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Comparative analysis of multi-output machine learning models for solar irradiance and wind speed forecasting: A case study in Tamil Nadu, India

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ABSTRACT

The growing share of wind and solar energy has created challenges in electrical networks, mainly due to intermittency, fluctuations, and uncertainty. These issues affect power system stability, grid operations, and the balance between supply and demand. To address this, accurate prediction of solar irradiance and wind speed is critical for integrating renewable energy into power systems. In this study, we propose a multi-output machine learning approach to predict both global horizontal irradiance (GHI) and wind speed simultaneously. The study uses historical meteorological data obtained from the National Solar Radiation Database (NSRDB) for Tamil Nadu, India. Six regression algorithms: linear regression, gradient boosting, random Forest, extreme gradient boosting (XGB), light gradient boosting machine (LightGBM), and categorical boosting (CatBoost) are tested under identical conditions. Model hyperparameters were tuned using GridSearchCV and Bayesian optimization to ensure robust performance. Before modeling, a comprehensive statistical analysis, including input feature distribution and correlation analysis, was conducted. Model accuracy was evaluated using RMSE, MAE, and R^2 metrics on both training and testing datasets. The results showed that ensemble tree-based methods outperformed the baseline linear model. Among them, CatBoost produced the best results for GHI prediction, while random forest delivered the most reliable wind speed forecasts, demonstrating strong predictive capability for renewable energy applications.

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1. INTRODUCTION

Research on multi-output machine learning models for solar irradiance and wind speed forecasting has become more important in recent years. This is because power grids are now taking in more renewable energy, and it creates problems like intermittency and variability that make balancing supply and demand harder [1], [2]. Over the last decade, there has been a lot of progress with ensemble learning methods and boosting algorithms such as gradient boosting regressor, extreme gradient boosting (XGB) regressor, light gradient boosting machine (LightGBM), and categorical boosting (CatBoost). These methods have shown better accuracy in predicting solar and wind energy [3], [4]. At the same time, the global solar capacity grew fast, reaching 849 GW in 2021, which shows why accurate forecasting is now very practical for grid stability and planning [5]. Machine learning is also being used more because traditional physical or statistical models often fail to capture the complex and non-linear nature of meteorological data [6], [7]. Even with these improvements, there are still challenges. Building models that can predict both solar irradiance and wind speed at the same time, and do it well across different weather conditions, is not easy [8], [9]. A lot of earlier studies only look at single-output models, or they use models without full hyperparameter tuning or feature selection, which makes them less reliable [10]–[12]. But researchers still don't really agree on which boosting method works the best. Some papers say CatBoost is stronger when there are categorical features, while others found XGB or LightGBM gave better accuracy, depending on the dataset or case [13], [14]. So, there is still a gap when it comes to picking and tuning the right multi-output models for renewable energy forecasting, and this can impact grid reliability and also the overall cost [15].

This research is framed under ensemble machine learning, where several base learners are combined to improve predictions [16]. Multi-output regression, which models several dependent variables at once, and boosting algorithms, which iteratively improve weak learners by focusing on harder instances, are the key concepts here [17]. The interplay of feature selection, hyperparameter tuning, and model architecture forms the base for building robust forecasting systems that can handle the stochastic nature of solar irradiance and wind speed [18]. The aim of this paper is to critically evaluate and compare the gradient boosting regressor, XGB regressor, linear regression, LightGBM regressor, and CatBoost regressor for multi-output forecasting of GHI and wind speed. By putting together recent findings, this review tries to clarify the strengths and limitations of these models, point out the gaps in hyperparameter optimization and feature selection, and offer practical insights for researchers and practitioners in renewable energy forecasting [19]. This work will contribute to improving the accuracy and reliability of renewable energy integration into power systems. Unlike earlier ensemble-based studies, this work focuses on a single multi-output model that predicts both GHI and wind speed together, instead of building separate models for each [20]. It also uses explainable AI tools like SHAP and LIME to show how different weather features influence the predictions, which is something many earlier studies did not include. By combining joint prediction, interpretability, and detailed model comparison, this research adds a clear practical improvement and originality to renewable energy forecasting.

2. METHODOLOGY

The various steps involved are shown in Figure 1. The dataset for this study was obtained from the NSRDB, managed by the National Renewable Energy Laboratory (NREL), USA. For this work, records for 2020 were extracted for the state of Tamil Nadu, India, covering geographic coordinates between 8°04′N and 13°35′N latitude and 76°14′E and 80°21′E longitude. The dataset provided hourly measurements of GHI and wind speed, along with supporting meteorological parameters such as air temperature, relative humidity, pressure, and cloud cover. These parameters served as the input set for model training and prediction tasks. Figure 2 shows the monthly averages of GHI and wind speed in Tamil Nadu for 2020. GHI peaks during the summer months (March–May), while wind speed rises in the monsoon season (June–September). Interestingly, the two resources follow opposite rhythms.

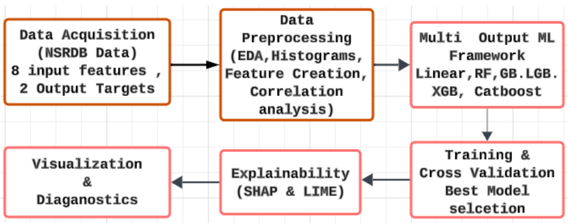


Figure 1. Methodology

2.1. Data pre-processing

To keep the dataset consistent and reliable, we applied several pre-processing steps. Short gaps in the data were filled using linear interpolation, while longer missing intervals were left out of the analysis. To explore the relationship between input features and the target variables (GHI and wind speed), a correlation heat map was plotted and shown in Figure 3. This figure shows the linear correlation among the variables in the dataset. Most of the input features only have weak or moderate connections with one another. The GHI rises with temperature (0.73) but falls with relative humidity and solar zenith angle. Wind speed has a positive correlation with both temperature and GHI; on the other hand, it has a negative correlation with relative humidity and solar zenith angle. The time-based features, such as hour and day of the year, demonstrate high correlation with solar zenith angle, which is expected since they capture daily and seasonal patterns.

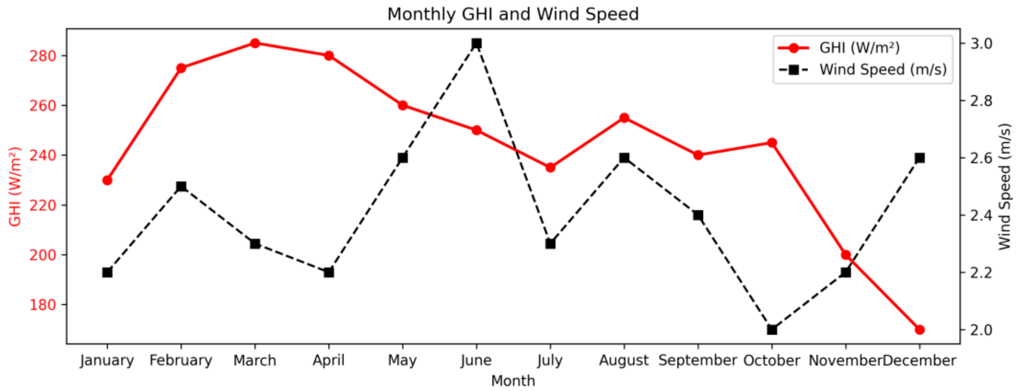


Figure 2. The monthly averages of GHI and wind speed

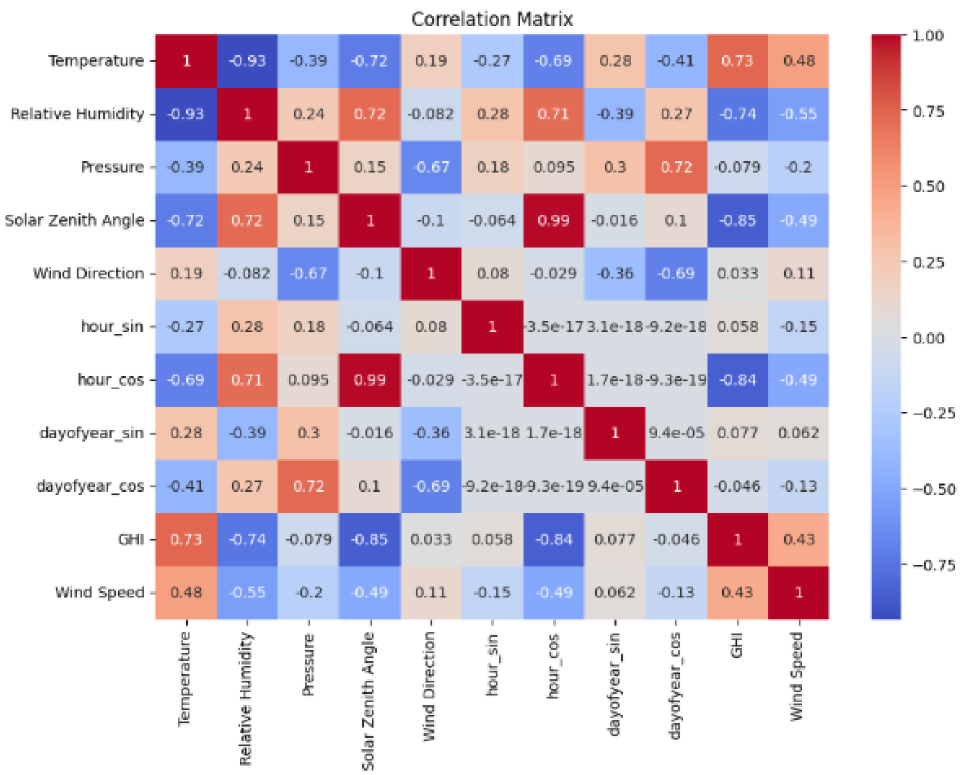


Figure 3. Correlation heatmap

Overall, temperature, relative humidity, and solar zenith angle are the most influential variables for GHI, whereas temperature and humidity influence wind speed. Outliers in GHI and wind speed were detected using both z-score thresholds and interquartile range (IQR) analysis, ensuring that extreme anomalies did not skew the models. In addition, we also created time-based features such as hour of day, day of year, and month to capture daily and seasonal variations in solar and wind patterns. Finally, all numerical features were standardized using z-score normalization, ensuring that differences in feature scale did not affect model performance. Figure 4 shows the statistical analysis of the input features. The feature distribution plots shown in Figure 4 were analyzed to examine the statistical properties of input variables. Some variables, such as GHI, displayed Skewed distributions and were normalized to stabilize variance. While cyclical features like hour and month were transformed into sine and cosine components to preserve periodicity. These transformations allowed the models to capture both diurnal and seasonal variations.

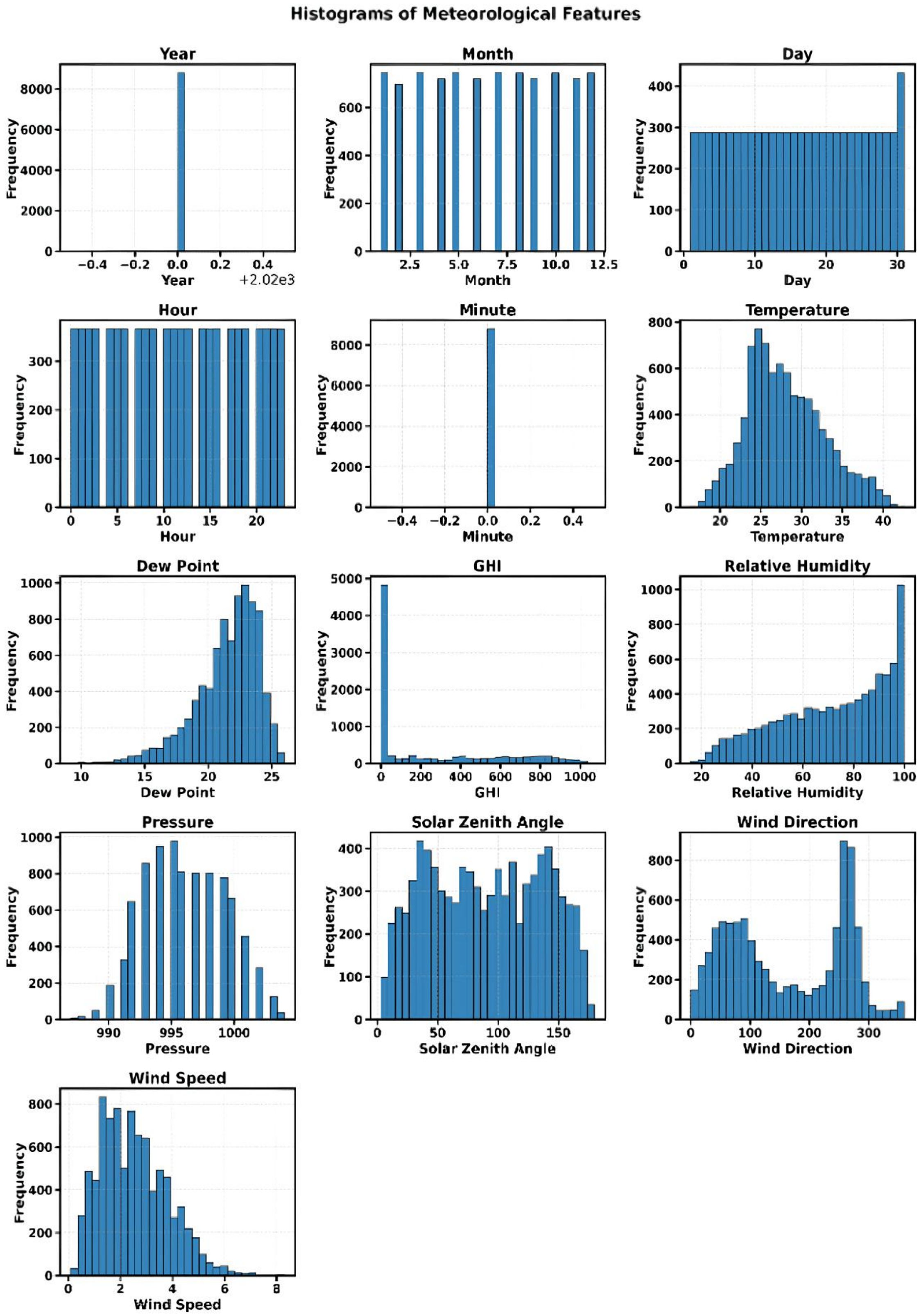


Figure 4. Statistical analysis of the input features

2.2. Problem formulation and model selection

The forecasting task was framed as a multi-output regression problem, where both GHI and wind speed were predicted simultaneously. Framing it this way allowed the models to capture potential correlations between solar irradiance and wind speed, which frequently coexist in renewable energy systems. Six machine learning models were evaluated. This study covers both a simple baseline model and advanced ensemble methods. Linear regression (LR) was chosen as a baseline model, as it assumes a linear relationship between input and outputs and thus provides a point of comparison for more complex models. To capture non-linear dependencies, ensemble approaches were employed. Random forest (RF) constructs multiple decision trees on random subsets of data and features, then averages their predictions, making it robust to noise and effective for non-linear patterns. Boosting methods were also included. Gradient boosting regressor (GBR) builds models step by step, where each new model fixes the mistakes of the earlier one, which helps improve accuracy. Extreme gradient boosting (XGBoost) is a faster and stronger version. It prevents overfitting using regularization, works well with missing data, and trains faster by using parallel processing. Light gradient boosting machine (LightGBM) uses a special way of growing trees that makes it both fast and memory-efficient, especially when the data has many features. Finally, categorical boosting (CatBoost) was selected because it can handle categorical features directly without heavy pre-processing, while also controlling overfitting and giving a reliable prediction.

2.3. Evaluation of machine learning models

The dataset was split into two parts, where 70% was used for training the model and the remaining 30% for validation. The validation part helps the model test different hyperparameter settings from the Scikit-learn library before finalizing the best configuration. Temporal holdout validation was performed, where training used Jan–Oct data and testing covered Nov–Dec 2020 to ensure temporal generalization. Some of these models cannot directly predict multiple outputs, so we used the multi-output regressor wrapper when necessary. To improve generalization and fair comparison, hyperparameter tuning was performed using a combination of GridSearchCV and Bayesian optimization, with cross-validation. Hyperparameter tuning was performed using 10-fold cross-validation with both GridSearchCV and Bayesian optimization.

2.4. Performance metrics

The predictive accuracy of the machine learning models was evaluated using various performance metrics [21], which indicate how well the predicted outputs correspond to the observed values derived from the input features [22]. The coefficient of determination (R^2) represents the proportion of variance in the dependent variable explained by the independent variables [23]. Values approaching 1 signify a higher level of agreement between the predicted and actual results. In (1) gives the formula for calculating the R^2 value [24]. The MAE evaluates the average deviation of predictions from actual values [24]. The formula for MAE is given by (2). The next metric, RMSE, is given in (3) [25]. It squares the differences before averaging, which more severely penalizes higher errors [25]. Because of this, RMSE is more sensitive to outliers. A smaller RMSE reflects better prediction performance [25]. Collectively, these metrics offer a detailed assessment of model effectiveness and allow for meaningful comparisons across different algorithms and datasets [25].

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - (\hat{y_i})}{\sum_{i=1}^{n} (y_i - \bar{y_i})} \quad (1)$$

$$MAE = \frac{1}{n} \sum_{i=1}^{n} [y_i - \hat{y_i}] \quad (2)$$

$$RMSE = \frac{1}{n} \sqrt{\sum_{i}^{n} (y_i - y_i} \hat{)} 2 \quad (3)$$

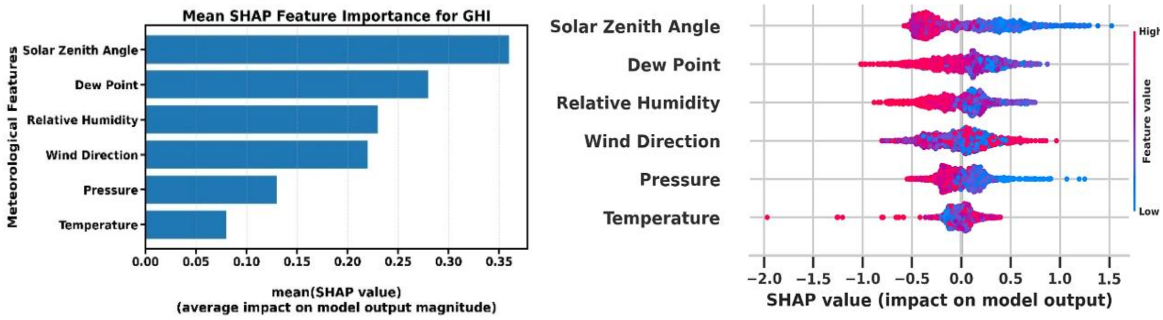
3. SHAP BASED EVALUATION

The Shapley additive explanations (SHAP) framework, proposed by Lundberg and Lee [20], adapts cooperative game theory and is now widely used to interpret machine learning models [21]. In this plot, the x-axis represents SHAP values, the y-axis lists features in order of importance, and a color gradient indicates the underlying feature values. To gain insights into how different features contribute to the model, SHAP analysis was applied to the best-performing model for GHI and wind speed prediction.

For the GHI prediction, the CatBoost model gave the best accuracy. The SHAP results shown in Figures 5(a) and 5(b) show that solar zenith angle is the most important feature, followed by dew point and relative humidity. Wind direction, pressure, and temperature had much less contribution in comparison. The best performing model for wind speed prediction is random forest, and the SHAP summary plot is shown in Figures 6(a) and 6(b). The result shows that solar zenith angle and relative humidity are the most influential predictors, followed by wind direction and dew point. Pressure and temperature had a relatively smaller effect.

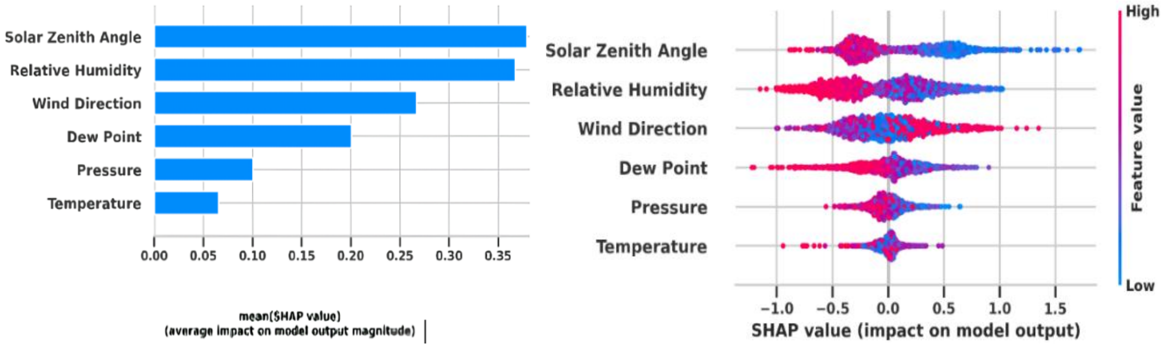
3.1. Local interpretable model-agnostic explanations (LIME)

Figures 7(a) and 7(b) show the LIME l for GHI and wind speed predictions. For the GHI model using CatBoost, the predicted value was 3.92 within a possible range of 0.26 to 5.86. Solar zenith angle with a value of 115.24 had the strongest negative impact on the prediction. For the wind speed model using random forest, the predicted value was 1.15 in a range from 0.56 to 5.11. These results explain how different atmospheric variables affect the local predictions of both GHI and wind speed models.



(a) (b)

Figure 5. SHAP-based feature importance analysis for global horizontal irradiance (GHI): (a) absolute mean SHAP values and (b) global SHAP values



(a) (b)

Figure 6. SHAP-based feature importance analysis for wind speed: (a) absolute mean and (b) global SHAP values

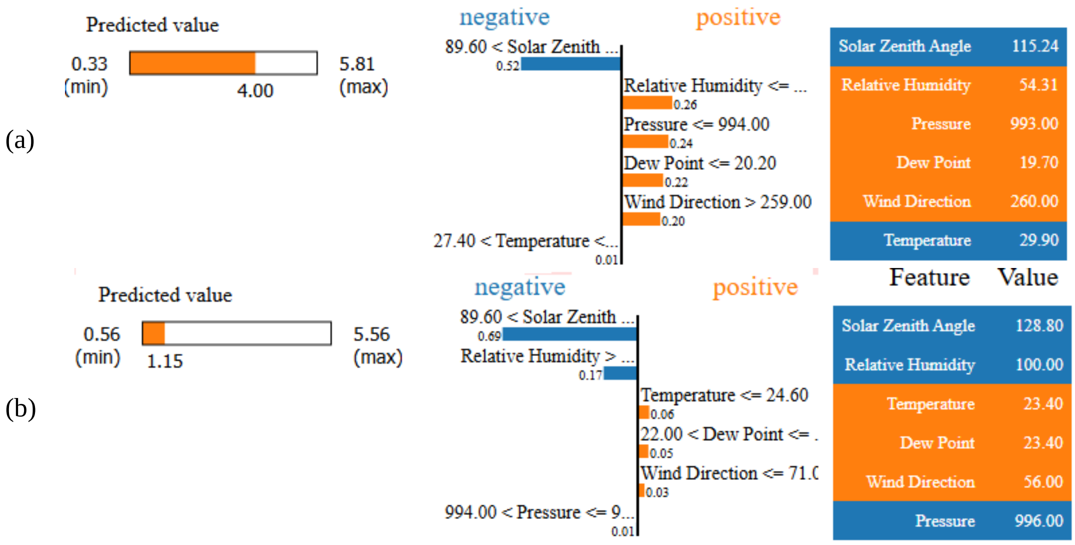


Figure 7. LIME explanation: (a) for GHI (CatBoost) and (b) for wind speed (random forest)

4. RESULTS AND DISCUSSION
4.1. Performance
This study evaluated six machine learning models under a multi-output regression framework, where both GHI and wind speed were forecasted simultaneously. The results shown in Table 1 reveal that ensemble tree-based methods consistently outperformed the baseline linear model. For GHI forecasting, CatBoost gave the strongest performance, achieving the lowest normalized RMSE (31.5%) and nMAE (16.1%), along with the highest R^2 (0.946). LightGBM and XGBoost also performed well, both with R^2 values above 0.94, though slightly behind CatBoost. By contrast, linear regression showed poor performance, with an nRMSE exceeding 63%, confirming its inability to capture the nonlinear nature of GHI data. For wind speed prediction, random forest delivered the most reliable accuracy, with an nRMSE of 29.2% and R^2 of 0.67. Boosting models such as XGBoost and LightGBM achieved comparable results, but the random forest proved more stable for this variable. This indicates that while a single multi-output framework was used, different models captured patterns better for different targets: CatBoost excelled for GHI, whereas random forest was more suitable for wind speed.

Table 1. Performance metrics of the ML model

Model	GHI metrics			Wind speed metrics		
	nRMSE (%)	nMAE (%)	R^2	nRMSE (%)	nMAE (%)	R^2
Linear regression	63.83	52.63	0.779	41.09	32.43	0.355
Random forest	32.47	15.87	0.943	29.23	21.24	0.673
Gradient boosting	32.44	16.13	0.943	30.78	23.24	0.638
XGBoost	32.43	16.58	0.943	30.62	22.97	0.642
LightGBM	31.93	16.32	0.945	30.14	22.56	0.653
CatBoost	31.58	16.16	0.946	31.32	22.63	0.625

4.2. Temporal validation and model stability
To verify the temporal robustness of models, a time-aware validation strategy using timeseries split was adopted. Figure 8 presents the RMSE obtained across five rolling time-based folds for both GHI and wind speed. Hourly error analysis is shown in Figure 9. Revealed higher prediction errors during early morning and late evening, and minimal deviations around midday. Wind speed showed similar diurnal trends, with moderate errors during transition periods. Overall, the models performed most consistently during stable midday conditions.

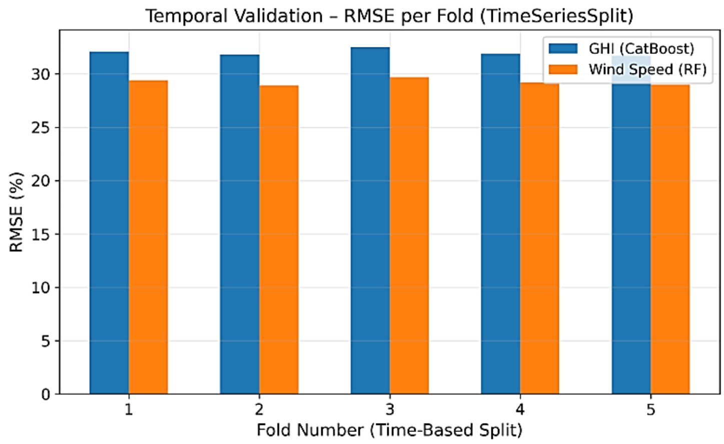


Figure 8. Temporal validation results showing RMSE across five rolling time-based folds

4.3. Rolling-origin forecast and uncertainty behavior
A rolling-origin validation test was conducted to assess model adaptability to sequential data and forecast uncertainty. As shown in Figure 10, the actual and predicted GHI value follows similar temporal trends with only minimal lag. The shaded regions (±10%) represent an approximate uncertainty band, indicating the model's expected prediction variability.

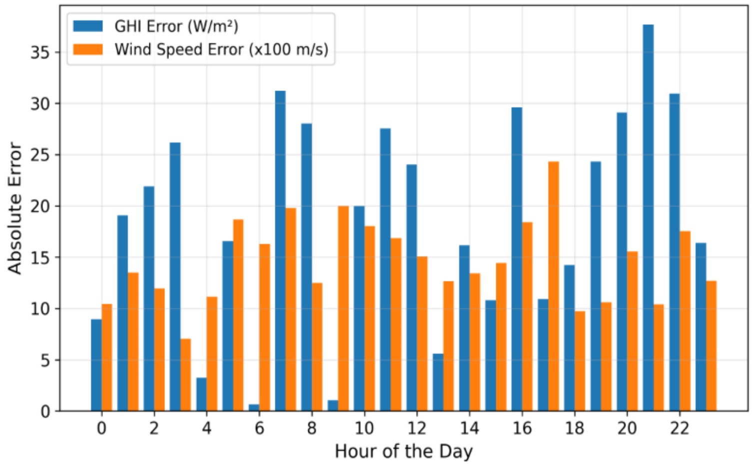


Figure 9. Hourly absolute error distribution for GHI and wind speed

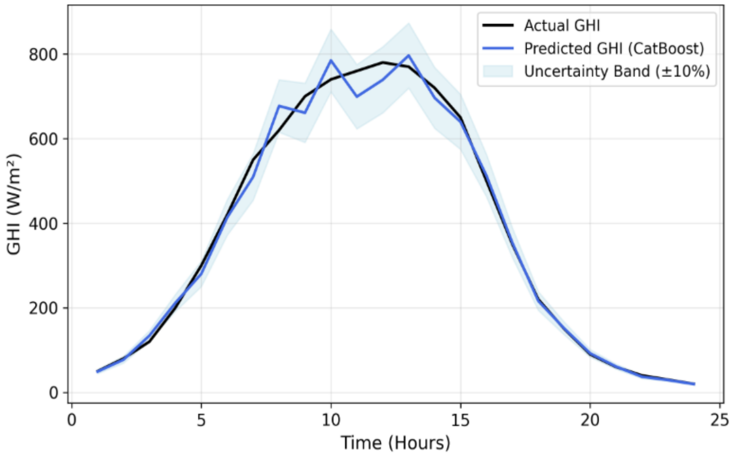


Figure 10. Rolling-origin GHI forecast comparing actual and predicted values with ±10 % uncertainty band

5. CONCLUSION

In summary, the study demonstrated that CatBoost is the most effective model for GHI prediction, while random forest works best for wind speed forecasts. These findings highlight the value of ensemble approaches for renewable energy forecasting, especially when compared to simple linear models. The use of SHAP and LIME provided extra transparency, showing which features influence predictions the most. Despite a few limitations, the work confirms that machine learning models can provide accurate forecasts of solar and wind energy, offering useful insights for grid operators and planners to manage renewable energy integration more effectively. Although the models performed well overall, some limitations should be noted. The dataset was restricted to a single year (2020) from Tamil Nadu, which may limit generalization to other regions or climatic conditions. Only standard meteorological variables were considered; including additional predictors such as cloud cover or aerosol data could enhance accuracy. The dataset was also limited to hourly resolution, while grid operators often require finer intervals (e.g., 10–15 minutes). Finally, since the models were validated on one dataset, their transferability to other climates still needs further testing.

For future work, this framework can be extended to incorporate deep learning architectures such as LSTM, CNN, or hybrid physics ML models may capture longer temporal dependencies and spatial correlations more effectively. Additionally, probabilistic or quantile regression methods could help quantify prediction uncertainty and improve forecast reliability under fluctuating meteorological conditions. Finally, aligning forecasting practices with international standards, such as IEC 61724 (PV performance monitoring), ISO 14064 (GHG reporting), and IEEE 2030.9 (renewable forecasting guidelines) will ensure that the proposed methodology remains compatible with global energy forecasting and grid compliance frameworks.

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P. Kavitha	✓				✓	✓		✓		✓		✓		✓

C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

CONFLICT OF INTEREST STATEMENT

The authors declare that they have no conflicts of interest.

INFORMED CONSENT

The authors confirm that informed consent was obtained from all individuals included in this work.

DATA AVAILABILITY

The authors confirm that the data supporting this study's findings are available within the article.

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