework improves prediction stability and enhances generalization across varying heating load ranges.

It is important to distinguish that the ensemble model operates within the forecasting stage only, whereas the hybrid framework refers to the broader integration of forecasting, optimization, and interpretability components.

The ensemble prediction is obtained using weighted averaging:

$$\hat{y}_{\text{ensemble}} = \sum_{j=1}^{M} w_j \, \hat{y}_j \tag{9}$$

where w_j are model weights such that:

$$\sum_{j=1}^{M} w_j = 1 \tag{10}$$

3.4. Optimization-Based Energy Allocation

The predicted heating load values generated by the ensemble model were integrated into an optimization framework designed to support energy allocation and demand balancing. The optimization process aims to minimize energy consumption cost while ensuring that energy supply meets forecasted demand and operational capacity constraints. The optimization model is formulated using a simplified linear objective function with basic demand and capacity constraints. While this formulation enables clear demonstration of the integration with forecasting outputs, it does not fully capture the complexity of real-world smart infrastructure systems, which may require multi-objective, stochastic, or dynamic optimization approaches.

The optimization objective is formulated as:

$$\min \sum_{t=1}^{T} C_t \; E_t \tag{11}$$

subject to:

$$\begin{aligned} E_t &\geq D_t, \quad \forall t = 1, \dots, T \\ E_t &\leq E_{\max}, \quad \forall t = 1, \dots, T \end{aligned} \tag{12}$$

where E_t represents the allocated energy at the time step t, D_t denotes the forecasted heating demand, and C_t represents the energy cost coefficient. This formulation enables the integration of predictive intelligence into operational resource allocation by ensuring demand satisfaction while minimizing total energy cost under capacity constraints.

3.5. Explainability and Model Interpretation

To enhance transparency and support decision interpretability, SHapley Additive exPlanations (SHAP) is applied as a post hoc interpretability method to analyze feature contributions to model predictions. SHAP values quantify the marginal impact of each building parameter on predicted heating load, enabling the identification of dominant structural features influencing energy demand and providing intuitive visual explanations of model behavior. It is important to note that SHAP does not directly influence the training of the predictive models or the optimization process; rather, it serves to improve transparency, support model understanding, and facilitate informed decision-making in intelligent energy management systems.

3.6. Model Evaluation

The performance of the predictive models is evaluated using three standard regression metrics: Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the coefficient of determination (R^2). These metrics are defined as follows:

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{y}_i| \tag{13}$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2} \tag{14}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{15}$$

where y_i represents the actual values, $\hat{y}_i$ denotes the predicted values, $\bar{y}$ is the mean of the actual values, and n is the total number of observations.

4. Results

The results of this study evaluate the performance of the proposed hybrid machine learning–optimization framework in terms of predictive accuracy, robustness, and operational effectiveness. The analysis is structured to assess both the forecasting capability of the machine learning models and the impact of integrating these predictions

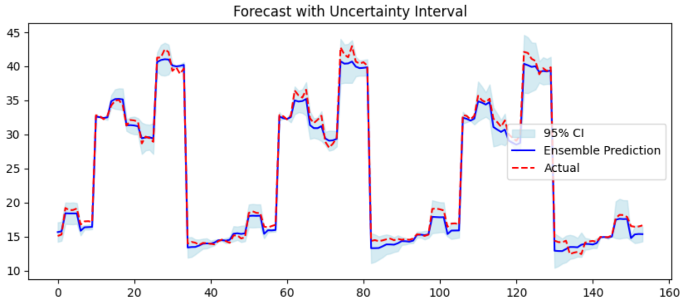

Figure 1. Ensemble-Based Heating Load Forecast and Uncertainty Quantification.

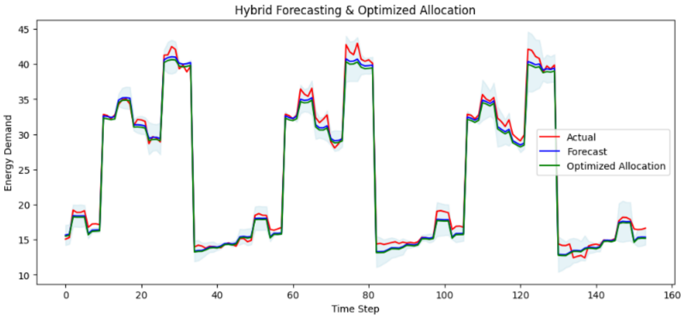

Figure 2. Hybrid Forecasting and Optimized Energy Allocation for Energy Demand.

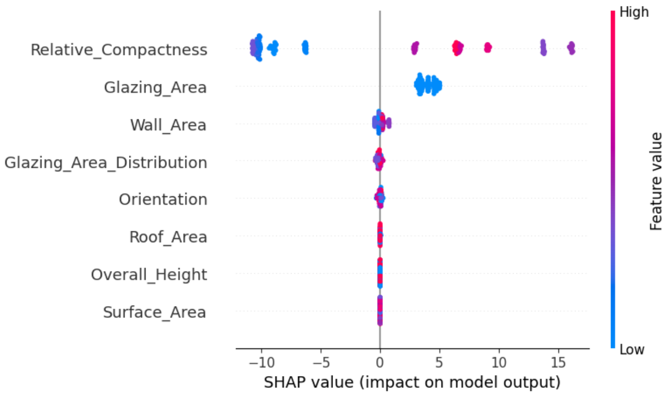

Figure 3. SHAP-Based Interpretation of Model Predictions for Heating Load.

Table 2. Regression Performance Metrics for Heating Load Prediction.

Model	MAE	RMSE	R^2
XGBoost	0.429	0.613	0.996
LSTM	1.240	1.516	0.978
Ensemble	0.666	0.810	0.994

into the optimization-based energy allocation process. Comparative evaluation of the XGBoost, Long Short-Term Memory (LSTM), and ensemble models is conducted using standard regression metrics, including Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and coefficient of determination (R^2). In addition, uncertainty quantification, residual analysis, and feature importance interpretation are employed to further examine model reliability and transparency. The results provide a comprehensive assessment of how the integrated framework enhances energy demand prediction and supports efficient decision-making in smart infrastructure systems.

To begin with, Table 2 summarizes the regression performance of the evaluated models for heating load prediction using mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R^2). The XGBoost model demonstrates the best overall performance, achieving the lowest error values (MAE = 0.429, RMSE = 0.613) and the highest explanatory power (R^2 = 0.996), indicating excellent predictive accuracy. The ensemble model also performs strongly, with low error metrics (MAE = 0.666, RMSE = 0.810) and an R^2 of 0.994, indicating robust generalization. In contrast, the LSTM model records comparatively higher prediction errors (MAE = 1.240, RMSE = 1.516) and a lower R^2 of 0.978, suggesting reduced accuracy for this task. Overall, the results confirm that tree-based and ensemble approaches are more effective than the standalone LSTM for continuous heating load regression.

Building on this comparative evaluation, Figure 1 demonstrates that the ensemble model accurately tracks actual heating load across all time steps, capturing both low and peak demand periods. The narrow uncertainty bands indicate high confidence and stable performance, with slight widening during peak transitions. Most actual values fall within the 95% interval, confirming the model's reliability and effective uncertainty quantification.

Furthermore, Figure 2 showing the comparison between actual energy demand, model forecast, and optimized allocation over time. The hybrid forecasting model closely follows the actual demand profile, accurately capturing both peak and off-peak periods. The optimized allocation curve further smooths demand fluctuations while remaining aligned with forecasted values, indicating effective allocation under system constraints. The narrow uncertainty band around the forecast reflects high confidence in the predictive model, while deviations between actual demand and optimized allocation highlight the impact of optimization in balancing demand and operational efficiency. Overall, the figure demonstrates the effectiveness of integrating forecasting with optimization for improved energy demand management.

In addition, Figure 3 shows the SHAP summary of feature contributions to heating load prediction. Relative compactness and glazing area are the most influential features, while wall area, glazing distribution, and orientation have moderate effects, and other features contribute less. The distribution of SHAP values highlights both the importance and variability of features, providing clear interpretability and confirming the dominance of building geometry in predictions.

Consistent with these findings, Figure 4 validates the predictive performance of the XGBoost model, showing that the model closely tracks the temporal dynamics of

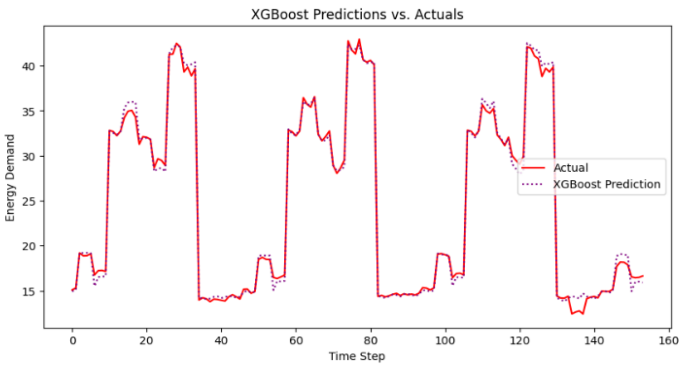

Figure 4. XGBoost-Based Energy Demand Forecasting: Predicted vs. Actual Values.

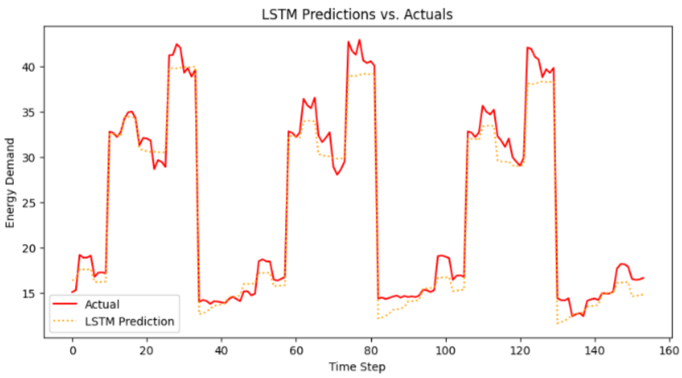

Figure 5. LSTM Model Predictions vs. Actual Energy Demand.

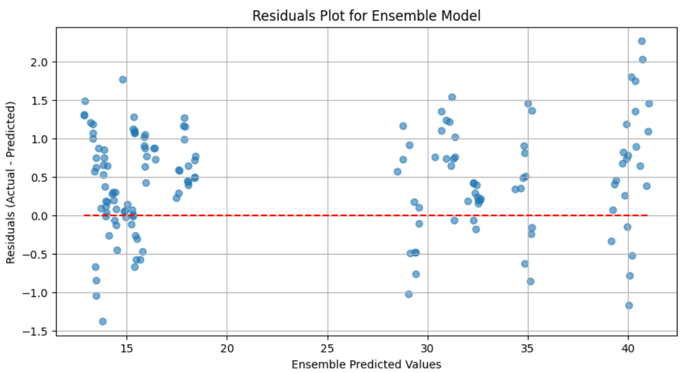

Figure 6. Residuals Analysis of the Ensemble Model Predictions.

actual energy demand. Peaks, troughs, and seasonal patterns are effectively captured, indicating that the model can serve as a reliable input for hybrid ML–optimization frameworks. The minimal deviations at abrupt transitions underscore potential areas for improvement through ensemble learning or temporal sequence models, such as LSTM or Transformer-based architectures.

By contrast, Figure 5 shows the performance of the Long Short-Term Memory (LSTM) model in forecasting energy demand over time. The solid red line represents the actual observed energy demand, while the dotted orange line shows the predictions generated by the LSTM model. The plot demonstrates how closely the LSTM predictions follow the general trend and fluctuations of the actual demand, capturing daily peaks and troughs, although some minor deviations are observed during sharp demand transitions.

To further examine model reliability, Figure 6 illustrates the residuals of the ensemble model, calculated as the difference between the actual and predicted values (Residuals = Actual − Predicted), plotted against the model's predicted values. The red dashed line at zero represents the ideal scenario where predictions perfectly match actual values. From the plot, it is evident that the residuals are not perfectly randomly scattered around zero. There is a visible pattern, with clusters at certain predicted value ranges (around 14–16, 29–30, 35, and 40), suggesting potential heteroscedasticity or regions where the model may underperform. However, most residuals lie within a ±1.5 range, indicating reasonably good predictive performance overall. This analysis helps in assessing model bias, variance, and potential improvements in the ensemble learning approach.

From a data perspective, Figure 7 shows the correlation among input features, with strong relationships observed between key structural variables. Relative compactness is negatively correlated with surface and roof area but positively with overall height, while surface area and roof area are strongly positively related. Most other features, particularly glazing and orientation variables, exhibit weak or minimal correlations, indicating their relative independence.

Moreover, Figure 8 shows a strong agreement between the ensemble model's predicted and actual heating load values. Most data points align closely with the ideal diagonal line, indicating high predictive accuracy. The clustering across low, medium, and high load ranges demonstrates consistent performance, with only minor deviations observed.

Finally, Figure 9 illustrates the frequency distribution of the actual heating load values in the test dataset. The histogram, combined with the density curve, shows how heating load values are spread across different ranges. The distribution reveals multiple clusters, with a noticeable concentration of values at lower heating loads (approximately 12–18 units) and another concentration at medium to higher ranges (approximately 28–42 units). The presence of these distinct clusters suggests variability in building energy demand, likely reflecting differences in structural characteristics and thermal properties across building samples.

5. Discussion

The performance of the developed machine learning models was evaluated using Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and coefficient of determination (R^2). The comparative results demonstrate strong predictive capability across all models, with tree-based methods showing superior performance for heating load prediction. The XGBoost model achieved the highest accuracy, with an MAE of 0.429, RMSE of 0.613, and R^2 of 0.996, indicating an excellent ability to capture nonlinear

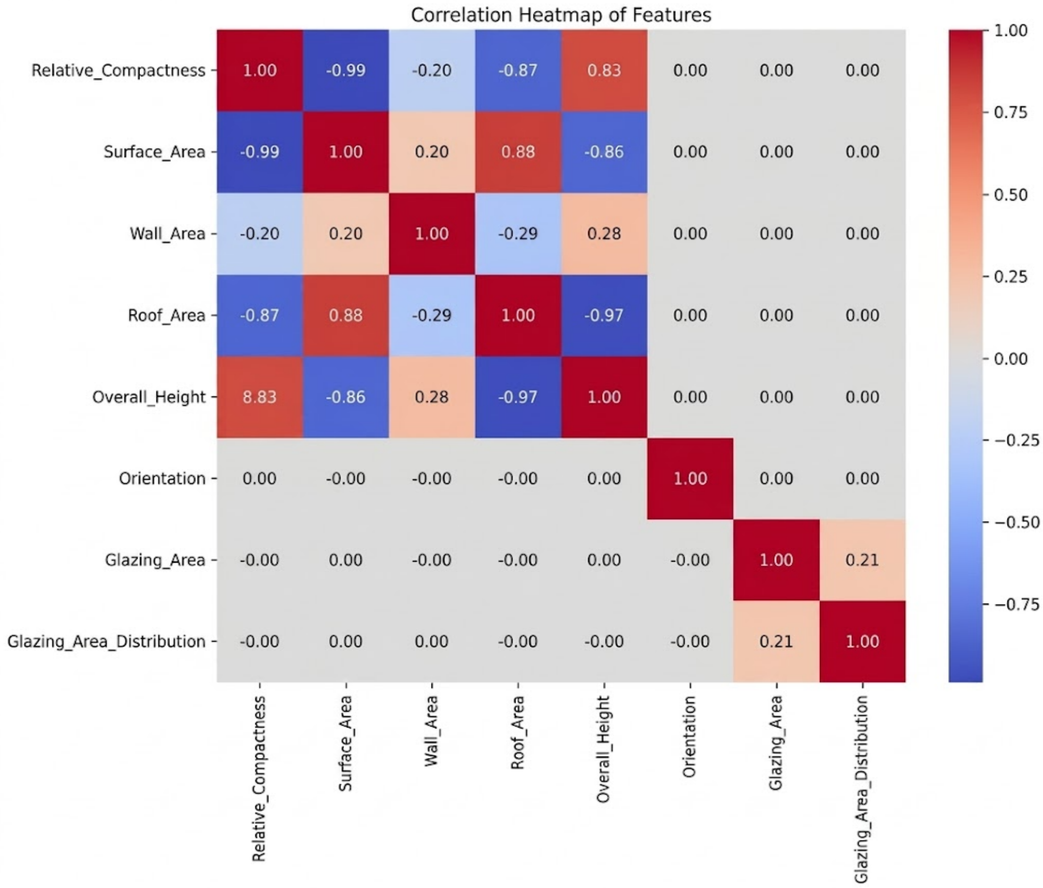

Figure 7. Correlation Heatmap of Building Energy Dataset Features.

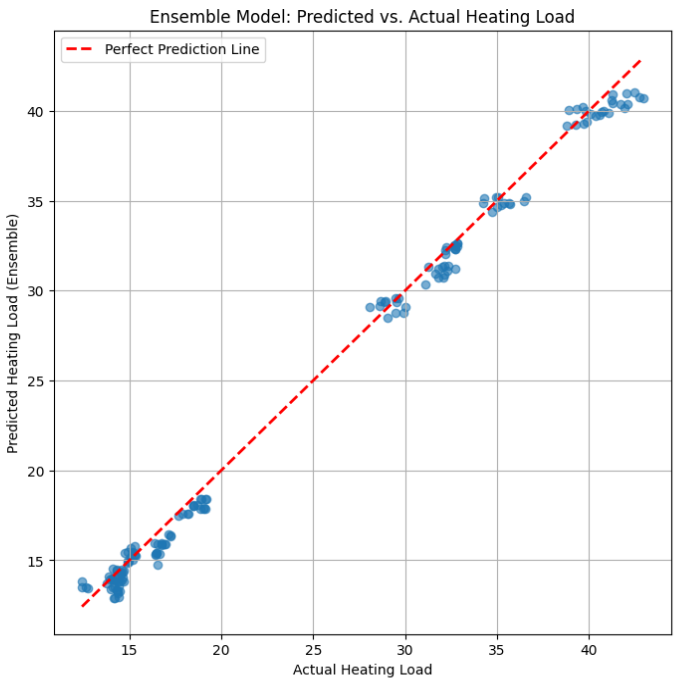

Figure 8. Ensemble Model Predicted vs. Actual Heating Load.

relationships between building parameters and heating load demand. The ensemble model also demonstrated strong predictive performance, achieving an MAE of 0.666, RMSE of 0.810, and R^2 of 0.994, confirming its robustness and generalization capability. In contrast, the LSTM model produced higher prediction errors, with an MAE of 1.240 and RMSE of 1.516, suggesting that sequential deep learning approaches may be less effective for this structured tabular dataset. The superior performance of XGBoost can be attributed to its gradient boosting mechanism, which effectively captures complex feature interactions and handles multicollinearity among structural variables [32]. The ensemble model improves reliability by combining the strengths of both tree-based and deep learning approaches, thereby reducing model variance and enhancing predictive stability.

The ensemble forecasting results demonstrate strong alignment between predicted and actual heating load values. The prediction curve closely tracks the observed demand profile across all building configurations, accurately capturing both low-load and peak-load scenarios [33]. The uncertainty quantification results further confirm the reliability of the ensemble framework, with most actual heating load values falling within the 95% confidence interval. Slight widening of uncertainty bands during peak transitions indicates increased variability under rapidly changing thermal conditions, which is expected in energy demand forecasting [34].

These findings highlight the effectiveness of ensemble learning in improving prediction robustness while providing reliable confidence estimates, which are critical for operational decision-making in energy management systems. The integration of forecasting outputs into the optimization module demonstrates significant improvements in energy demand management [35]. The optimized

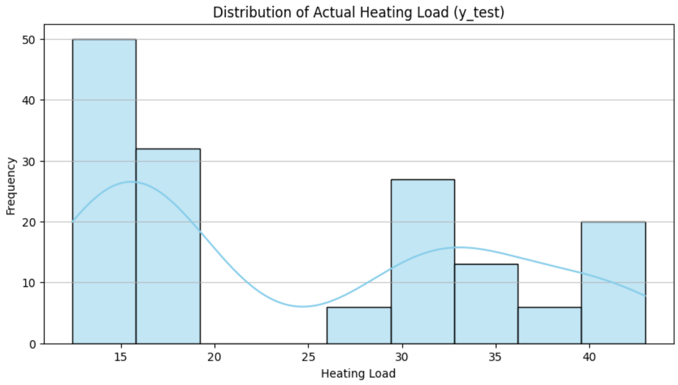

Figure 9. Distribution of Actual Heating Load.

allocation curve smooths demand fluctuations while remaining closely aligned with forecasted heating load patterns. This smoothing effect reduces abrupt energy consumption peaks and enhances system stability by ensuring efficient resource distribution under operational constraints. The results confirm that embedding predictive intelligence within optimization frameworks enables more adaptive and cost-effective energy allocation strategies. The optimization framework also demonstrates the capability to balance energy demand variability while maintaining supply reliability. This integration bridges the gap between predictive modeling and real-world infrastructure operations, allowing forecasting outputs to directly influence energy scheduling and load balancing decisions [36]. Compared to existing studies that focus solely on forecasting accuracy or standalone optimization, the proposed framework provides a structured integration of both components within a single pipeline. While prior works emphasize either predictive performance or operational efficiency independently, this study highlights the importance of linking these stages to improve overall system functionality.

The SHAP-based interpretability analysis provides valuable insights into the relative importance of building structural parameters in heating load prediction. Relative compactness and glazing area emerged as the most influential features, indicating that building geometry and envelope transparency significantly affect thermal energy demand. Higher values of relative compactness generally contribute to increased heating load, reflecting structural heat retention characteristics. Similarly, glazing area influences heat transfer and solar radiation absorption, thereby impacting indoor thermal conditions. Wall area, glazing distribution, and orientation demonstrate moderate contributions to heating load variability, while roof area, overall height, and surface area exhibit comparatively lower influence [37]. The interpretability results confirm that heating load demand is primarily driven by structural design features and building envelope characteristics [38]. The ability to explain feature contributions enhances transparency and supports informed infrastructure design and energy efficiency planning. Residual analysis of the ensemble model reveals that most prediction errors remain within a narrow range, indicating strong model accuracy and stability. Although residual clustering is observed at certain heating load ranges, the overall distribution remains centered around zero, suggesting minimal systematic prediction bias. These clusters may indicate regions where structural parameter combinations introduce additional complexity in thermal behavior, highlighting potential areas for further model refinement.

The distribution of actual heating load values demonstrates the presence of multiple demand clusters representing low, medium, and high energy consumption scenarios. This variability confirms the dataset's suitability for evaluating model generalization across diverse building energy conditions. The ability of the ensemble model to maintain accuracy across these demand ranges further validates its robustness. Correlation analysis reveals strong multicollinearity among geometric building parameters, particularly between relative compactness, surface area, roof area, and overall height [39]. These interdependencies reflect inherent architectural design relationships and confirm that structural building characteristics collectively influence heating load behavior. In contrast, glazing-related and orientation features exhibit relatively low correlation with structural parameters, suggesting that they provide complementary and independent predictive information. While the proposed framework demonstrates the potential to support energy allocation decisions, the current implementation focuses on methodological integration rather than full system-level deployment. Therefore, the results should be interpreted as indicative of decision-support capability rather than validated operational performance in real-world environments.

The inclusion of these independent variables contributes to improved model learning and forecasting accuracy [37]. The results demonstrate that integrating machine learning forecasting, optimization-based allocation, and interpretability analysis provides a comprehensive decision-support framework for smart infrastructure energy management. The hybrid framework not only improves prediction accuracy but also translates predictive insights into actionable operational strategies. The interpretability component further enhances model transparency, supporting trust and adoption of intelligent decision-support systems in energy planning and infrastructure design. The findings confirm that hybrid machine learning optimization frameworks can significantly improve heating load prediction, energy allocation efficiency, and decision transparency in smart infrastructure systems.

6. Conclusion

This study presented a hybrid machine learning optimization framework for energy demand forecasting and intelligent decision support in smart infrastructure systems. By integrating predictive modeling, operational optimization, and explainable artificial intelligence within a unified architecture, the proposed approach addresses the structural disconnect between standalone forecasting models and real-world energy management processes. Empirical evaluation using the UCI Building Energy Efficiency dataset demonstrated that tree-based learning, particularly XGBoost, achieved superior predictive performance ($R^2 = 0.996$), while the ensemble model provided strong robustness and generalization capability. The integration of forecasting outputs into the optimization module enabled effective energy allocation, reduced demand fluctuations, and improved operational cost efficiency under system constraints.

The incorporation of SHAP-based interpretability further enhanced transparency by identifying relative compactness and glazing area as dominant contributors to heating load demand. Residual and uncertainty analyses confirmed the reliability and stability of the hybrid framework across varying demand ranges. The findings demonstrate that combining machine learning, optimization, and explainable AI within a single coherent framework significantly improves predictive accuracy, operational efficiency, and decision transparency. The proposed methodology provides a scalable and trustworthy foundation for intelligent energy management in smart grids, intelligent buildings, and data-driven infrastructure systems. The proposed framework is hybrid in terms of methodological integration, while its implementation follows a sequential pipeline that ensures clear information flow between prediction and optimization stages. Future research may extend this framework to real-time deployment scenarios, renewable integration, and multi-objective optimization environments.

7. Limitations and Future Work

This study has several limitations that provide opportunities for future research. First, the experimental evaluation is conducted on a relatively small, simulation-based dataset, which may not fully represent the complexity of real-world smart infrastructure systems. Second, the framework follows a sequential pipeline without incorporating feedback mechanisms or adaptive learning between forecasting and optimization stages. Third, the optimization model is simplified and does not account for multi-objective, stochastic, or real-time constraints commonly found in practical energy systems. Additionally, the use of SHAP is limited to post hoc interpretability and does not influence the decision-making process.

Future work will focus on extending the framework to real-time environments, incorporating dynamic and large-scale datasets, developing more advanced optimization models, and integrating feedback-driven learning mechanisms. Furthermore, comparative benchmarking against existing hybrid approaches and inclusion of additional evaluation metrics will enhance the robustness and applicability of the framework.

8. Declarations

8.1. Author Contributions

Godfrey Perfectson Oise: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing, Original Draft, Supervision, Project administration; **Tejiri Jessa:** Formal analysis, Investigation, Data Curation, Writing – Original Draft; **Evans Mintah:** Formal analysis, Investigation, Resources, Data Curation; **Felix Oshiorenoya Uloko:** Validation, Writing – Review & Editing, Visualization; **Oludare Sokoya:** Supervision, Writing – Review & Editing, Project administration; **Osahon Ukpebor:** Supervision, Writing , Review & Editing, Funding acquisition.

8.2. Institutional Review Board Statement

Not applicable.

8.3. Informed Consent Statement

Not applicable.

8.4. Data Availability Statement

The data presented in this study are available at: https://www.kaggle.com/datasets/ujjwalchowdhury/energy-efficiency-data-set.

8.5. Acknowledgment

Not applicable.

8.6. Conflicts of Interest

The authors declare no conflicts of interest.

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