APPLICATION OF MACHINE LEARNING (kNN) WITH AUTOHYPERPARAMETER TUNING FOR HYDROGEN PRODUCTION PROBABILISTIC FORECASTING FROM WIND ENERGY

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Abstract

One of the main challenges for the energy transition is knowing how to deal with the variability of solar and wind sources, as this poses risks for renewable engineering projects. In this sense, this work presents the application of self-adjusting tuning for the k-Nearest Neighbors (kNN) machine learning model in a wind energy and green hydrogen production scenario. The methodology adopted consisted of a literature review to develop time series ensembles, and the results obtained were compared with the literature on the same subject. Three types of analyses were performed: wind speed prediction, direct prediction of green hydrogen production, and indirect prediction of hydrogen using the optimized values of the lag columns and kNN hyperparameter for wind speed. The distinctive feature of this approach is the combination of the bagging mechanism with the algorithm developed to auto-adjust the hyperparameter “n_neighbors” until the model stabilizes without supervision, which is proved useful and applicable to Artificial Intelligence models with more hyperparameters, allowing simulations to be performed for a large number of models and lag columns (values from previous time steps). The proposed methodology obtained better results in terms of prediction error (RMSE and nRMSE) and optimal values for R^2, indicating advances over existing approaches compared in the literature.

Keywords: wind energy, green hydrogen, machine learning, self-adjusting tuning, hyperparameter optimization.

1. Introduction

Decarbonization is one of humanity's greatest demands today, which has intensified the search for sustainable and efficient sources to generate energy. In this way, green hydrogen stands out as an advantageous solution for the energy transition, whose production is based on renewable sources such as solar irradiance and wind energy. Therefore, hydrogen is an important strategy, as it has more energy and environmental contributions than carbon-based fuels (Maka and Mehmood, 2024). However, the variability of renewable sources is an aggravating factor for the hydrogen production chain, given the risks and costs that fluctuating energy availability brings to the plant (Branco et al., 2023; Hassan et al., 2024; Oliveira et al., 2025). Thus, with the aim of contributing to and boosting the development of the hydrogen production chain, this study sought to improve on the results found by Leal et al. (2025), a study that stood out for its application of Dynamic Linear Models in the probabilistic forecasting of wind speed in the context of hydrogen production. Leal et al. (2025) studied wind time series using three wind-hydrogen conversion models (named C1, C2, and C3) found in the literature to estimate hydrogen production. Three Brazilian states were studied: Ceará, Bahia, and Rio Grande do Sul. Given this, the work presented by the authors of this abstract uses the same database and conversion techniques as the aforementioned research. The objective is to evaluate the behavior of self-adjusting tuning for three different scenarios:

1 - Wind speed prediction (using conversion methods, it is then possible to determine hydrogen production);

2 - Directly predicting green hydrogen production (hydrogen production is estimated using the

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conversion methods applied by (Leal et al., 2025), and these values are then passed on to the algorithm);

3 - Indirectly predicting green hydrogen production. Using hydrogen production estimates together with the optimized values of lag columns and "n_neighbors" found for speed prediction, the behavior of the algorithm is analyzed to relate hydrogen to wind speed.

1.1 k-Nearest Neighbors (kNN) Algorithm

For the comparison with Dynamic Linear Models, k-Nearest Neighbors (kNN) was chosen, a Machine Learning algorithm that makes predictions based on the assumption that the distance to some samples (k) is sufficient to make an inference (Harrison, 2019). kNN is a supervised instance-based algorithm that depends on calculating the similarity between the target and the nearest neighbor(s) (Grus, 2019; Muhammad Ali, 2022; James et al., 2023). In the case of regression, kNN defines the new value based on the average of the k nearest neighbors. This is an algorithm model with applications in various areas of science, which is why this research seeks a new perspective for this machine learning technique to further enhance its use.

1.2 Bagging and Moving Block Bootstrap (MBB)

The code developed was based on bagging, a mechanism for training multiple models of the same type to improve the stability and accuracy of machine learning models (Moeini, 2024; Nie et al., 2025). Bagging is a technique in which, instead of fitting multiple models to the same data, each model is fitted to a bootstrap sample (Bruce and Bruce, 2019). However, it is worth remembering that traditional bagging breaks the total order, which drastically affects the results of time series analyses. Thus, to enable the application of ensemble in the context of wind energy and green hydrogen, we chose to use the Moving Block Bootstrap methodology, which is based on the decomposition of the original series into multiple contiguous and overlapping blocks. With this, these blocks are sampled with replacement, and the concatenation of the selected blocks results in the formation of the bootstrap sample (Bandara et al., 2021; Bertail and Dudek, 2022). This procedure ensures the preservation of the intrinsic serial dependency structure, providing greater robustness and consistency to the variance estimates and ensemble-based predictive models that use it (Sroka, 2022). The figure below was created by (El Anbari, Abeer Fadda and Ptitsyn, 2015) and shows how the MBB works. Each block can start at any position, as long as it is smaller than (database size - ideal block size). Each color indicates a new subset of the data. Finally, the blocks are reorganized to form a new training set, ensuring that each bagging model sees the data differently.

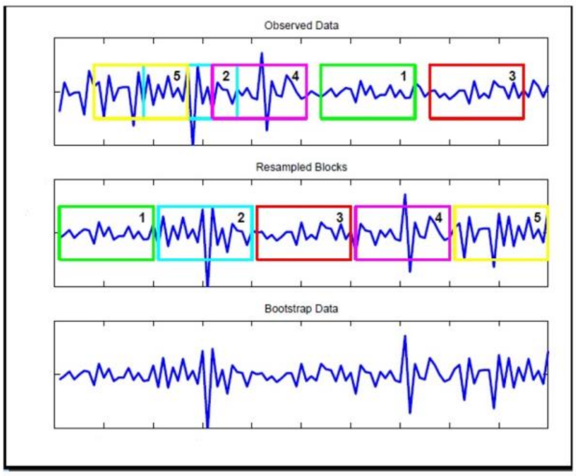

Figure 1: Representation of the use of Moving Block Bootstrap in a database. Each color highlights a different block representing a new subset of the data.

1.3 Methods for converting wind speed into hydrogen production.

Table 1 shows the three conversion methods found in (Leal *et al.*, 2025) that will be discussed in this article.

P% represents the ratio between the theoretical power reaching the electrolyzer and the nominal power of this equipment. This ratio is important in methods C2 and C2 for defining the efficiency of the electrolyzer. The major difference between C1 and the other methods is that the efficiency of the electrolyzer is considered to be fixed at 75%.

Table 1: Key information about wind energy-green hydrogen conversion models as seen by (Leal *et al.*, 2025).

Method	Name/Main Reference	Wind Turbine Power Curve	Electrolyzer Efficiency (ηELE)
C1	(Javaid et al., 2022)	It is not considered.	Constant. Set at 75%.
C2	(Zhu et al., 2022)	It is considered.	Variable, by trapezoidal linearization. Varies from 0% to 82% depending on the input power range.
C3	(Hofrichter et al., 2022)	It is considered.	Variable and Conditional. Uses a 5th order polynomial function (for 10% < P% < 15%) or a linear function (for P% > 15%).

1.4 Wind speed database

Leal et al. (2025) did not specify the cities from which the data were collected, only the Brazilian states in which they are located. Figure 2 shows the temporal distribution of wind speed data from Ceará and the corresponding histogram. Figure 3 presents the speed data for Bahia, and finally, Figure 4 shows the behavior of the data for Rio Grande do Sul.

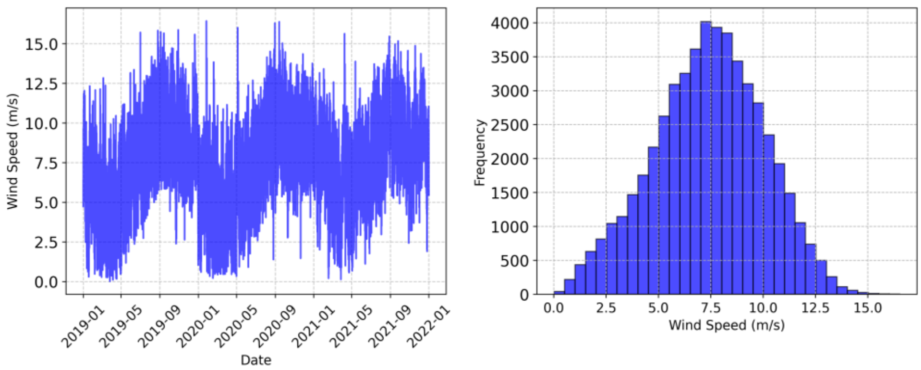

Figure 2: (Left) Wind speed time series for Ceará and (right) corresponding histogram showing the temporal evolution and statistical distribution of observed values

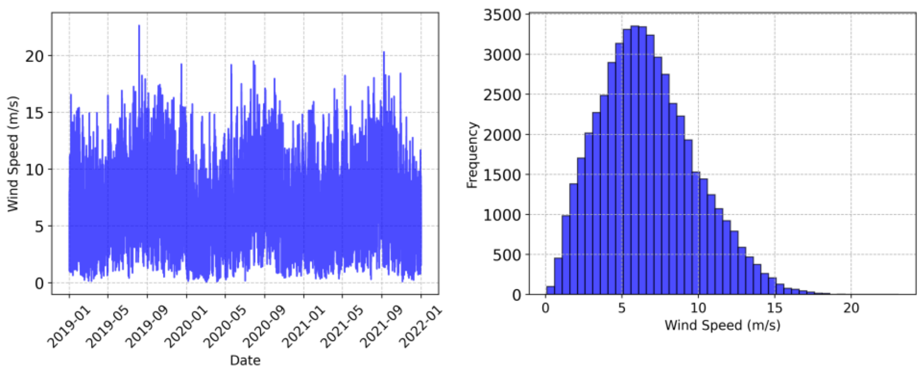

Figure 3: (Left) Wind speed time series for Bahia and (right) corresponding histogram showing the temporal evolution and statistical distribution of observed values.

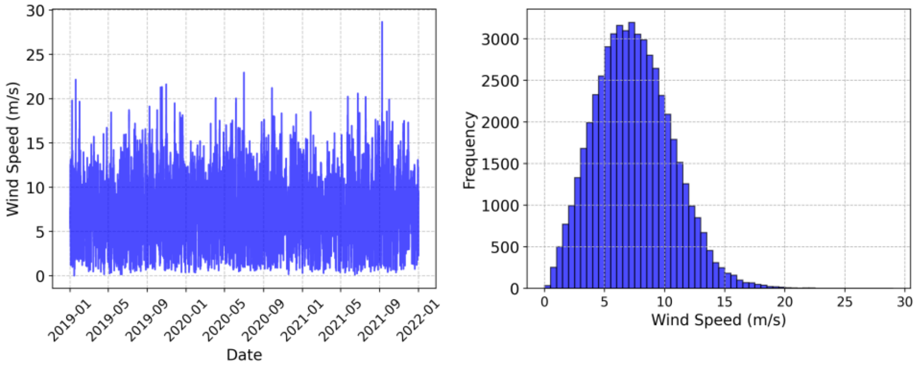

Figure 4: (Left) Wind speed time series for Rio Grande do Sul and (right) corresponding histogram showing the temporal evolution and statistical distribution of observed values.

2. Methodology

The four main stages of the research were: selecting the ideal block size for the Moving Block Bootstrap, creating the self-adjusting tuning mechanism, selecting the performance metrics, and defining the bagging modeling and training structure.

2.1 Block Size Definition

After choosing the MBB technique, the next step was to define the optimal size for the blocks. (Bertail and Dudek, 2022) studied different assembly methods for periodic time series (e.g., daily or seasonal) and showed that the block size (b) must respect the periodic structure, being a multiple of the period (d) of the series plus 1. This relationship can be seen in Equation 1.

$$b = v_b d + 1 \qquad \text{(eq. 1)}$$

This ensures that each block contains complete cycles, preserving temporal dependencies. The goal is to choose the (b) that minimizes the mean squared error (MSE) of the bootstrap variance, balancing bias and variance. Thus, with d set at 48, since the data were collected every half hour, v_b values from 1 to 10 were tested. We chose 10 as the limit so that the blocks would not become too large. For each v_b value, 30 bootstrap replications were generated in order to stably estimate the variance, bias, and empirical mean squared error (MSE). The number of bootstrap replications is a factor that depends on the complexity of the problem, and 30 proved to be adequate for the scenario studied.

The block size is defined each time the code is executed, so the optimal size changes depending on whether wind speed or hydrogen production is being analyzed. Figure 5 shows the MSE results obtained for the three wind speed databases for training, where it can be seen that the ideal size for the data from Ceará is 99 samples, for Bahia it is 145 samples, and for Rio Grande do Sul it is 481 samples.

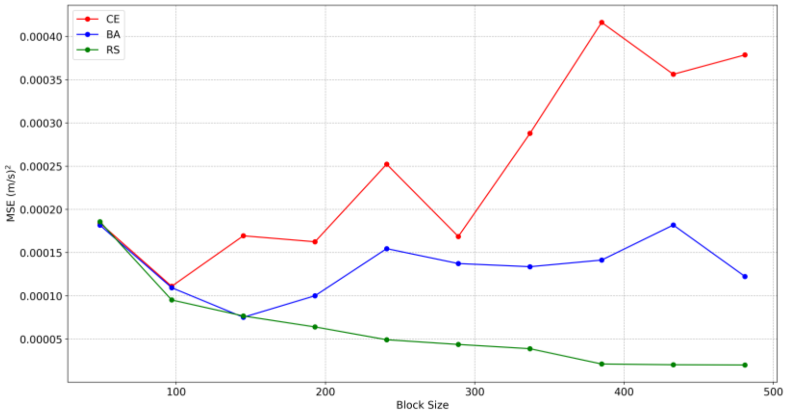

Figure 5: MSE analysis to determine the optimal block size for each velocity dataset.

2.2 Self-adjusting Hyperparameter Tuning

- Initially, three values for the hyperparameters "n_neighbors" are tested: e.g., 4, 5, 6
- If the best value is the middle one (e.g., 5), autotuning stabilizes.
- If the best value is at the higher or lower extreme:

  A new set is generated around that value:

  Best = 6 → new: 5, 6, 7

  Best = 4 → new: 3, 4, 5
- The process repeats until it finds an optimal and stable value without supervision.

2.3 The Performance Metrics

Equation 2 brings the Root Mean Squared Error (RMSE), which measures the mean squared error between predicted and observed values.

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

Where:

- y_i = observed value;
- $\hat{y}_i$ = predicted value;
- N = number of observations.

Normalized Root Mean Squared Error (nRMSE) is defined as:

$$nRMSE = \left(\frac{RMSE}{\bar{y}}\right) \cdot 100 \qquad \text{(eq. 3)}$$

Where:

- $\bar{y}$ = average of observed values.

Coefficient of determination (R^2), which measures the proportion of variability explained by the model, is defined by the equation below.

$$R^2 = 1 - \frac{\Sigma(y_i - \hat{y}_i)^2}{\Sigma(y_i - \bar{y})^2} \qquad \text{(eq. 4)}$$

Equation 5 presents the Prediction Interval Coverage Probability (PICP), which measures the percentage of observed values that fall within the prediction interval.

$$PICP = (\frac{1}{N}) \cdot \Sigma C_i \qquad \text{(eq. 5)}$$

Where:

- $C_i = 1$ if $(L_i \leq y_i \leq U_i)$, otherwise 0;
- Ui = upper bound → upper limit of the forecast interval for the i-th observation;
- Li = lower bound → lower limit of the forecast interval for the i-th observation.

Prediction Interval Normalized Average Width (PINAW), which measures the normalized average width of prediction intervals, is defined as:

$$PINAW = (\frac{1}{N \cdot R}) \cdot \Sigma(U_i - L_i) \qquad \text{(eq. 6)}$$

Where:

- $R = \max(y_i) - \min(y_i)$

2.3 Bagging Modeling and Training Framework

In this work, a kNN bagging methodology was developed to predict green hydrogen production time series, in which the dataset was initially divided into training data and test data. The database consists of 52,608 records collected every 30 minutes, from 00:00 on January 1, 2019, to 23:30 on February 5, 2021, corresponding to the training data (70%), and from 00:00 on February 6, 2021, to 23:30 on December 31, 2021 (30%), to the test data. Thus, the training data was subdivided to train and test the different kNN models created for bagging, taking care to use Moving Block Bootstrap so that each model had data in a different arrangement to be evaluated. This helps in creating a bagging structure that increases the stability/reliability of the results. The columns day of the year, time of day, and lag (values from previous time steps to capture the temporal dependence of the data) were chosen as predictors.

Specifically, each kNN model undergoes an automatic adjustment of "n_neighbors," in which attempts are made to improve this value until the code automatically concludes that varying this parameter for each model and each lag column configuration is no longer advantageous. All simulations in the Results section were performed with bagging of 10 kNN models with up to 10 lag columns for each, so that each simulation underwent 100 self-adjusting tuning operations. As a result, the developed code is able to capture the best value for "n_neighbors", lag columns, RMSE, and nRMSE (RMSE divided by the mean), so that each optimal configuration can be reused to evaluate the initial test data set. In this work, variable importance analysis was also performed using the SHAP library. Finally, with each kNN model already optimized, a prediction is made using these models for the initial test data set. With the average of the model results, it is possible to compare the results of the various kNN models created and the actual data for wind speeds and for each wind-to-hydrogen conversion technique using performance metrics.

3. Results

3.1 Results for Wind Speed Simulations

Table 2 shows the results obtained for bagging in the three wind speed databases. Ceará had the best results in all metrics, both for training and test data. It should be noted that Bahia had the worst results for both training and test data, which shows that the performance of self-adjusting tuning depends heavily on the location analyzed.

Table 2: Performance metric results for training and testing using wind speed.

Metric	Ceará		Bahia		Rio Grande do Sul	
	Train	Test	Train	Test	Train	Test
RMSE (m/s)	0.9339	0.9828	1.3532	1.426	1.037	1.108
nRMSE	0.1289	0.1272	0.2018	0.2161	0.1394	0.1491
R^2	0.8814	0.8295	0.813	0.7943	0.8899	0.8873

Figure 6 shows the histograms for the test data for the three wind speed databases. It can be seen how close the distribution of the true data is to the bagging ensemble data.

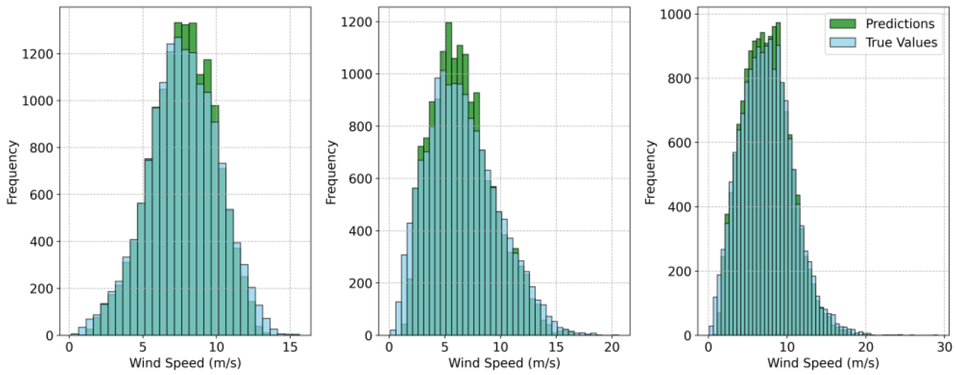

Figure 6: (Left) Histogram for wind speed test data of true and predicted values for Ceará. (Center) Histogram for wind speed test data of true and predicted values for Bahia. (Right) Histogram for wind speed test data of true and predicted values for Rio Grande do Sul.

3.1.1 Data obtained for bagging models for wind speed in Ceará

The models that generated the results in Table 2 for Ceará are shown in Table 3. It is possible to analyze the number of optimal lag columns for each model created and the SHAP score for all features. Although each model sees the data differently due to Moving Block Bootstrap, the RMSE and nRMSE results do not vary greatly from each other.

Table 3: Bagging results for Ceará.

				SHAP Values						
Model	**k**	**RMSE (m/s)**	**nRMSE (%)**	**hour**	**day of year**	**lag_1**	**lag_2**	**lag_3**	**lag_4**	**lag_5**
1	14	1.06	14.38	0.09	0.33	0.95	0.42	0.28	---	---
2	26	1.07	15.10	0.09	0.37	1.12	0.59	---	---	---
3	14	1.08	14.89	0.10	0.36	1.14	0.57	---	---	---
4	6	1.08	15.46	0.11	0.27	0.84	0.36	0.20	0.15	0.14
5	23	1.07	14.58	0.09	0.37	1.12	0.59	---	---	---
6	10	1.06	14.51	0.11	0.37	1.15	0.56	---	---	---
7	10	1.06	14.37	0.11	0.37	1.15	0.56	---	---	---
8	9	1.05	15.52	0.10	0.30	0.97	0.41	0.22	0.20	---
9	17	1.06	15.06	0.10	0.37	1.13	0.58	---	---	---
10	18	1.06	14.87	0.10	0.37	1.13	0.58	---	---	---

3.1.4 Compilation of results for nRMSE in the daily time window for wind speed

Leal et al. (2025) analyzed the nRMSE in a daily window. That is, they calculated this metric for each day of the test data. Table 4 compares the results obtained in this article with those of (Leal et al., 2025) for the three wind speed databases. It can be seen that the self-adjusting tuning methodology with bagging and Moving Block Bootstrap achieves better results in all nRMSE parameters. The standard deviation is in relation to the nRMSE results.

Table 4: nRMSE for the daily time window.

Parameter	$nRMSE_{CE}$		$nRMSE_{BA}$		$nRMSE_{RS}$	
	(Leal et al., 2025)	Achieved	(Leal et al., 2025)	Achieved	(Leal et al., 2025)	Achieved
Minimum	7.6%	6.82%	10.31%	9.97%	7.73%	6.36%
Median	18.54%	11.80%	35.77%	21.34%	33.57%	13.32%
Mean	22.18%	13.37%	36.24%	23.60%	40.95%	15.28%
Maximum	96.37%	40.66%	97.88%	62.26%	97.71%	43.45%
Standard Deviation	0.12	0.05	0.17	0.09	0.20	0.07

3.1.5 Compilation of results for nRMSE in the weekly time window for wind speed.

Leal et al. (2025) also analyzed the nRMSE for each week in the test data. Table 5 shows a comparison between the results. Only (Leal *et al.*, 2025)'s minimum results were better than those obtained from bagging.

Table 5: nRMSE for the weekly time window.

Parameter	$nRMSE_{CE}$		$nRMSE_{BA}$		$nRMSE_{RS}$	
	(Leal et al., 2025)	Achieved	(Leal et al., 2025)	Achieved	(Leal et al., 2025)	Achieved
Minimum	6.25%	9.25%	13.04%	14.87%	6.08%	10.40%
Median	15.01%	11.83%	32.72%	21.08%	28.55%	15.01%
Mean	17.31%	13.26%	34.47%	23.13%	31.73%	14.86%
Maximum	77.77%	27.12%	95.69%	43.76%	96.27%	23.06%
Standard Deviation	0.08	0.04	0.13	0.06	0.16	0.03

3.1.6 Compilation of results for PICP in the daily time window for wind speed.

Table 6 shows the results for the PICP metric, which was the only metric for which (Leal *et al.*, 2025) obtained the best results. PICP should not be analyzed separately from the other metrics, because if only the values in the table below are considered, it may appear that the performance of kNN is not good, which is not correct. In fact, what is happening is that the prediction interval constructed by the bagging models is narrow, as can be seen in Table 7 by the PINAW values. Despite the narrow prediction intervals, the daily (Table 4), weekly (Table 5), and overall (Table 2) nRMSE results indicate good bagging performance. PICP had low results, but this does not mean that the predicted results are not good.

Table 6: PCIP for the daily time window.

Parameter	$PICP_{CE}$		$PICP_{BA}$		$PICP_{RS}$	
	(Leal et al., 2025)	Achieved	(Leal et al., 2025)	Achieved	(Leal et al., 2025)	Achieved
Minimum	27.08%	2.08%	2.08%	2.08%	12.50%	4.17%
Median	97.92%	22.92%	79.17%	20.83%	70.83%	25%
Mean	93.31%	23.16%	76.10%	21.13%	71.80%	25.43%

Maximum	100.00%	40.00%	100.00%	37.50%	100.00%	50%
Standard Deviation	0.0969	0.07	0.2072	0.06	0.2401	0.08

3.1.7 Compilation of results for PINAW in the daily time window for wind speed.

The following table shows the results of the PINAW metric. It can be seen that the results were better than those of (Leal *et al.*, 2025), which means that the prediction intervals are narrower than those constructed by the Linear Dynamic Models.

Table 7: PINAW for the daily time window.

Parameter	**$PINAW_{CE}$**		**$PINAW_{BA}$**		**$PINAW_{RS}$**	
	(Leal et al., 2025)	**Achieved**	**(Leal et al., 2025)**	**Achieved**	**(Leal et al., 2025)**	**Achieved**
Minimum	50.44%	5.66%	38.14%	3.87%	44.41%	4.31%
Median	69.15%	9.43%	65.66%	8.15%	73.94%	8.46%
Mean	72.84%	9.86%	68.84%	8.40%	76.01%	9.11%
Maximum	100.00%	18.29%	100.00%	15.53%	100.00%	21.95%
Standard Deviation	0.13	0.02	0.17	0.02	0.14	0.03

3.2 Results of the direct simulation of green hydrogen forecasting

3.2.1 Results of direct hydrogen forecasting for Ceará

Bagging was also applied to directly predict green hydrogen production. Table 8 shows the results for Ceará for methods C1, C2, and C3. C2 obtained the most consistent results, while C1 had RMSE and nRMSE results far from C2 and C3. Comparing these results with those of wind speed for Ceará, it can be concluded that the results are worse. This means that bagging has difficulty dealing with the simplifications and uncertainties associated with each conversion method.

Table 8: Performance metric results for training and testing using green hydrogen production data for Ceará.

Metric	**C1**		**C2**		**C3**	
	Train	**Test**	**Train**	**Test**	**Train**	**Test**
RMSE (m/s)	179.11	198.05	66.25	71.20	96.26	107.37
nRMSE	0.38	0.38	0.21	0.21	0.28	0.28
R^2	0.84	0.78	0.87	0.81	0.82	0.75

3.2.2 Results of direct hydrogen forecasting for Bahia

The following table shows the results of the direct hydrogen forecast for Bahia. C1 also obtained results that were far from C2 and C3. When comparing these results with Table 2, it can be seen that forecasting wind speed yields better results than directly forecasting green hydrogen production.

Table 9: Performance metric results for training and testing using green hydrogen production data for Bahia.

Metric	**C1**		**C2**		**C3**	
	Train	**Test**	**Train**	**Test**	**Train**	**Test**
RMSE (m/s)	200.95	208.38	83.66	90.96	106.12	119.42
nRMSE	0.59	0.63	0.37	0.42	0.44	0.50
R^2	0.80	0.78	0.79	0.76	0.77	0.71

3.2.2 Results of direct hydrogen forecasting for Rio Grande do Sul.

The results of the hydrogen forecast for Rio Grande do Sul are shown in Table 10. Once again, C1 showed a large disparity in relation to C2 and C3. For this region, too, forecasting wind speed yields better results than directly forecasting hydrogen.

Table 10: Performance metric results for training and testing using green hydrogen production data for Rio Grande do Sul.

Metric	C1		C2		C3	
	Train	Test	Train	Test	Train	Test
RMSE (m/s)	263.77	318.95	68.00	70.51	96.88	100.69
nRMSE	0.47	0.54	0.22	0.23	0.29	0.30
R^2	0.85	0.84	0.87	0.87	0.83	0.82

3.3 Results of the indirect simulation of green hydrogen forecasting

The last forecast scenario studied was to use the models that generated the results in Table 2 to forecast green hydrogen production. Therefore, each model, already with the numbers of lag columns and k neighbors defined in the simulations for wind speed, was trained with the green hydrogen production data. The results in Table 11 are for the indirect prediction of the test data. This was the scenario that generated the worst results (compared to Tables 2, 8, 9, and 10), indicating that the optimal amounts of lag columns and k neighbors for wind speed are different from the optimal amounts for hydrogen production.

Table 11: Results of performance metrics from test data for indirect forecasting of green hydrogen production.

Metric	Ceará			Bahia			Rio Grande do Sul		
	C1	C2	C3	C1	C2	C3	C1	C2	C3
RMSE (m/s)	195.81	71.29	107.58	208.17	90.31	118.64	318.16	70.90	100.65
nRMSE	0.38	0.21	0.28	0.63	0.41	0.50	0.54	0.24	0.30
R^2	0.79	0.81	0.75	0.78	0.76	0.72	0.84	0.86	0.82

4. Conclusion

Although the results for wind speed prediction were better compared to direct and indirect green hydrogen production, it can be concluded that the objective of this research, to show that self-adjusting tuning can be a reasonable way to improve the use of the kNN algorithm was achieved. It can also be concluded that hydrogen forecasting presented greater errors because the algorithm was unable to capture the non-operating ranges of the electrolysers for very low wind speeds or for input powers above the nominal power of the wind turbines and the electrolyser.

It is important to note that they prove that the optimal values for lag columns and neighboring k are different when analyzing wind speed or green hydrogen production. Therefore, depending on the variable being analyzed, self-adjusting tuning tends to adjust differently.

The fact that method C1 presented worse results than C2 and C3 is expected, since C1 does not consider the power curve of wind turbines, being based entirely on an unrealistic case.

PICP is a metric that requires careful observation, as, if studied separately, it can lead to misinterpretations of the algorithms' performance.

As a suggestion for future research, the same optimization methodology could be applied to artificial intelligence models with more hyperparameters, which should produce better results. It is also recommended to apply automatic adjustment to solar data to compare whether performance can be improved. Another perspective to be studied is to use hydrogen production data from real electrolyzers, which will give more reliability to the results, as this article used methods from the literature that adopted simplifications and have built-in errors.

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