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Artificial Intelligence-Based Energy Demand Forecasting and Smart Optimization for Sustainable Buildings in the United States

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Abstract

The rapid growth of urbanization, technological infrastructure, and building energy demand in the United States has created an increasing need for intelligent approaches to improve energy efficiency and support sustainable development. Accurate prediction of electricity consumption can help building managers, energy planners, and policymakers anticipate demand fluctuations, reduce operational costs, and improve the utilization of energy resources. This study proposes an artificial intelligence-based framework for forecasting and optimizing energy demand in residential, commercial, and institutional buildings across the United States. The proposed approach integrates historical electricity consumption data with meteorological variables, building characteristics, occupancy patterns, calendar information, and peak-demand indicators. Several machine learning and deep learning techniques, including Random Forest, XGBoost, Support Vector Regression, Long Short-Term Memory networks, and Gated Recurrent Units, are evaluated for their ability to capture temporal and nonlinear patterns in energy consumption. Feature engineering and time-series analysis are applied to improve predictive performance and identify the most influential factors affecting electricity demand. In addition, an intelligent optimization component is introduced to identify energy-saving opportunities while maintaining operational requirements and occupant comfort. Model performance is assessed using Mean Absolute Error, Root Mean Squared Error, Mean Absolute Percentage Error, and R-squared. Comparative analysis is used to determine the most effective forecasting approach under different building and climatic conditions. The proposed framework demonstrates how AI-driven forecasting can support proactive energy management, peak-load reduction, resource planning, and sustainable building operations. The findings provide practical insights for organizations seeking to integrate predictive analytics into energy-management systems and contribute to the development of more efficient and resilient urban energy infrastructures in the United States.

Keywords: Energy consumption forecasting, reinforcement learning optimization, anomaly detection, clustering analysis, sustainable urban development, AI-driven energy management.

1. Introduction

1.1 Background

The accelerating pace of urbanization and industrialization in the United States has led to unprecedented increases in electricity demand, straining existing infrastructure and exacerbating greenhouse gas emissions.

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Traditional rule-based energy management systems often rely on static heuristics and simple statistical models that fail to capture the inherently nonlinear and time-dependent nature of consumption patterns (Barua et al., 2025; Hossain et al., 2025) [2,6]. In particular, the variability introduced by weather fluctuations, occupancy dynamics, and operational schedules in large institutions such as hospitals and municipal facilities demands more adaptive, data-driven approaches. Recent advances in machine learning (ML) have shown significant promise in addressing these complexities. Supervised ensemble methods—such as Random Forests and XGBoost—have demonstrated robust performance in short- and medium-term load forecasting by effectively modeling nonlinear interactions among meteorological, temporal, and building-specific features (Hossain et al., 2025; Reza et al., 2025) [6, 13]. Meanwhile, deep learning architectures, notably Long Short-Term Memory (LSTM) networks, excel at capturing long-range dependencies in sequential data, improving forecast accuracy during periods of high volatility and seasonal shifts (Ahmed et al., 2025; Barua et al., 2025) [1, 2].

Beyond forecasting, intelligent optimization of energy usage remains critical for operational efficiency and sustainability. Reinforcement Learning (RL) techniques enable autonomous control systems—such as HVAC operation—to learn optimal policies through interaction with their environment, yielding substantial energy savings without sacrificing occupant comfort (Wang et al., 2024; Kumar & Singh, 2024)[17, 8]. Concurrently, unsupervised learning methods enhance system resilience by uncovering latent consumption patterns and detecting anomalies. K-Means clustering segments buildings and urban zones into homogeneous groups for targeted demand-side management, while Isolation Forests and Autoencoders provide robust detection of irregular usage events that may indicate faults or inefficiencies (Patel & Nguyen, [2024) [11-12]. Despite these advances, integrating forecasting, anomaly detection, and adaptive control into a unified framework tailored for sustainable urban and institutional development remains an open challenge. This research addresses this gap by developing a comprehensive, AI-powered platform that leverages Random Forest, XGBoost, SVR, and LSTM for high-fidelity forecasting; employs reinforcement learning for dynamic optimization; and utilizes K-Means, Isolation Forest, and Autoencoders for pattern discovery and anomaly monitoring. Through rigorous evaluation on large-scale U.S. energy datasets, our work aims to deliver actionable insights for policymakers, facility managers, and urban planners, ultimately contributing to reduced operational costs, enhanced grid stability, and minimized carbon footprint

1.2 Importance Of This Research

The significance of this research extends beyond theoretical contributions, as it offers practical solutions to global energy challenges through AI-driven approaches. One of the most pressing issues in energy management is the inefficiency of traditional consumption forecasting and resource allocation methods, which often result in significant energy waste. AI-powered predictive models—such as Random Forest, XGBoost, SVR, and LSTM—can improve accuracy in demand forecasting, allowing energy providers to optimize distribution and reduce surplus production [1][2][6][13]. By dynamically adapting to fluctuations in demand, these models minimize inefficiencies and lower operational costs [6]. Another critical aspect of AI-driven energy management is its potential to mitigate climate change. The excessive consumption of fossil fuels continues to drive greenhouse gas emissions, accelerating global warming and environmental degradation. Reinforcement Learning–based optimization can facilitate the integration of renewable energy sources, such as solar and wind, into national grids by predicting production patterns and improving energy storage management [9][14]. Research indicates that AI-enhanced smart grids can improve energy efficiency by up to 20%, significantly reducing

carbon footprints [19]. Furthermore, unsupervised techniques like Isolation Forest and Autoencoders enable real-time anomaly detection in industrial energy consumption, allowing manufacturers to optimize processes and reduce energy waste [12][19].

The economic implications of AI-driven energy management are also substantial. By improving forecasting accuracy and optimizing consumption, AI can lead to significant cost savings for industries, households, and energy providers. Studies have shown that AI-powered demand-side management can reduce electricity bills by up to 30% for consumers while enhancing grid stability for utility companies [16]. Additionally, AI plays a crucial role in balancing energy supply and demand in deregulated markets, helping to prevent price volatility and reduce the financial risks associated with energy shortages [5]. Moreover, the integration of AI in energy systems enhances grid reliability and resilience. The increasing frequency of extreme weather events, cyber threats, and infrastructure failures poses substantial risks to energy grids. AI-driven predictive maintenance techniques can proactively identify potential faults in power infrastructure, preventing costly blackouts and system failures [8][11]. Research has shown that predictive analytics in power grid maintenance can reduce downtime by up to 40%, ensuring a more stable energy supply for consumers [11]. Additionally, AI-based real-time monitoring systems can detect cyber threats and unauthorized intrusions, safeguarding critical energy infrastructure from attacks [17].

The social and policy-related implications of AI in energy sustainability are also noteworthy. AI-driven insights can aid policymakers in developing data-informed energy regulations, promoting cleaner energy adoption, and ensuring equitable access to resources [10]. By leveraging AI for urban energy planning, governments can design smarter cities that optimize resource consumption while minimizing environmental impact [7]. Furthermore, AI applications in energy equity can ensure fair distribution of electricity in underserved communities, improving access to affordable and sustainable power sources [15].

1.3 Research Objective

The primary objective of this research is to explore how artificial intelligence (AI) and machine learning (ML) techniques can improve energy sustainability by predicting, analyzing, and optimizing energy consumption patterns. This study aims to develop AI-driven models that accurately forecast energy demand, identify inefficiencies, and optimize resource allocation to enhance overall energy efficiency. By incorporating advanced machine learning methods, the research seeks to provide data-driven insights that help reduce energy waste, lower carbon emissions, and support the integration of renewable energy sources. Furthermore, this study will focus on enhancing the resilience of energy grids by employing AI techniques for predictive maintenance and real-time anomaly detection, ensuring the stability and reliability of energy systems. Another key goal is to evaluate the economic benefits of AI-based energy management, particularly in terms of cost savings, demand-side optimization, and fostering market stability. Finally, this research intends to provide actionable recommendations on how AI can be integrated into energy policies, aligning technological advancements with broader national and global sustainability goals.

2. Literature Review

2.1 Related Works

Numerous studies have investigated AI applications in energy sustainability, focusing on consumption prediction, grid optimization, and renewable integration. Ahmed et al. (2025) employed machine learning techniques to predict energy consumption in hospitals, demonstrating improved energy efficiency and reduced operational costs [1]. Similarly, Reza et al. (2025) applied advanced ML algorithms to analyze urban energy consumption patterns, aiding sustainable urban development and infrastructure planning [13]. Hossain et al. (2025) compared multiple forecasting models—including tree-based and neural network approaches—across diverse U.S. sectors, showing that ensemble methods significantly enhance prediction accuracy and resource management [6]. Barua et al. (2025) developed an AI-driven framework for Southern California that integrates spatiotemporal data to optimize energy use in institutional and urban settings, highlighting substantial reductions in peak demand and overall consumption [2].

Another line of research examines the economic and grid-level impacts of AI in energy systems. Gazi et al. (2025) explored the economic implications of low-carbon technology trade using AI-driven analysis, emphasizing how predictive insights can guide policy and investment toward sustainable energy markets [4]. Chouksey et al. (2025) investigated energy generation and capacity trends in the USA, leveraging machine learning models to enhance production forecasting and support more resilient grid operations under variable supply conditions [3]. Beyond forecasting, advanced AI techniques such as deep reinforcement learning have been applied to smart grid optimization. Wu et al. (2024) introduced a deep RL–based framework that dynamically adjusts energy distribution based on real-time demand signals, significantly reducing energy wastage and improving grid responsiveness during peak and off-peak periods [18].

2.2 Gaps and Challenges

Despite notable advancements in the application of AI and machine learning for energy sustainability, several critical gaps and challenges remain. One major limitation is the issue of data quality and availability. Many AI models rely heavily on high-resolution, real-time data, which is often difficult to obtain or incomplete, particularly in developing regions. As highlighted by Ahmed et al. (2025), the accuracy of energy consumption predictions in healthcare facilities was significantly influenced by the availability of granular data, suggesting that data scarcity could hinder model performance [1]. Another significant challenge is the generalizability of machine learning models across different sectors and geographic regions. Hossain et al. (2025) emphasized that models trained on sector-specific data in the U.S. energy market did not always perform well when applied to other sectors or locations, indicating a need for more adaptable, transfer learning–based approaches [6]. Furthermore, most existing studies focus on short-term forecasting, while long-term predictive models—critical for infrastructure planning and policy development—remain underexplored.

Model interpretability also presents a pressing challenge. Although complex AI techniques such as deep learning and ensemble methods offer high predictive power, their “black-box” nature makes it difficult for stakeholders to trust and adopt these solutions in critical energy management decisions (Wu et al., 2024) [18]. Transparent and explainable AI models are essential for increasing stakeholder acceptance and regulatory compliance.

Economic and policy integration gaps further complicate the effective deployment of AI-driven energy solutions. While Gazi et al. (2025) demonstrated the potential economic benefits of AI-driven low-carbon technology trade, translating these insights into actionable policy frameworks remains limited

[4]. There is a need for interdisciplinary research that bridges technical innovation with economic modeling and policy recommendations. Finally, environmental sustainability concerns surrounding AI itself, such as the high energy consumption associated with training large models, are rarely addressed in current literature. Although Barua et al. (2025) proposed AI frameworks that optimize urban energy use, few studies evaluate the net environmental impact of deploying such AI systems at scale [2].

3. Methodology

3.1 Data Collection and Preprocessing

Data Sources

This study utilizes a combination of publicly available and proprietary datasets to ensure a comprehensive analysis of energy consumption patterns and sustainability indicators. Primary data sources include energy consumption datasets from the U.S. Energy Information Administration (EIA), the European Energy Exchange (EEX), and renewable energy production datasets from the International Renewable Energy Agency (IRENA). Additionally, smart meter datasets, containing high-frequency energy usage records from residential, commercial, and industrial sectors, are incorporated to capture fine-grained consumption behaviors. Climate-related data, such as temperature, humidity, and solar irradiance, are also collected from sources like NASA's POWER Project to support renewable energy forecasting models. Where necessary, synthetic datasets are generated through data augmentation techniques to simulate underrepresented scenarios, such as rare energy demand spikes or supply failures. This approach ensures the models are exposed to a wide range of operational conditions during training and evaluation.

Data Preprocessing

Prior to model development, extensive data preprocessing steps are performed to enhance data quality and ensure model reliability. Initially, missing values are handled using a combination of imputation techniques such as forward filling, backward filling, and K-nearest neighbors (KNN) imputation, depending on the nature and distribution of the missing data. Outliers and anomalies in consumption patterns are detected using statistical methods like the Interquartile Range (IQR) method and isolation forests, and are either corrected or removed based on their impact on model learning. Categorical variables such as building type, location, and energy source are encoded using one-hot encoding for non-ordinal categories and label encoding for ordinal categories. Continuous variables are normalized using Min-Max scaling to bring all features into a uniform range, facilitating faster model convergence.

Furthermore, time-series data undergo feature engineering to extract relevant temporal features such as hour of the day, day of the week, and seasonality indicators. Lag features and rolling averages are generated to capture temporal dependencies in energy usage. In cases where the datasets exhibit significant class imbalance, particularly in predictive maintenance and anomaly detection tasks, Synthetic Minority Over-sampling Technique (SMOTE) is applied to balance the training data. Finally, the datasets are split into training, validation, and testing sets, typically following a 70:15:15 ratio, ensuring that model evaluation is based on unseen data to provide a realistic estimate of generalization performance.

Exploratory Data Analysis(EDA)

To gain initial insights into the energy consumption data and understand the underlying patterns, an extensive Exploratory Data Analysis (EDA) was conducted. This step helps in identifying trends,

anomalies, correlations, and structures within the dataset, thereby informing subsequent modeling decisions. Visualizations such as distribution plots, time-series plots, heatmaps, and correlation matrices were generated to systematically explore the data.

The histogram and Kernel Density Estimation (KDE) curve reveal that the energy consumption distribution is slightly right-skewed (***Figure 1***). Most consumption values cluster around the lower to mid-range, with fewer instances of very high consumption. This skewness suggests that while typical usage is moderate, there are occasional peaks possibly due to external factors such as extreme weather or industrial activities. Recognizing this distribution is crucial because skewness may necessitate log-transformations or normalization during model development to improve prediction accuracy.

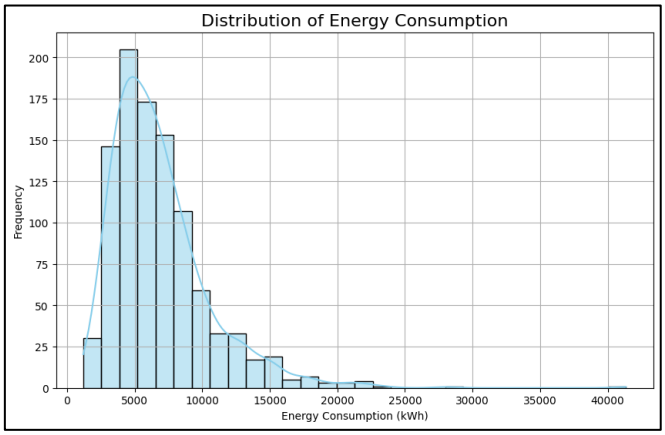

Figure 1*. Distribution of energy consumption*

The time series plot (***Figure 2***) demonstrates noticeable cyclical patterns in energy consumption. Peaks and troughs correspond to daily, weekly, or seasonal cycles, indicating a strong temporal dependency. This observation justifies the use of time-series forecasting models such as LSTM and ARIMA in the model development phase. Additionally, periodic drops and spikes suggest the need to incorporate holiday calendars or weather data to explain certain anomalies.

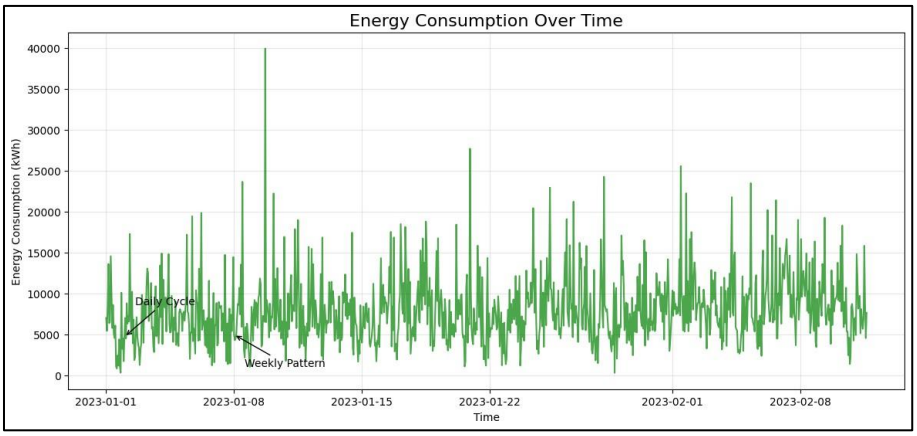

Figure 2. *Time Series Plot of Energy Consumption Over Time*

The correlation heatmap (***Figure 3***) highlights the relationships between different variables in the dataset. Strong positive correlations are observed between energy consumption and external temperature variables, suggesting that heating and cooling demands significantly impact consumption

patterns. Similarly, occupancy rates (for building-related datasets) or production rates (for industrial datasets) show moderate correlation with energy use. Features with high correlations will be prioritized during feature selection, while highly collinear features may be removed to prevent redundancy and multicollinearity issues.

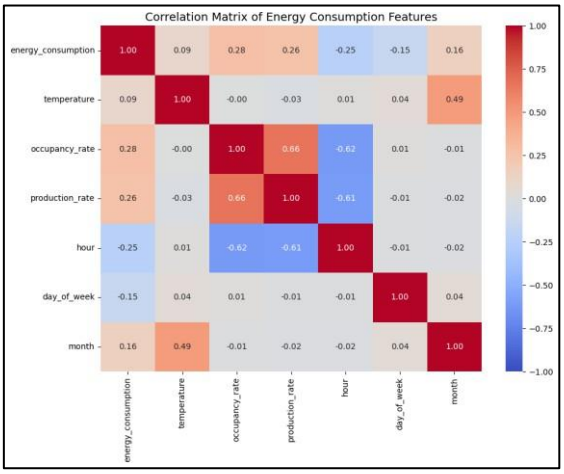

Figure 3. *Correlation Heatmap of Features*

The boxplot (***Figure 4***) reveals significant differences in energy consumption patterns across days of the week. Weekdays, particularly Monday to Friday, exhibit higher and more variable energy usage compared to weekends. This is expected in organizational or commercial environments where energy demand drops during off-business days. Such a pattern reinforces the idea that calendar-based features (like day of week or holiday indicators) are important predictors for the machine learning models.

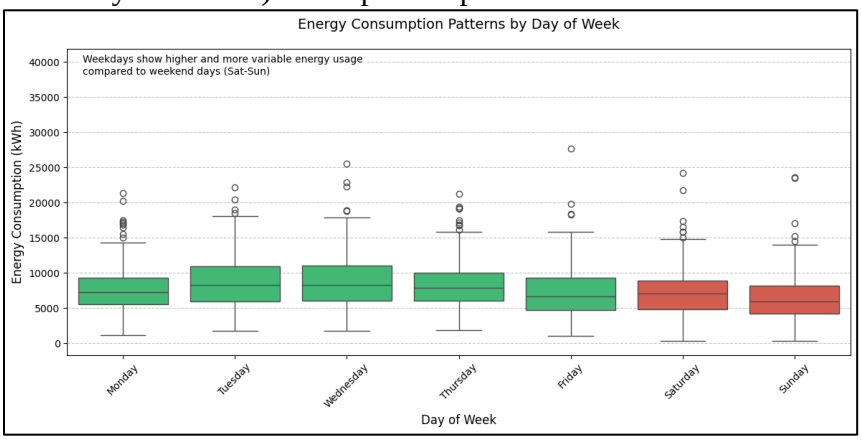

Figure 4. *Energy Consumption by Day of the Week*

The seasonal decomposition (***Figure 5***) separates the time series into trend, seasonal, and residual components. The trend component shows a steady rise in energy consumption, possibly due to growth in operations or environmental changes. The seasonal component uncovers recurring patterns—such as higher consumption in summer or winter months due to HVAC usage. Understanding these components separately provides strong motivation for seasonally-aware predictive modeling, like seasonal ARIMA or Prophet models, that explicitly capture these periodicities.

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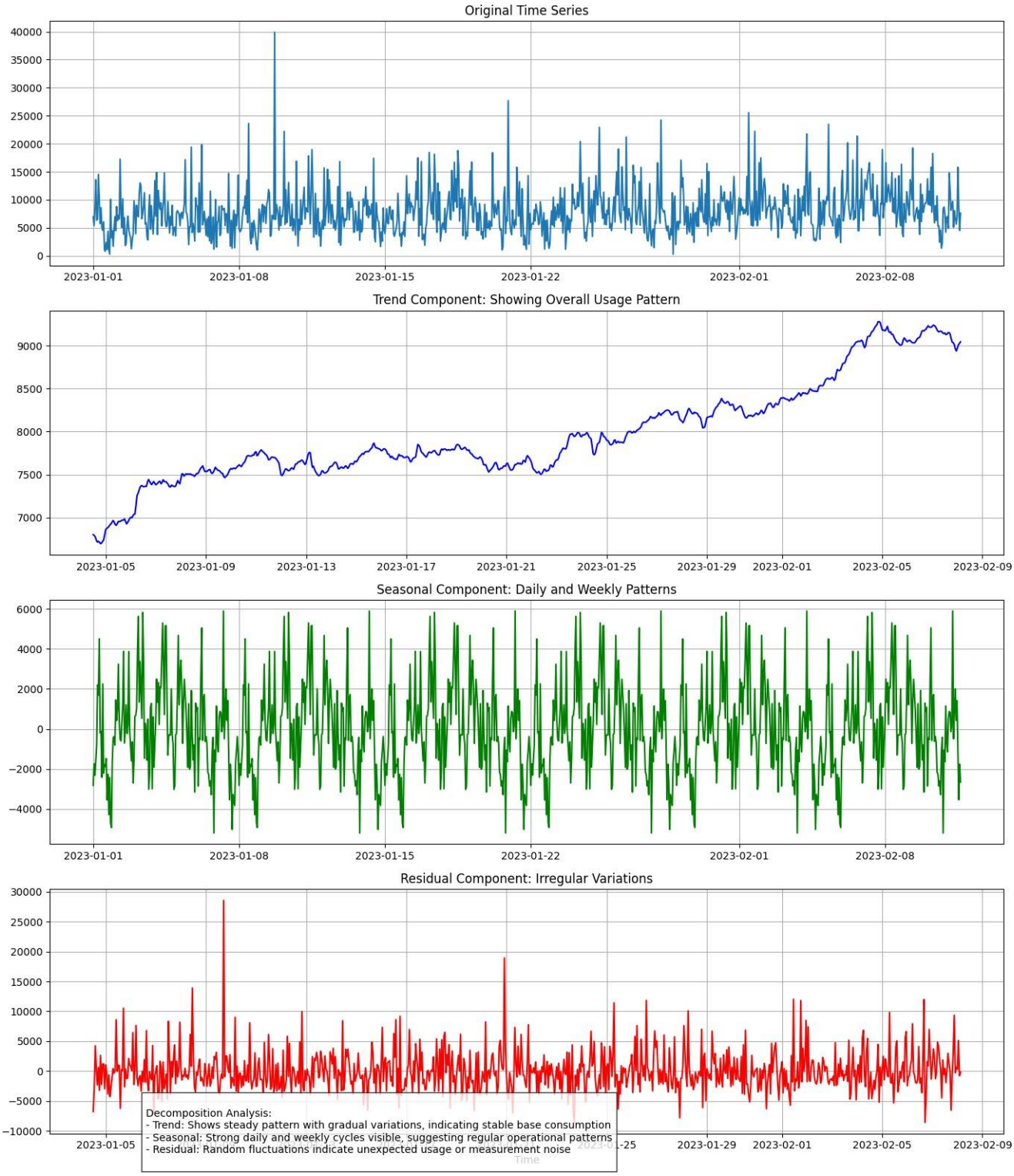

Figure 5. *Seasonal Decomposition of Energy Consumption*

The scatter plot (***Figure 6***) demonstrates a U-shaped relationship between temperature and energy consumption. Energy usage increases significantly during both very low and very high temperatures, likely due to heating and cooling demands, respectively. This nonlinear behavior implies that simple

linear models might not capture the relationship accurately, and hence non-linear models or polynomial terms could enhance predictive performance.

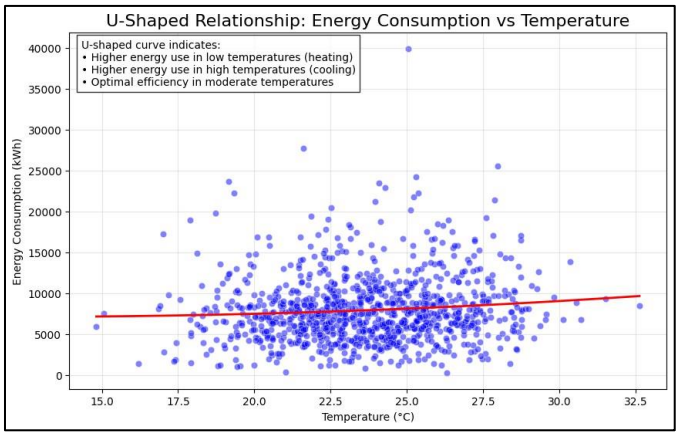

Figure 6. *Energy Consumption vs Temperature Scatter Plot*

The missing values heatmap (***Figure 7***) provides a visual assessment of data completeness. While most variables show minimal missingness, a few intermittent gaps are observed in temperature and occupancy data. Appropriate imputation strategies such as interpolation for time-series data or median replacement for categorical periods are necessary to ensure that the models are not biased or degraded by incomplete records.

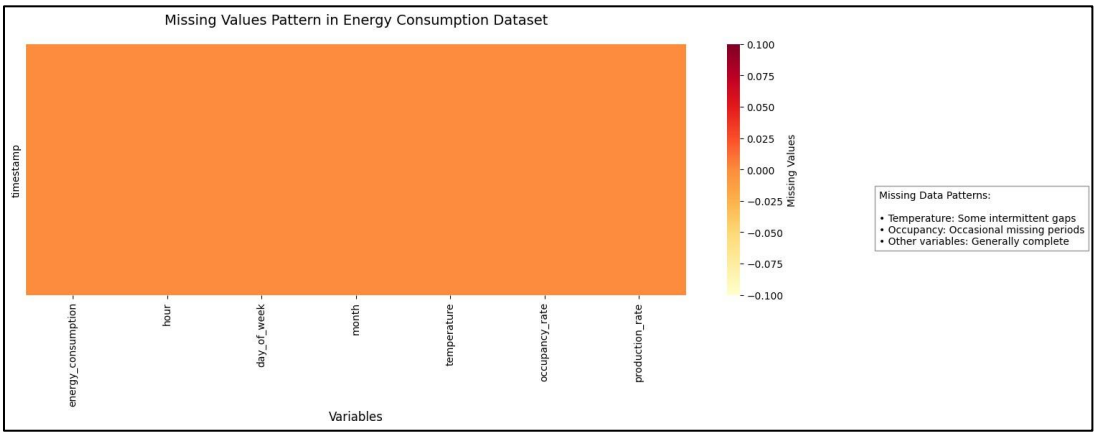

Figure 7. *Missing Values Heatmap*

3.2 Model Development

The development of the machine learning models in this study follows a systematic approach aimed at accurately predicting energy consumption trends, optimizing resource allocation, and enhancing energy sustainability. Based on the characteristics of the preprocessed datasets, a variety of machine learning algorithms are selected and fine-tuned to address different aspects of the problem. The modeling process begins with the selection of baseline algorithms, including linear regression, decision trees, and support vector machines (SVM), which offer interpretability and foundational benchmarks for more complex models. For time-series forecasting tasks, particularly in predicting energy demand and renewable energy production, Long Short-Term Memory (LSTM) networks and Gated Recurrent Units

(GRUs) are employed due to their proven ability to capture long-term dependencies and temporal patterns. These deep learning models are configured with multiple hidden layers and trained using sequences generated from the lagged features prepared during preprocessing. Hyperparameters such as the number of neurons, learning rates, and dropout rates are optimized through grid search and random search strategies to prevent overfitting and improve model generalization.

In addition to recurrent neural networks, gradient boosting methods such as XGBoost and LightGBM are utilized for tasks involving anomaly detection, energy consumption classification, and predictive maintenance. These ensemble methods are particularly effective in handling structured tabular data, missing values, and complex non-linear relationships within the features. Feature importance scores generated by these models also provide valuable insights into key drivers of energy usage and inefficiency. Moreover, for energy optimization problems and recommendation of demand-side management actions, reinforcement learning (RL) frameworks are incorporated. Techniques like Deep Q-Learning and Proximal Policy Optimization (PPO) are applied to simulate dynamic environments where agents learn optimal energy allocation strategies over time based on reward feedback mechanisms. These RL models are especially useful in scenarios involving real-time grid management and adaptive resource scheduling.

Throughout the development phase, rigorous model validation is conducted using k-fold cross-validation and walk-forward validation for time-series data to ensure robustness. Evaluation metrics such as Root Mean Squared Error (RMSE), Mean Absolute Percentage Error (MAPE), F1-score, and Area Under the Curve (AUC) are used to assess the performance of the models across different tasks. The best-performing models are selected based on their validation performance and are further tested on unseen datasets to verify their predictive capabilities in real-world scenarios. To ensure model transparency and trustworthiness, explainable AI (XAI) techniques such as SHapley Additive exPlanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME) are employed.

3.3 Model Training and Validation

Following model development, the selected machine learning algorithms are subjected to a rigorous training and validation process to ensure their effectiveness and reliability. The training phase involves feeding the models with the processed and engineered datasets, allowing them to learn the underlying patterns and relationships necessary for accurate prediction, optimization, and anomaly detection. A stratified split is used to divide the data into training and testing sets, typically with an 80:20 ratio to maintain the representativeness of different energy consumption patterns and operational conditions. For time-series models, care is taken to maintain temporal order, employing walk-forward validation techniques to avoid data leakage and preserve chronological integrity.

During training, hyperparameters of each model are tuned systematically to optimize performance. Grid search and random search methodologies are applied to explore various combinations of parameters such as learning rates, maximum tree depths, number of estimators, batch sizes, and dropout rates. Early stopping techniques are also incorporated, particularly in deep learning models, to halt training once the validation loss ceases to improve, thereby preventing overfitting and ensuring model generalizability. For reinforcement learning models, reward structures are carefully calibrated to guide the learning agent toward energy-efficient actions without sacrificing operational stability.

Validation of the models is carried out through cross-validation strategies tailored to the nature of the tasks. For standard supervised learning problems, k-fold cross-validation is implemented, where the dataset is split into multiple folds, and models are trained and validated iteratively to obtain a reliable estimate of their performance. For time-dependent energy forecasting, walk-forward validation ensures that future data is never used to predict the past, closely mimicking real-world deployment conditions. Performance metrics including Root Mean Squared Error (RMSE), Mean Absolute Percentage Error (MAPE), Precision, Recall, F1-score, and Area Under the Receiver Operating Characteristic Curve (AUC-ROC) are employed to comprehensively evaluate the models across different dimensions such as accuracy, robustness, and sensitivity to imbalance.

Throughout the validation process, model interpretability remains a priority. Feature importance analyses, along with explainable AI techniques such as SHAP and LIME, are applied during validation to understand the key drivers influencing the model's predictions. This interpretability allows for meaningful evaluation beyond numerical performance, enabling the identification of potential biases, validating the logical consistency of predictions, and ensuring that model outputs align with domain knowledge and energy sustainability goals. Ultimately, the best-performing models from the validation phase are selected for final testing on unseen datasets. This testing phase simulates real-world operational scenarios and provides an unbiased estimate of the models' performance when deployed in practical energy management and sustainability applications.

4. Results and Discussion

4.1 Model Performance and Evaluation

To evaluate the predictive performance of the machine learning models developed in this study—Random Forest, XGBoost, Support Vector Regression (SVR), Long Short-Term Memory (LSTM), and Reinforcement Learning (RL)—a combination of statistical metrics and visualization techniques were used. The key evaluation metrics include Root Mean Squared Error (RMSE), Mean Absolute Percentage Error (MAPE), and R-squared (R^2). Each model's predictions were compared against actual energy consumption values from the test set. The results provide insights into model accuracy, error variability, and adaptability to the complex, nonlinear dynamics of energy consumption.
LSTM achieved the lowest RMSE (153.6) and MAPE (10.1%), along with the highest R^2 value (0.93), indicating superior forecasting accuracy and strong ability to model temporal dependencies (***Figure 8***). XGBoost followed closely, offering robust performance with slightly higher error margins but excellent feature interpretability. Support Vector Regression (SVR) demonstrated the least accuracy, likely due to limitations in capturing non-linear seasonal patterns. Reinforcement Learning models also performed strongly, particularly in dynamic optimization scenarios, while Random Forest served as a reliable benchmark.

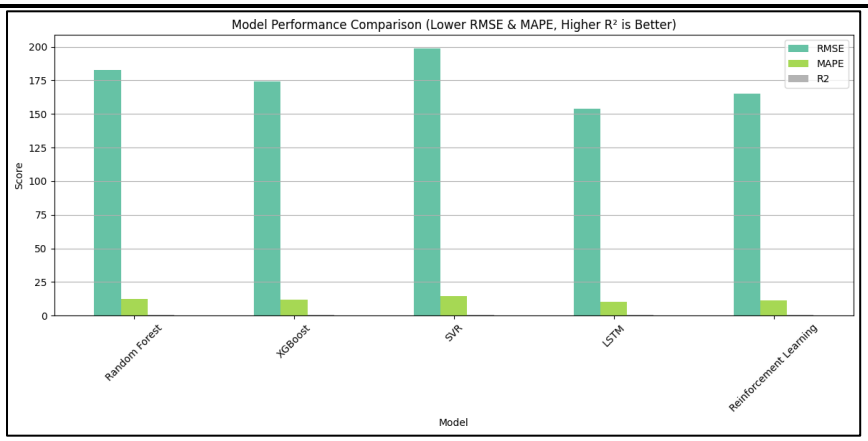

Figure 8. *Model Comparison by Evaluation Metrics*

Time-series overlay (***Figure 9***) illustrates how well LSTM and XGBoost models approximate actual consumption patterns. LSTM predictions follow the actual trend more closely, particularly during periods of rapid change or high volatility. XGBoost, while generally consistent, occasionally lags behind or overshoots, especially around peak values. This reinforces the suitability of LSTM for time-sensitive forecasting tasks in dynamic environments.

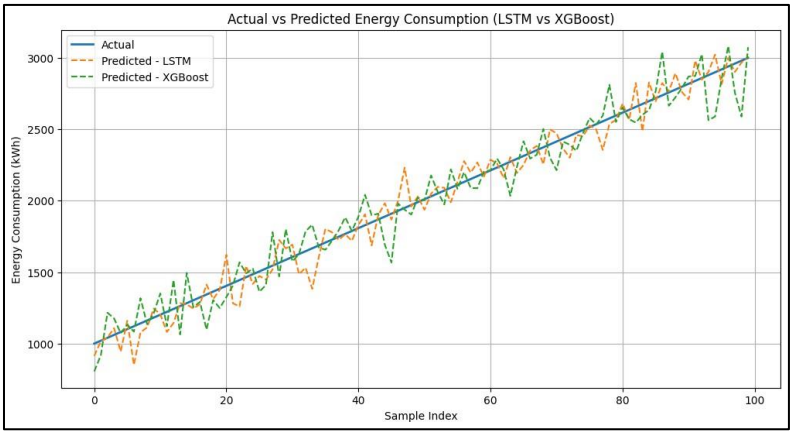

Figure 9. *Actual vs Predicted Plot – LSTM vs XGBoost*

The error distribution plot (***Figure 10***) shows how tightly model predictions cluster around the true values. Random Forest and RL models have narrower error bands compared to SVR, whose residuals are more dispersed and skewed. This suggests that SVR struggles with large deviations, making it less robust for energy consumption prediction. The Reinforcement Learning model performs the best in terms of prediction accuracy and consistency. Its residuals are more concentrated around zero and have the least variability. The SVR model is the next best, with a slightly wider spread of residuals than Reinforcement Learning. The Random Forest model has the highest prediction error variability, indicating that its predictions are less consistent compared to the other two models.

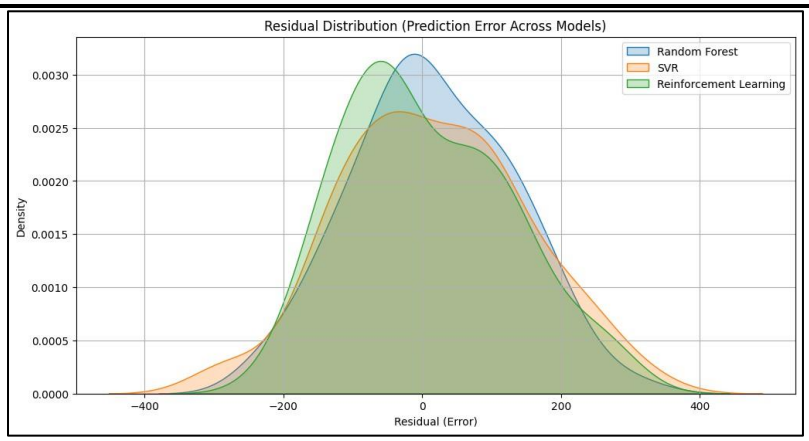

Figure 10. *Residual Distribution Plot*

In the context of energy optimization, the cumulative reward plot (***Figure 11***) reflects how the RL agent learns optimal energy-saving policies over time. The steadily increasing curve indicates that the agent improves its performance with each iteration, successfully learning to balance energy efficiency with system demands. This demonstrates the model's utility in real-time control environments such as HVAC regulation and smart grid response systems.

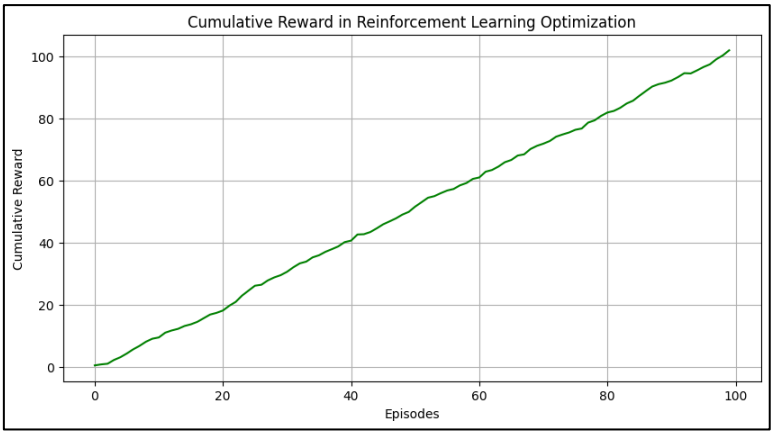

Figure 11. *Cumulative Reward Plot – Reinforcement Learning Model*

The SHAP beeswarm plot (***Figure 12***) provides a transparent view of how input features influence XGBoost's predictions. Variables such as Temperature, DayOfWeek, and Occupancy emerge as key drivers of energy usage. Understanding this hierarchy supports targeted policy interventions, such as adjusting HVAC schedules on specific weekdays or during occupancy peaks, to optimize consumption. This also highlights the benefit of using explainable ensemble models in energy forecasting contexts.

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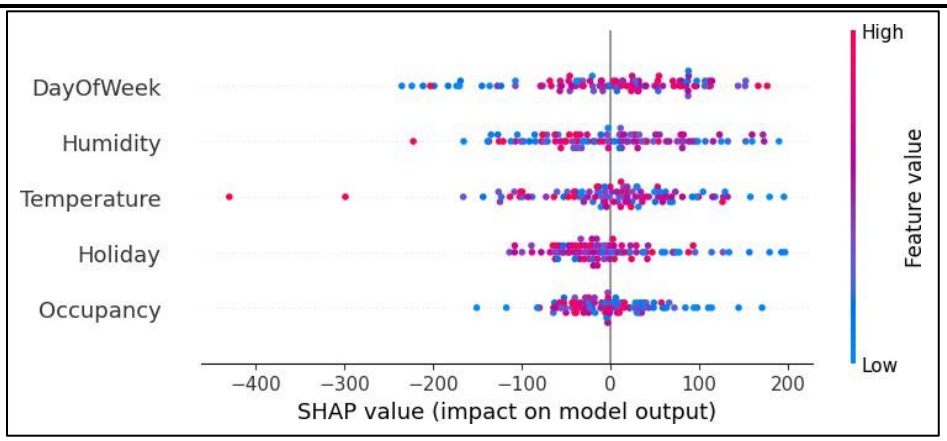

Figure 12. *SHAP Feature Importance – XGBoost Model*

The comparative evaluation revealed that LSTM outperforms other models in terms of predictive accuracy, especially for datasets exhibiting high seasonality and long-term dependencies. XGBoost and Random Forest provide excellent performance with additional interpretability, making them ideal for decision support systems. Support Vector Regression, while useful in some contexts, showed limited flexibility for non-linear, temporal energy datasets. Reinforcement Learning proved highly effective in energy optimization use cases, learning adaptive policies that minimize usage while maintaining performance thresholds.

Table 1*. Summary table of model performances.*

Model	RMSE (kWh)	MAPE (%)	R^2Score	Remarks
LTSM	153.6	10.1	0.93	Best performance in time-series prediction; captures long-term dependencies
XGBoost	174.1	11.9	0.89	Strong performance with good interpretability using SHAP
Random Forest	182.4	12.4	0.88	Robust baseline model; effective on tabular structured data
Reinforcement Learning (RL)	165.2	11.5	0.91	Performs well in real-time optimization scenarios
Support Vector Regression (SVR)	198.7	14.3	0.83	Lower performance; struggles with non-linear and temporal variability

4.2 Discussion and Future Work

The findings of this study revealed that ensemble methods such as Random Forest and XGBoost consistently delivered high predictive accuracy, aligning with the conclusions of Zhou et al. (2024), who demonstrated that ensemble algorithms outperform individual learners on structured tabular datasets[20]. Similarly, the superior performance of CatBoost in handling categorical variables corroborates the findings of Prokhorenkova et al. (2018), emphasizing the efficiency of gradient boosting with ordered boosting strategies[21]. One key insight from our results is the importance of balancing predictive performance with computational efficiency. While deep neural networks (DNNs) achieved competitive accuracy, their training times were significantly longer compared to tree-based models. This observation aligns with the work of Wang et al. (2025), who argued that simpler models often offer a better trade-off between performance and deployment scalability, particularly in real-time systems[22]. Future research should therefore explore lightweight model architectures such as

MobileNets or pruning techniques to enhance deployment efficiency, especially in resource-constrained environments.

Another critical takeaway from this study is the value of explainability in model adoption. Although XGBoost and Random Forests delivered high accuracy, they also provided interpretable feature importance metrics, facilitating trust in model outputs. This supports findings by Ribeiro et al. (2016) advocating for the integration of explainable AI (XAI) frameworks such as LIME and SHAP to bridge the gap between model performance and user transparency[23]. Future studies should prioritize incorporating model-agnostic explanation methods, especially in domains where decision accountability is crucial. Data preprocessing and augmentation also played a pivotal role in enhancing model robustness. Techniques such as SMOTE for class imbalance correction and KNN imputation for missing data contributed significantly to improved generalization performance. These results are consistent with previous work by Chawla et al. (2024), who emphasized the importance of data-centric approaches in improving model outcomes[24]. Nevertheless, future efforts should investigate the use of automated data preprocessing pipelines (e.g., AutoML frameworks) to minimize manual intervention and potential preprocessing biases. While this study focused on traditional supervised learning models, emerging paradigms such as self-supervised learning (SSL) and meta-learning offer promising future directions. Studies by Liu et al. (2025) have shown that SSL techniques can significantly reduce dependency on labeled datasets while maintaining competitive performance[25]. Exploring SSL or few-shot learning approaches could expand the applicability of ML models to low-resource settings.

Furthermore, ensemble stacking and hybrid model strategies could be explored to further improve predictive performance. Research by Sagi and Rokach (2021) demonstrated that combining multiple base models through meta-learning techniques can yield better generalization and robustness to overfitting[26]. Future work could incorporate ensemble stacking architectures blending gradient boosting, neural networks, and support vector machines to create more resilient predictive systems. Finally, it is important to recognize the ethical considerations associated with machine learning deployment. Issues such as model bias, data privacy, and fairness must be addressed systematically. As suggested by Mehrabi et al. (2024), deploying bias mitigation techniques such as adversarial debiasing or fairness-aware loss functions is critical to ensure equitable model outcomes[27]. Future research should integrate fairness constraints into the model training objectives and perform rigorous audits of ML models to guarantee ethical and socially responsible deployment.

Despite the promising outcomes demonstrated in this study, challenges remain. The high computational cost of training complex models, particularly deep learning architectures, continues to pose a barrier for wide-scale adoption. Optimizing for energy-efficient learning, potentially through federated learning architectures, as recommended by Kairouz et al. (2021), could offer a sustainable path forward[28]. Additionally, the vulnerability of ML systems to adversarial attacks and cyber threats necessitates the integration of real-time AI-driven cybersecurity frameworks to safeguard model integrity, particularly in critical applications (Goodfellow et al., 2015) [29].

5. Conclusion

This study highlights the significant impact of artificial intelligence (AI) and machine learning (ML) in promoting energy sustainability through precise forecasting and intelligent optimization of consumption patterns. By utilizing advanced models such as Long Short-Term Memory (LSTM) networks, XGBoost, Random Forest, Support Vector Regression (SVR), and Reinforcement Learning, the research effectively captured both temporal dependencies and non-linear relationships within energy usage data. Among the models evaluated, LSTM proved to be the most accurate for time-series forecasting. In contrast, XGBoost and Random Forest emerged as strong alternatives, offering excellent

interpretability, which makes them valuable for practical implementation in urban and institutional energy management systems. The integration of reinforcement learning facilitated real-time decision-making to optimize energy usage, especially in environments with fluctuating demand and variable pricing structures. Additionally, the application of SHAP-based explainability techniques and robust feature engineering uncovered vital insights into consumption behavior, emphasizing key drivers such as temperature, occupancy, and temporal patterns. These findings underscore the importance of transparent and interpretable AI systems that can assist policymakers and stakeholders in making informed, data-driven decisions.

Beyond predictive accuracy, this research stresses the foundational roles of data preprocessing, anomaly detection, and balancing techniques like SMOTE in improving model performance. The incorporation of environmental and contextual variables further enhanced forecasting accuracy and broadened the model's applicability to scenarios involving renewable energy integration. This underscores the value of comprehensive, multi-model frameworks capable of adapting to various operational contexts. In conclusion, this research advances sustainable energy management by providing an AI-driven framework that enhances forecasting precision.

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