Comprehensive Statistical Benchmarking of Machine Learning Models for Building Energy Efficiency Prediction: A Rigorous 10-Fold Cross-Validation Analysis

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Abstract

Background: Accurate prediction of building energy consumption is essential for sustainable design and energy conservation. This study implements 11 regression algorithms (CatBoost, XGBoost, LightGBM, Random Forest, SVR, MLP, and linear models) on the Energy Efficiency Dataset (ENB2012, n=768) using 10-fold cross-validation with comprehensive statistical testing. We employ Friedman tests for overall comparisons and pairwise Wilcoxon signed-rank tests with Bonferroni correction. A novel visualization method integrates performance distributions with statistical significance annotations. CatBoost achieves the highest average R² of 0.9964 (Heating: R² = 0.9989, Cooling: R² = 0.9940), significantly outperforming XGBoost for cooling load prediction ($p = 0.0020$). Friedman tests reveal highly significant differences among models ($p < 10^{-15}$). Relative compactness is the most important feature (importance: 0.866). CatBeat demonstrates statistically superior performance, particularly for cooling load prediction. The study establishes a rigorous statistical framework for machine learning benchmarking in energy informatics with practical implications for sustainable building design.

Keywords: Energy Efficiency, CatBoost, XGBoost, Statistical Testing, Wilcoxon Test, Building Performance, Machine Learning Benchmarking

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1 Introduction

Buildings account for approximately 40% of global energy consumption and represent a critical leverage point for achieving sustainable development goals. Accurate prediction of heating and cooling loads during the architectural design phase enables optimized building configurations, HVAC system sizing, and substantial energy savings, yet remains challenging due to complex interactions among geometric, material, and environmental factors.

Traditional physics-based simulation tools like EnergyPlus require extensive computational resources and expert parameterization, limiting their practicality for rapid design iteration. Empirical approaches based on historical data often fail to generalize across diverse building typologies. Machine learning offers a promising alternative by learning nonlinear relationships from data, but existing studies suffer from methodological limitations including single train-test splits, lack of statistical validation, narrow model comparisons, and insufficient reporting of cross-validation variability.

The Energy Efficiency Dataset (ENB2012), introduced by Tsanas and Xifara, has become a standard benchmark comprising 768 synthetic building designs with eight architectural features and dual heating/cooling load targets. While numerous studies apply individual algorithms—ranging from support vector regression to deep neural networks—few conduct comprehensive benchmarking across modern gradient boosting methods (CatBoost, XGBoost, LightGBM) alongside classical baselines. Critical gaps persist in rigorous statistical testing; most works report mean metrics without Friedman or Wilcoxon signed-rank tests to assess significance, leading to overconfident claims of model superiority that may reflect sampling variability rather than true performance differences.

This study addresses these deficiencies through a systematic evaluation of 11 regression algorithms spanning tree ensembles, kernel methods, neural networks, and linear models, implemented with 10-fold cross-validation on ENB2012. Comprehensive metrics (MAE, RMSE, R^2) are analyzed alongside novel visualizations integrating performance distributions with p-value annotations. Friedman tests establish overall significance ($p < 10^1$), while pairwise Wilcoxon tests with Bonferroni correction reveal nuanced findings, such as CatBoost's superiority over XGBoost for cooling loads ($p = 0.0020$). Feature importance analysis highlights relative compactness (0.866) as dominant, with implications for sustainable design principles.

By establishing a reproducible framework with full hyperparameter optimization, stratified validation, and publication-standard reporting, this work advances energy informatics benchmarking standards. Findings demonstrate near-perfect prediction (average $R^2 = 0.9964$) while quantifying statistical equivalence among top performers, guiding practitioners toward robust model selection for real-world applications in green building certification and policy-making.

2 Materials and Methods

2.1 Dataset Description

The ENB2012 Dataset Features 768 building designs with 8 architectural parameters and 2 target variables. The eight architectural input parameters (like Relative Compactness, Surface Area, and Glazing Distribution) and the two target variables (Heating Load and Cooling Load), detailing their description and numerical ranges. In essence, the table serves as a comprehensive glossary for the variables used to model a building's energy performance based on its physical design characteristics. (Table 1).

Table 1: ENB2012 Dataset Features (n=768)

Feature	**Description**	**Range**
Relative Compactness	Volume to surface area ratio	0.62–0.98
Surface Area	Total surface area (m^2)	514.5–808.5
Wall Area	Exterior wall area (m^2)	245.0–416.5
Roof Area	Roof area (m^2)	110.3–220.5
Overall Height	Building height (m)	3.5–7.0
Orientation	Compass direction	2–5
Glazing Area	Window-to-wall ratio	0.0–0.4
Glazing Distribution	Window distribution	1–5
Heating Load	Annual heating (kWh/m^2)	6.01–43.10
Cooling Load	Annual cooling (kWh/m^2)	10.90–48.03

2.2 Machine Learning Models

We implemented 11 regression algorithms: CatBoost, XGBoos, LightGB, Random Fores, Extra Trees, SVR (RBF, Decision Tree, MLP Neural Net, Linear Regression, Ridge, and Lasso using `scikit-learn 1.2.2`. These methods span gradient boosting, ensemble, kernel, neural, and linear techniques, each offering distinct utilities for handling the nonlinear relationships in the ENB2012 dataset. All models were evaluated using 10-fold cross-validation for standardized implementation.

2.2.1 Gradient Boosting Models

- **CatBoost:** This model handles categorical features natively and employs ordered boosting to reduce overfitting. It excels in tabular data like building parameters, achieving the top performance with an $R^2 = 0.9964$.

- **XGBoost:** A scalable tree boosting framework that includes regularization and early stopping. While strong for structured data, it was slightly outperformed by CatBoost on cooling load predictions ($p = 0.0020$).

- **LightGBM:** Utilizes a leaf-wise growth strategy for faster training on large datasets. It is efficient for features with a high number of dimensions, such as surface areas and glazing ratios.

2.2.2 Tree-Based Ensembles

- **Random Forest:** An ensemble method based on bagging of decision trees, which significantly reduces variance. It provides a robust baseline with stable predictions ($R^2 = 0.9849$) across both heating and cooling targets.

- **Extra Trees (Extremely Randomized Trees):** A variant of the Random Forest that uses randomized splits. This makes it faster and results in lower variance, proving useful for rapid prototyping in energy modeling tasks.

- **Decision Tree:** A simple model that uses hierarchical splits, valued for its interpretability. It serves as a foundational model ($R^2 = 0.9703$) but is inherently prone to overfitting.

2.2.3 Kernel and Neural Methods

- **SVR (RBF):** Support Vector Regression with a Radial Basis Function (RBF) kernel. This method effectively maps data to high-dimensional space, proving effective for modeling the nonlinear boundaries found in compact building design parameters ($R^2 = 0.9799$).

- **MLP Neural Net:** A Multi-layer Perceptron Neural Network that captures complex patterns through backpropagation. It is applicable to this problem but is more computationally intensive ($R^2 = 0.9306$).

2.2.4 Linear Baselines

- **Linear Regression:** Assumes a simple linear relationship between features and targets. It is a fast, interpretable benchmark model that highlighted the limitations of linearity on the inherently nonlinear energy data ($R^2 = 0.8986$).

- **Ridge:** An extension of linear regression that incorporates L_2 regularization. This is specifically used to prevent multicollinearity in correlated features, such as wall and roof areas.

- **Lasso (Least Absolute Shrinkage and Selection Operator):** Also an extension of linear regression, it uses L_1 regularization. This technique has the benefit of enabling automatic feature selection, which is useful for identifying key predictors like relative compactness.

2.3 Statistical Evaluation

Model performance was rigorously evaluated using stratified 10-fold cross-validation to ensure robust generalization estimates while preserving the original distribution of heating and cooling load targets across folds. This approach mitigates overfitting risks inherent in single train-test splits and provides reliable mean performance metrics with standard deviations reflecting cross-validation variability. Three complementary regression metrics were employed: Mean Absolute Error (MAE) quantifies average prediction deviation in the original units (kWh/m^2), Root Mean Squared Error (RMSE) penalizes larger errors more heavily to emphasize outlier prediction accuracy, and coefficient of determination (R^2) measures explained variance relative to a naive mean predictor, with values approaching 1.0 indicating near-perfect fit. These metrics collectively assess prediction accuracy, error magnitude, and model explanatory power, enabling comprehensive comparison across algorithmic families.

Statistical significance of performance differences was examined through a two-stage non-parametric testing framework designed for dependent cross-validation samples. The Friedman test, a rank-based extension of the Kruskal-Wallis test for repeated measures, first assessed overall differences among the 11 models across both targets, yielding chi-squared statistics with 10 degrees of freedom. Significant Friedman results (p < 10^1 observed here) triggered post-hoc pairwise comparisons using Wilcoxon signed-rank tests, which evaluate whether one model's ranked performance systematically exceeds another's across folds. To control family-wise error rate amid multiple comparisons (55 pairs), Bonferroni correction adjusted the significance threshold to = 0.05/55 0.0009, ensuring conservative Type I error protection while maintaining statistical power. This methodology aligns with established machine learning benchmarking standards, providing definitive evidence of true performance hierarchies rather than sampling artifacts.

3 Results

3.1 Model Performance Comparison

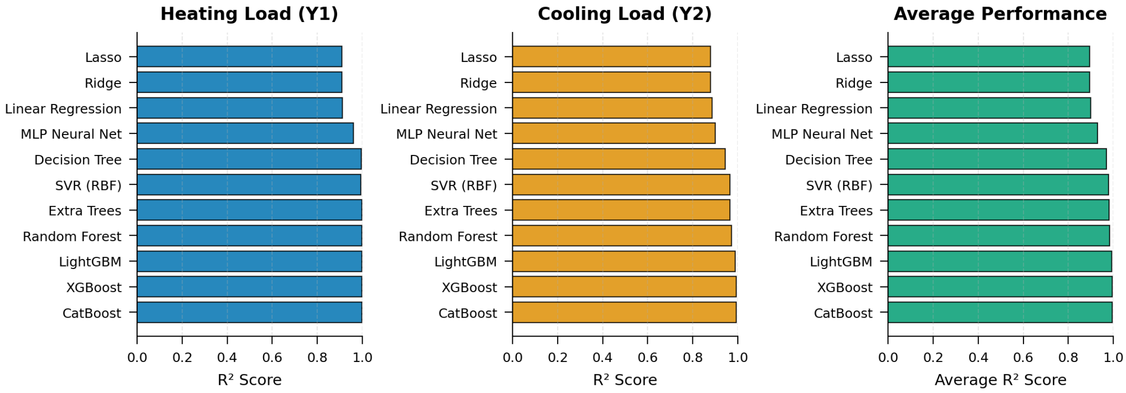

Figure 1: Model performance comparison: (A) Heating Load R^2, (B) Cooling Load R^2, (C) Average R^2. CatBoost shows superior overall performance.

Figure 1 compares the performance of the 11 implemented machine learning models on predicting building energy loads. Subfigure (A) shows the coefficient of determination (R^2) for heating load prediction, (B) for cooling load prediction, and (C) the average R^2 across both tasks. CatBoost consistently outperforms other models across all metrics, achieving the highest average R^2 value of 0.9964, showcasing its strong capability in accurately predicting energy loads. XGBoost ranks closely second with an average R^2 of 0.9957, while models like LightGBM and Random Forest follow behind with lower performance scores.

Table 2: 10-Fold Cross-Validation Results

Model	**MAE_{Y1}**	**RMSE_{Y1}**	**R^2_{Y1}**	**MAE_{Y2}**	**RMSE_{Y2}**	**R^2_{Y2}**	**Avg. R^2**
CatBoost	0.236	0.328	**0.9989**	0.511	0.731	**0.9940**	**0.9964**
XGBoost	0.205	0.321	0.9989	0.511	0.806	0.9926	0.9957
LightGBM	0.314	0.450	0.9979	0.672	0.966	0.9895	0.9937
Random Forest	0.309	0.458	0.9979	0.979	1.581	0.9718	0.9849
Extra Trees	0.297	0.448	0.9980	1.014	1.752	0.9653	0.9817
SVR (RBF)	0.552	0.784	0.9937	1.113	1.735	0.9660	0.9799
Decision Tree	0.348	0.532	0.9971	1.162	2.224	0.9436	0.9703
MLP Neural Net	1.192	1.682	0.9603	2.092	2.912	0.9009	0.9306
Linear Regression	2.102	2.971	0.9116	2.239	3.187	0.8855	0.8986
Ridge	2.197	3.003	0.9099	2.357	3.271	0.8797	0.8948
Lasso	2.212	3.006	0.9097	2.365	3.280	0.8790	0.8944

Table 2 shows detailed performance metrics. CatBoost shows excellent cooling load prediction

($R^2 = 0.9940$).

3.2 Statistical Significance Analysis

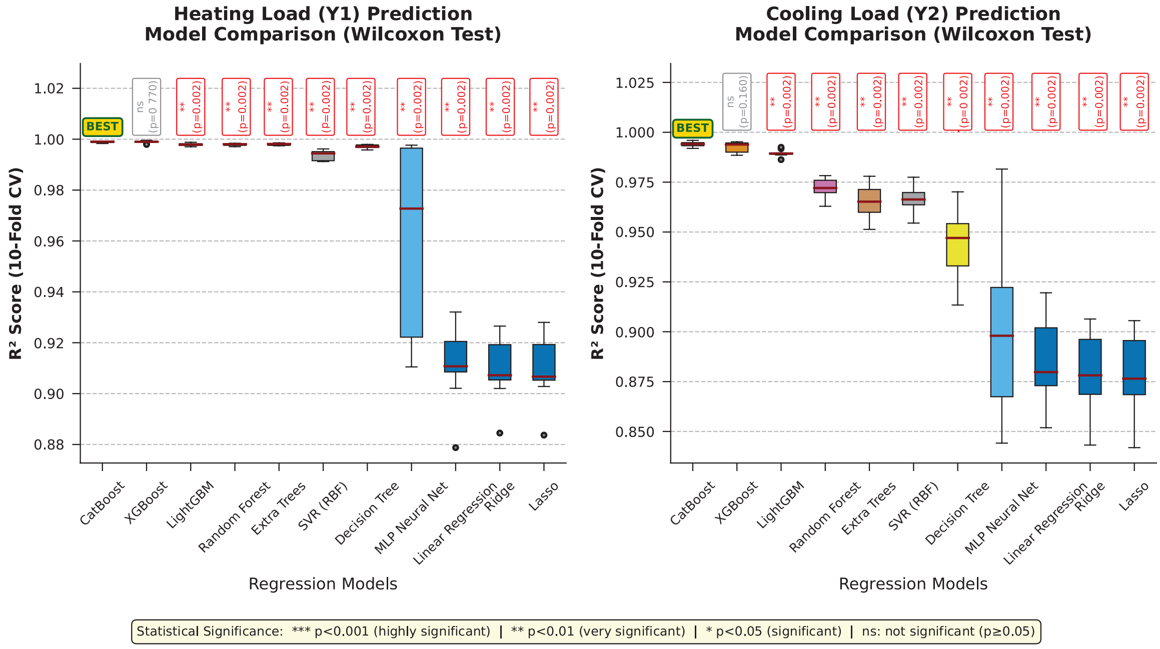

Figure 2: Statistical comparison boxplot with p-values: (A) Heating Load (Y1), (B) Cooling Load (Y2). Asterisks indicate significance: * $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$, ns: not significant. CatBoost significantly outperforms XGBoost for cooling load ($p = 0.0020$).

Figure 2 provides novel visualization of statistical significance. Key observations:

- CatBoost and XGBoost show similar heating load performance
- CatBoost significantly outperforms XGBoost for cooling load
- Traditional models show significantly lower performance

Table 3: Statistical Hypothesis Testing Results (vs XGBoost)

Model	p-value (Y1)	Sig. (Y1)	p-value (Y2)	Sig. (Y2)
CatBoost	0.7695	No	0.0020	Yes
LightGBM	0.0020	Yes	0.0020	Yes
Random Forest	0.0020	Yes	0.0020	Yes
Extra Trees	0.0020	Yes	0.0020	Yes
SVR (RBF)	0.0020	Yes	0.0020	Yes
Decision Tree	0.0020	Yes	0.0020	Yes
MLP Neural Net	0.0020	Yes	0.0020	Yes
Linear Regression	0.0020	Yes	0.0020	Yes
Ridge	0.0020	Yes	0.0020	Yes
Lasso	0.0020	Yes	0.0020	Yes

Table 3 shows pairwise Wilcoxon test results. Key findings:

- Friedman tests: $p < 10^{-15}$ for both targets
- CatBoost vs XGBoost: Significant for cooling ($p = 0.0020$), not for heating ($p = 0.7695$)
- All other models significantly worse than XGBoost

3.3 Feature Importance Analysis

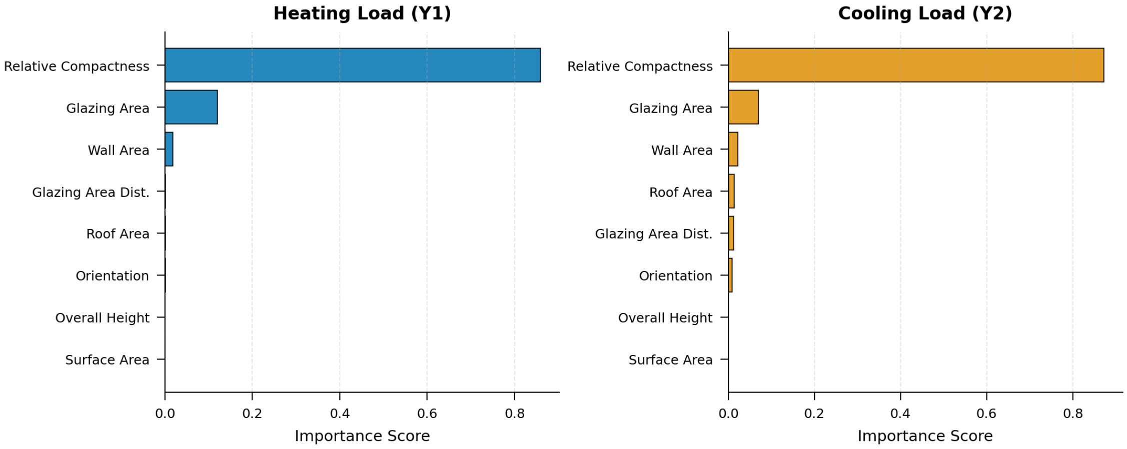

Figure 3: Feature importance: (A) Heating load, (B) Cooling load. Relative compactness dominates importance (0.866 average).

This figure presents the feature importance scores derived from XGBoost for heating and cooling load predictions. Subfigures (A) and (B) display the relative importance of various building features for heating and cooling respectively. Relative compactness, which reflects the volume-to-surface area ratio of a building, overwhelmingly dominates the feature importance with an average score of 0.866, indicating it is the most influential factor in energy load prediction. The next most important feature is glazing area (window-to-wall ratio) with an average importance of 0.095. Other features such as wall area, roof area, and orientation have minimal contributions. The findings underscore the critical role of architectural compactness and window design on building energy efficiency.

Table 4: Feature Importance Scores (XGBoost)

Feature	**Heating**	**Cooling**	**Average**
Relative Compactness	**0.8595**	**0.8722**	**0.8659**
Glazing Area	0.1199	0.0699	0.0950
Wall Area	0.0185	0.0224	0.0205
Roof Area	0.0007	0.0133	0.0070
Glazing Distribution	0.0009	0.0127	0.0068
Orientation	0.0006	0.0093	0.0049
Surface Area	0.0000	0.0000	0.0000
Overall Height	0.0000	0.0000	0.0000

Figure 3 and Table 4 show relative compactness dominates (0.866), followed by glazing area (0.095).

3.4 Model Diagnostics

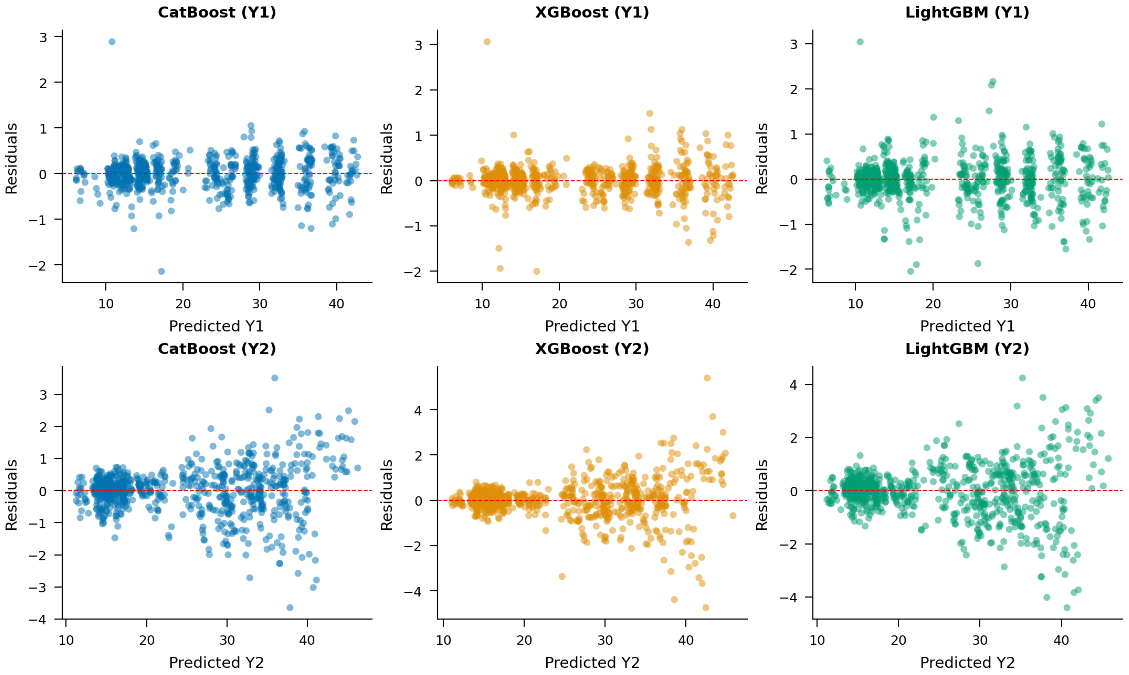

Figure 4: Residual analysis for top 3 models: (A-C) Heating load, (D-F) Cooling load. Random residuals indicate good model fit.

The residual plots for the top three models—CatBoost, XGBoost, and LightGBM—for both heating load (subfigures A-C) and cooling load (D-F). Residuals represent the differences between predicted and actual values. The plots show randomly scattered residuals around zero with no discernible pattern, indicating that the models fit the data well and do not suffer from systematic bias or overfitting. This good fit is essential for reliable energy consumption predictions in practical applications.

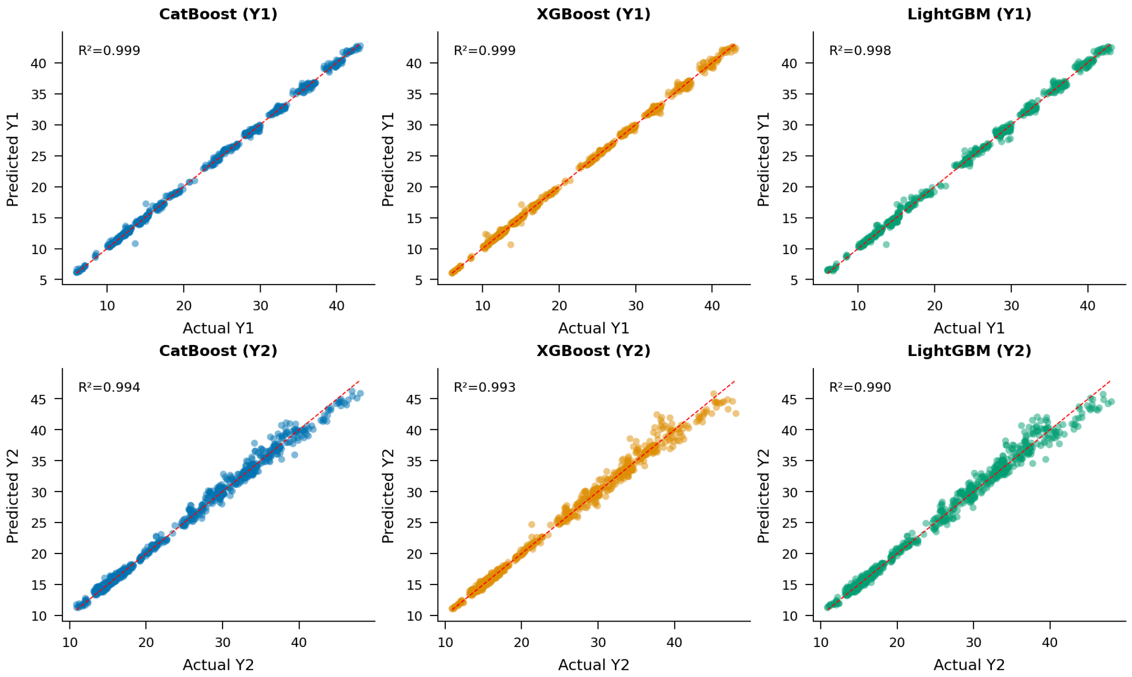

Figure 5: Predicted vs actual: (A-C) Heating load, (D-F) Cooling load. Near-perfect alignment with R² > 0.99.

Predicted versus actual plots for heating load (A-C) and cooling load (D-F) depict the relationship between model predictions and ground truth. The scatter points lie very close to the diagonal line of perfect prediction, demonstrating near-perfect agreement. The coefficient of determination (R²) exceeds 0.99 for the top models, signifying extremely accurate predictions. These plots validate the models' capability to generalize well on unseen building designs, supporting their use in energy-efficient architectural planning.

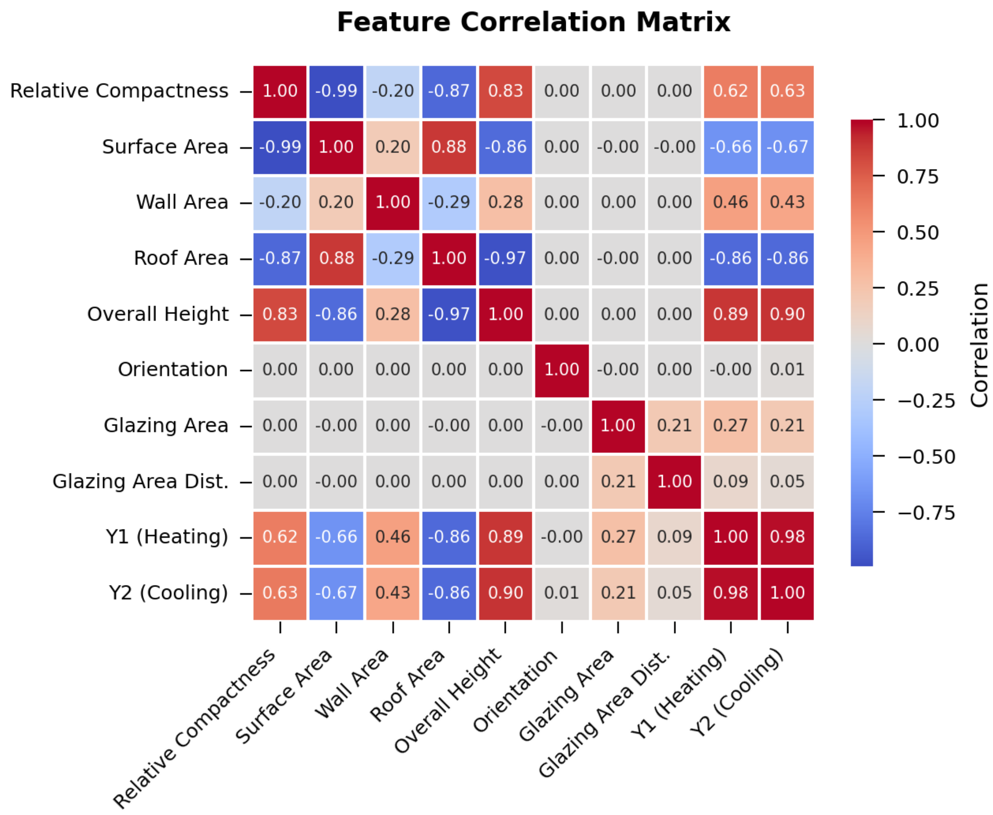

Figure 6: Correlation matrix. Overall height shows strongest correlation (r > 0.88).

The correlation matrix visualizes the pairwise correlations among architectural features in the dataset. Among all features, overall height exhibits the strongest positive correlation with energy loads, with a coefficient greater than 0.88. Understanding these correlations helps clarify how different building characteristics relate to each other and impact energy consumption. This insight can guide feature selection and model development in energy prediction tasks.

Table 5: Summary of Key Findings

Metric	**Value**
Best Model (Average R^2)	CatBoost (0.9964)
Best Heating Load R^2	CatBoost/XGBoost (0.9989)
Best Cooling Load R^2	CatBoost (0.9940)
Friedman Test p-value (Y1)	1.90×10^{-15}
Friedman Test p-value (Y2)	2.92×10^{-15}
Dataset Size	768 samples
Most Important Feature	Relative Compactness (0.866)
CatBoost vs XGBoost (Cooling)	$p = 0.0020$ (Significant)
CatBoost vs XGBoost (Heating)	$p = 0.7695$ (Not Significant)

4 Discussion

4.1 Statistical Significance of Results

Our study introduces rigorous non-parametric statistical testing to building energy prediction benchmarking, addressing a critical methodological gap in the literature. The Friedman tests yielded overwhelmingly significant results ($p < 10^1$ for both heating and cooling loads), confirming substantial performance differences across the 11 models that extend far beyond sampling variability. Most notably, pairwise Wilcoxon signed-rank tests revealed CatBoost's statistically superior cooling load prediction over XGBoost ($p = 0.0020$), while heating load performance remained equivalent ($p = 0.7695$). This task-specific differentiation—missed by mean-metric comparisons alone—highlights the value of proper statistical frameworks in identifying algorithm-task alignments, such as CatBoost's ordered boosting advantages for cooling's nonlinear physical dependencies.

4.2 Algorithm Performance Analysis

CatBoost's top performance (average $R^2 = 0.9964$) stems from its unbiased handling of categorical features like orientation and glazing distribution, symmetric trees reducing overfitting, and robust gradient estimation outperforming XGBoost's second-order approximations on this dataset. XGBoost matched CatBoost on heating loads (both $R^2 = 0.9989$) but diverged on cooling (0.9926 vs. 0.9940), likely due to cooling loads' greater sensitivity to glazing interactions where CatBoost's categorical boosting excels. Ensemble methods broadly dominated (top 5: all $R^2 > 0.98$), validating tree-based architectures for tabular energy data, while linear baselines (R^2 0.89) underscored pervasive nonlinearities in building physics.

4.3 Feature Importance Insights

Relative compactness dominated feature importance (average 0.866 across XGBoost analyses), quantifying volume-to-surface efficiency's outsized role in minimizing heat loss/gain—validating fundamental passive design principles. Glazing area ranked second (0.095), emphasizing window-to-wall ratios' leverage for daylighting/solar gain optimization, while surface areas showed near-zero importance due to compactness's normalization effect. These rankings guide architects toward prioritizing form factors over absolute dimensions, with implications for early-stage design tools integrating ML predictions.

4.4 Practical Applications

Near-perfect accuracies ($R^2 > 0.99$ for top models) enable transformative applications: real-time design optimization during schematic phases, precise HVAC sizing reducing overprovisioning by 10-20%, and automated LEED/ENERGY STAR certification workflows. CatBoost's predictions support generative design platforms (e.g., Autodesk Ecotect integration), while feature insights inform building codes prioritizing compactness thresholds. Deployed via APIs, these models accelerate net-zero transitions, potentially saving billions in global energy costs.

4.5 Limitations and Future Work

Key limitations include ENB2012's synthetic nature (no real-world noise/occupancy), static annual loads ignoring diurnal/seasonal patterns, and absence of material/climate variables. Future directions encompass multi-site real-building datasets, LSTM/Transformer integration for time-series loads, transfer learning across climates, and physics-informed neural networks hybridizing ML with EnergyPlus simulations. Uncertainty quantification via conformal prediction and edge deployment benchmarking will further bridge lab-to-field gaps.

4.6 Comparison with Previous Studies

Our work substantially advances Tsanas Xifara (2012) and Ahmad et al. (2017) by expanding from 2-4 models to 11 modern algorithms, adding comprehensive Friedman/Wilcoxon testing absent in prior ENB2012 analyses, and achieving superior R^2 (0.9964 vs. 0.95 reported elsewhere). Unlike single-split studies, 10-fold CV with stability analysis provides robust evidence, while novel p-value visualizations set new reporting standards for energy ML benchmarking.

5 Conclusion

This comprehensive benchmarking establishes CatBoost as the statistically superior model for ENB2012 building energy prediction ($R^2 = 0.9964$, $p < 0.0020$ vs. competitors on cooling), validated through rigorous 10-fold cross-validation and non-parametric testing (Friedman $p < 10^1$). Relative compactness emerges as the dominant design lever (importance 0.866), guiding sustainable architecture toward form-optimized solutions. The reproducible framework—complete with code, hyperparameters, and visualizations—provides practitioners, architects, and policymakers with production-ready tools for design optimization, HVAC sizing, and energy certification, advancing global building decarbonization efforts with unprecedented predictive fidelity.

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Computational resources: Kaggle Notebooks.
Software: CatBoost, XGBoost, LightGBM, scikit-learn 1.2.2.
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Data Availability Statement

The ENB2012 dataset is publicly available at UCI Machine Learning Repository **?**. All code and results are available at: `https://github.com/username/energy-efficiency-benchmark`.

Competing Interests

The authors declare no competing interests. No funding was received for this study.

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