Performance Analysis of Intelligent Computational Algorithms for Biomass Higher Heating Value Prediction

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ABSTRACT: Higher heating value (HHV) is an essential parameter to consider when evaluating and choosing biomass substrates for combustion and power generation. Traditionally, HHV is determined in the laboratory using an adiabatic oxygen bomb calorimeter. Meanwhile, this approach is laborious and cost-intensive. Hence, it is essential to explore other viable options. In this study, two distinct artificial intelligence-based techniques, namely, a support vector machine (SVM) and an artificial neural network (ANN) were employed to develop proximate analysis-based biomass HHV prediction models. The input variables comprising ash, volatile matter, and fixed carbon were paired to form four separate inputs to the prediction models. The overall findings showed that both the ANN and the SVM tools can guarantee accurate prediction in all the input combinations. The optimal prediction performances were observed when fixed carbon and volatile matter were paired as the input combination. This combination showed that the ANN outperformed the SVM, having presented the least root mean squared error of 0.0008 and the highest correlation coefficient of 0.9274. This study, therefore, concluded that the ANN is more preferred compared to SVM for biomass HHV prediction based on the proximate analysis.

KEYWORDS: Artificial intelligence; calorific value; machine learning; neural network; proximate analysis

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I. INTRODUCTION

The increasing energy demand, the depletion of fossil fuel reserves, and the pressing desire for ecologically friendly energy sources necessitated the global interest in renewable energy (RE). RE sources such as wind, solar, hydro, and biomass are clean energy sources and are in abundance with prospects to replace fossil energy sources for the generation of thermal energy and electricity (Olatomiwa *et al*., 2022). Biomass is credited to be the most widely available RE source after wind and solar and it comprises sewage sludge, energy grasses, algae, wood, food wastes, bagasse, straw, forest wastes, agro residues, and others (Dodo *et al*., 2021).

For optimal design and operation of biomass-fuelled energy systems, certain properties of the feedstock must be investigated and analyzed. Foremost is the calorific value also known as the heating value, as it expresses the energy content of the biomass substrate (Ezzahra Yatim *et al*., 2022; Dodo and Ashigwuike, 2023). The heating value is reported to be either a higher heating value (HHV) or a lower heating value (LHV). The HHV accounts for the condensation enthalpy of water when a unit weight/volume of fuel is combusted to release thermal energy while the LHV is found when the condensation enthalpy of water is not accounted for.

By tradition, the heating value is determined in the laboratory using an oxygen bomb calorimeter at standard conditions. Meanwhile, the energy audience is embracing the approaches that rely on the proximate or ultimate analyses for prediction since the experimental procedures are costly, strenuous, and require skillful personnel for sample preparation to avoid erroneous results (Dodo *et al*., 2022; Güleç *et al*., 2022). The ultimate analysis states the nitrogen, hydrogen, carbon, sulphur, and oxygen contents while the proximate analysis defines the ash, fixed carbon, volatile matter, and moisture content of the biomass fuel. Similarly, the cost of an elemental analyzer and the skill requirements for its operation in addition to sample preparation under certain stringent conditions are impediments to reliance on ultimate analysis to predict the heating value. As a result, seeking an alternative approach capable of providing optimal results with minimum stress and economy has become an imperative task and the proximate analysis fits into these descriptions (Ezzahra Yatim *et al*., 2022).

Furthermore, the application of artificial intelligence (AI) to solve complex problems in various fields has gained novel interest in recent years. Thus, AI techniques such as the artificial neural network (ANN), adaptive neuro-fuzzy inference system, Gaussian process regression, and so on can serve as robust alternatives to the laboratory investigation of the biomass heating value. For instance, Ezzahra Yatim *et al*. (2022) developed ANN algorithms to estimate the HHV of biomass. The root mean square error and the correlation

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coefficient of the optimal model were 1.17527 and 0.75377 respectively. Qian *et al*. (2018) employed 49 lines of proximate analysis data to predict the HHV of poultry waste. The best-fit regression model was better in accuracy based on the error metrics. Rostami and Baghban (2018) developed machine learning prediction models using 100 data points of ultimate analysis variables. Güleç *et al*. (2022) Implemented ANN models trained by combining ultimate-proximate analysis variables to estimate the HHV of biomass. The sigmoidal transfer functions provided superior prediction results compared to the linear activation function. The model developed by Dai *et al*. (2021) showed the promising features of extreme machine learning to predict biomass HHV. García Nieto *et al*. (2022) employed an experimental dataset to develop HHV prediction models based on SVM with the grid search (GS) optimizer, and a multilayer perceptron neural network. The SVM-GS model proved superior in accuracy.

It is a common practice to utilize a few sets of experimental data or implement heating value predictive models using only one biomass substrate. Meanwhile, the prediction models implemented for such investigation cannot guarantee accurate prediction performances especially when the heating values of a variety of biomass materials are to be predicted (Dodo *et al*., 2022). Furthermore, the review of related studies has shown the trend of AI application to biomass heating value prediction being dominated by an ANN technique. Hence, it is imperative to explore another AI technique to see if it can provide more precise prediction performance.

Therefore, the present study aimed to develop and compare the accuracies of two AI-based models (support vector machine and artificial neural network) to predict the higher heating value (HHV) of biomass using a large pool of experimental datasets covering a wide-ranging feedstock as a function of the proximate analysis. The moisture-free proximate analysis variables comprising ash, fixed carbon (FC), and volatile matter (VM) in wt.% were selected to form four different inputs to the models. The dataset was calibrated to have 75% reserved for training and the remaining 25% for testing in line with the notion that the more training data, the better the prediction model performances. Finally, the precisions of the implemented models were appraised using statistical metrics. It is anticipated that the results of this study will serve as a paradigm for the energy audience in seeking viable, fast, and economical routes for determining the HHV of broad categories of biomass materials.

II. MATERIALS AND METHODS

A. Data Pre-processing

In this research, two AI-based techniques, namely, SVM and an ANN were implemented to predict the HHV of biomass from the moisture-free proximate analysis parameters which include FC, ash, and VM. The experimental datasets comprising 474 instances credited to Nhuchhen and Salam (2012), Phichai *et al.* (2013), Estiati *et al.* (2016), Gunamantha (2016), Uzun *et al.* (2017), and Qian *et al.* (2018) were utilized for model implementation. The biomass contained in the dataset encompasses a wide range of feedstock, such as grasses (57 samples), seed hulls (34 samples), sewage sludge (41 samples), sawdust (28 samples), animal manure (71 samples), agro wastes (111 samples), wood wastes (40 samples) and solid wastes (92 samples). The prediction models were implemented in *MATLAB_R2019b_9.7.0x64:* 2019 Version, 64 Bit (x64) while the analyses were performed in *Microsoft Excel:* 2013 version, 64-Bit Edition.

The Eqn. (1) was applied to normalize the dataset to a standard scale with an array of 0 to 1 to strengthen the integrity of the data and guarantee that deviations in the signals of the various parameters have the same influences on the characteristics of the networks regardless of their magnitudes.

$$x_n = \frac{x_i - x_{\min}}{x_{\max -} x_{\min}} \quad (1)$$

x_n and x_i represent the normalized and unnormalized variables, the maximum and minimum variables of the dataset, respectively are represented by $x_{\max}$ and $x_{\min}$.

In the development of predictive models, some independent variables have significant effects on the target variable, while some have little to no effects. Therefore, it is crucial to identify the combination of these independent variables that could produce the optimal prediction accuracy. Given this, the FC, VM, and ash were selected for sensitivity analysis based on Table 1 for consequent implementation in the ANN and SVM tools.

Table 1: Input selection

Model input	Variable combination
M1	VM, ash
M2	FC, ash
M3	FC, VM, ash
M4	FC, VM

By convention, the ANN frameworks and their counterparts in MATLAB employ data division of 20%, 20%, and 60 % respectively for validation, testing, and training which can be folded into 40% and 60% following common testing-training divisions. The common data divisions in various studies are 30% and 70% or 25% and 75% respectively for testing and training purposes in line with the notion that prediction models function more effectively with more training data (Dodo *et al.*, 2022). Therefore, this study considered a division of dataset for testing and training respectively as 25% and 75%. The prediction effectiveness of the developed models was evaluated using statistical indices. The flowchart depicting the study methodology is shown in Figure 1.

B. Support vector machine

Support vector machine (SVM) is an often discussed machine learning algorithm for requiring little tuning to achieve high-level performance. First created in 1995 by Vladimir Vapnik, SVM is a supervised machine learning model primarily used to solve problems involving regression and classification, namely, support vector classification and support vector regression (Dodo *et al.*, 2022). The concepts behind the SVM are structural risk reduction and statistical learning theory, which revolve around the mapping of the initial samples of the training data into a higher dimensional

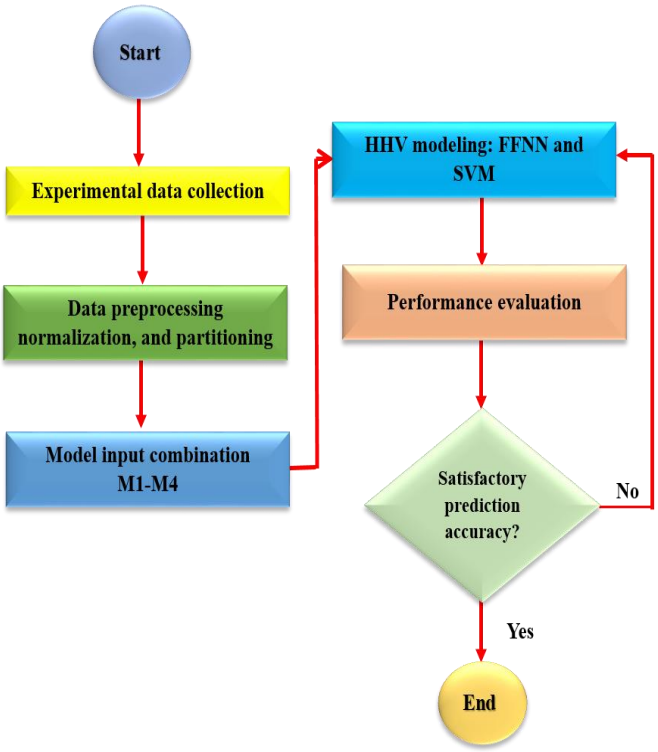


Figure 1: Study flowchart

feature space by employing non-linear kernel functions. This approach facilitates the transformation of the problems from non-linear to linear for an optimal solution. The regression function of the SVM is expressed in Eqn. (2) (Elmaz *et al.*, 2019).

$$f(x) = b + w\phi(x) \quad (2)$$

Here, Here, b and w stand for the bias and weight vectors respectively, while the non-linear function for mapping the initial input vectors into a higher dimensional feature space is represented by $\phi(x)$. The Lagrange multipliers and optimality constraints expressed in Eqn. (3) are used to determine the regression function of Eqn. (2) (Dodo *et al.*, 2022). and w stand for the bias and weight vectors respectively, while the non-linear function for mapping the initial input vectors into a higher dimensional feature space is represented by $\phi(x)$

The Lagrange multipliers and optimality constraints expressed in Eqn. (3) are used to determine the regression function of Eqn. (2) (Dodo *et al.*, 2022).

$$f(x) = \sum_{k=1}^{n} (\beta_k - \beta_k^*) Q(x, x_k) + b \quad (3)$$

Where $Q(x, x_k)$ represents the kernel function and the term $\beta_k - \beta_k^*$ represents the Lagrange multipliers.

In the selection of the appropriate kernel function for modeling the HHV of the biomass from the proximate analysis, a trial-and-error strategy utilizing root mean square error as the performance evaluation index was adopted since there have not been any established criteria for kernel selection in the literature. As such, this approach accorded more credence to the linear kernel function. Furthermore, a common technique for appraising the effectiveness of an SVM model is cross-validation. In particular, the 10 k-fold cross-validation which is more popular in the literature for replicating the prediction models' generalization and accuracy was used to validate the dataset (Dodo *et al.*, 2022a; Elmaz *et al.*, 2019). The architecture of the SVM model served by the proximate analysis parameters (FC, VM, and ash) is shown in Figure 2.

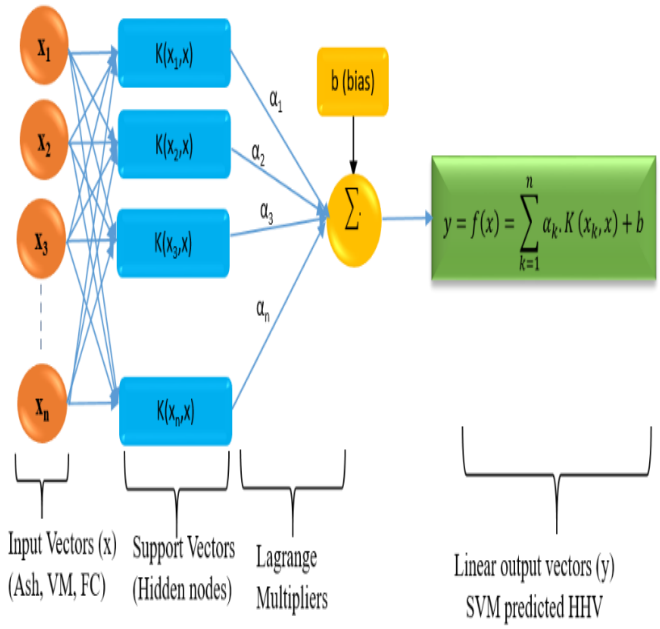


Fig. 2: SVM model

C. *Artificial neural network*

Artificial neural network (ANN) was developed as a technology based on the study of the human brain and nervous system. Particularly, ANN models mimic the electrical activity of the nervous and brain system. Processing elements also referred to as neurons are connected by weighted links (Dodo et al. 2022). They are typically stacked in layers or vectors, with the output from one layer providing input for the subsequent layer and perhaps other layers. Feed-forward back-propagation network (FFBN), recurrent neural network, radial basis function neural network, Kohonen self-organizing neural network, convolutional neural network, and modular neural network are just a few of the many ANN structures that can be

used for various problems (Dodo *et al*. 2022). However, FFBN was chosen for this study because it has the credit of being the most effective architecture for pattern prediction and pattern-matching problems (Abba *et al*., 2019).

An FFBN is shown in Figure 3, which consists of three layers: an input layer with nodes representing the input parameters (i.e. ash, FC, and VM); a hidden layer with nodes for detecting nonlinearity in the data; and an output layer with nodes for the output parameter (i.e. higher heating value). Each layer's neuron in an FFBN is coupled unidirectionally, combining the weighted sum of inputs with a bias and an activation or transfer function to create an output that does not provide feedback to the input neurons.

The generalized expression for FFBN is represented in Eqn. (4) (Olatunji *et al.*, 2019).

$$y = k\left\{B_2 + h\left[B_1 + f\left(x\right)W_1\right]W_2\right\} \tag{4}$$

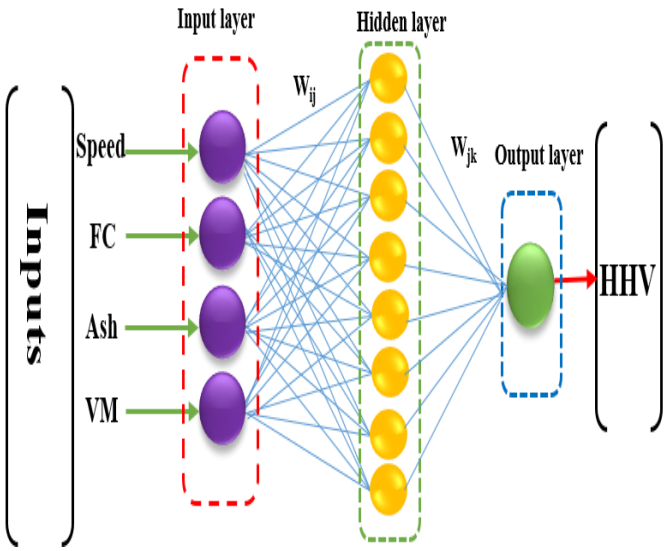


Fig. 3: Feed-forward neural network structure

The input and output vectors were represented by y and k respectively. f, h, and k are the transfer functions while B_i and W_i are the weight and bias vectors.

The most crucial factors influencing the success of a model in ANN were the number of hidden layers and hidden neurons, as well as transfer functions. Therefore, proper selection of these variables is crucial. A hidden layer is often chosen for the majority of the process since using two hidden layers when modeling data with discontinuities can greatly increase the likelihood of convergence in local minima (Abba *et al.*, 2019). As a result, an FFBN with a single hidden layer was utilized in this work. In addition, the number of neurons will have a substantial influence on the network's accuracy. The training data will perform well with a large number of hidden neurons, but the training period will be extremely stretched, and worse, over-fitting could arise. On the other hand, under-fitting or inadequate convergence could occur if there are insufficient hidden neurons. The ideal number of neurons typically lies between 1 and 20, according to Wong *et al.* (2020). As a result, the number of hidden neurons in this study was determined by trial-and-error by altering the neurons from 1 to 20. The tangent-sigmoid (tansig) transfer function $\varphi(x)$ shown in Eqn. (5) was used in this study. It is a non-linear function that is differentiable and has a range between -1 and +1. This function is used more frequently when speed is a concern (Dodo *et al.*, 2022).

$$\varphi(x) = \frac{2}{e^{-2x}+1} \tag{5}$$

The FFBN training function adopted in this study is the Leverberg-Marquardt (trainlm). Being the fastest FFBN formalism in the toolkit, trainlm is widely recommended as a preferred supervised learning algorithm despite the requirements for more memory compared to other algorithms (Olatunji *et al.*, 2019).

D. Performance evaluation

The metrics used to assess the predictive potential of the models included the mean square error (MSE), root mean square error (RMSE), coefficient of determination (R^2), and correlation coefficient (R) expressed in Eqns. (6 - 9). These evaluation criteria were chosen because they have been successfully used in a lot of studies of a similar nature to demonstrate a prediction model's accuracy (Dodo *et al.*, 2022). The prediction model is generally better and more accurate when the MSE and RMSE have lower values. The R and R^2 vary from 0 to 1. They reveal the degree to which a model matches the data. Higher R^2 and R values signify that the implemented model has a high degree of accuracy.

$$R^2 = 1 - \frac{\left(HHV_{e(i)} - HHV_{p(i)}\right)^2}{\left(HHV_{e(i)} - \overline{HHV}_{e(i)}\right)^2} \tag{6}$$

$$R = \sqrt{1 - \frac{\left(HHV_{e(i)} - HHV_{p(i)}\right)^2}{\left(HHV_{e(i)} - \overline{HHV}_{e(i)}\right)^2}} \tag{7}$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(HHV_{e(i)} - HHV_{p(i)}\right)^2 \tag{8}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(HHV_{e(i)} - HHV_{p(i)}\right)^2} \tag{9}$$

$HHV_{e(i)}$ is the experimental HHV, $HHV_{p(i)}$ is the predicted HHV, and $\overline{HHV}_{e(i)}$ is the mean value of the experimental HHV.

III. RESULTS AND DISCUSSION

A. Prediction performances of the standalone models

Quantitative and visual representations of the results were crucial for evaluating the effects of various input combinations and the precision of the predictive models in computational analysis. Hence, as shown in Table 2, all the input combinations (M1-M4) in both the ANN and SVM techniques can guarantee precise prediction owing to their high coefficient

Table 2: Prediction models performance evaluation results

		Training Phase				Testing Phase			
		R^2	R	MSE	RMSE	R^2	R	MSE	RMSE
SVM	M1	0.7851	0.8861	0.0022	0.0471	0.8429	0.9181	0.0010	0.0323
	M2	0.8018	0.8954	0.0020	0.0453	0.8488	0.9213	0.0010	0.0317
	M3	0.8034	0.8963	0.0020	0.0451	0.8508	0.9224	0.0010	0.0315
	M4	**0.7973**	**0.8929**	**0.0021**	**0.0458**	**0.8527**	**0.9234**	**0.0010**	**0.0313**
ANN	M1	0.8029	0.8960	0.0020	0.0453	0.8689	0.9322	0.0009	0.0295
	M2	0.8095	0.8997	0.0020	0.0445	0.8699	0.9327	0.0009	0.0294
	M3	0.8025	0.8958	0.0021	0.0453	0.8257	0.9087	0.0012	0.0340
	M4	**0.8154**	**0.9030**	**0.0019**	**0.0438**	**0.8786**	**0.9374**	**0.0008**	**0.0284**

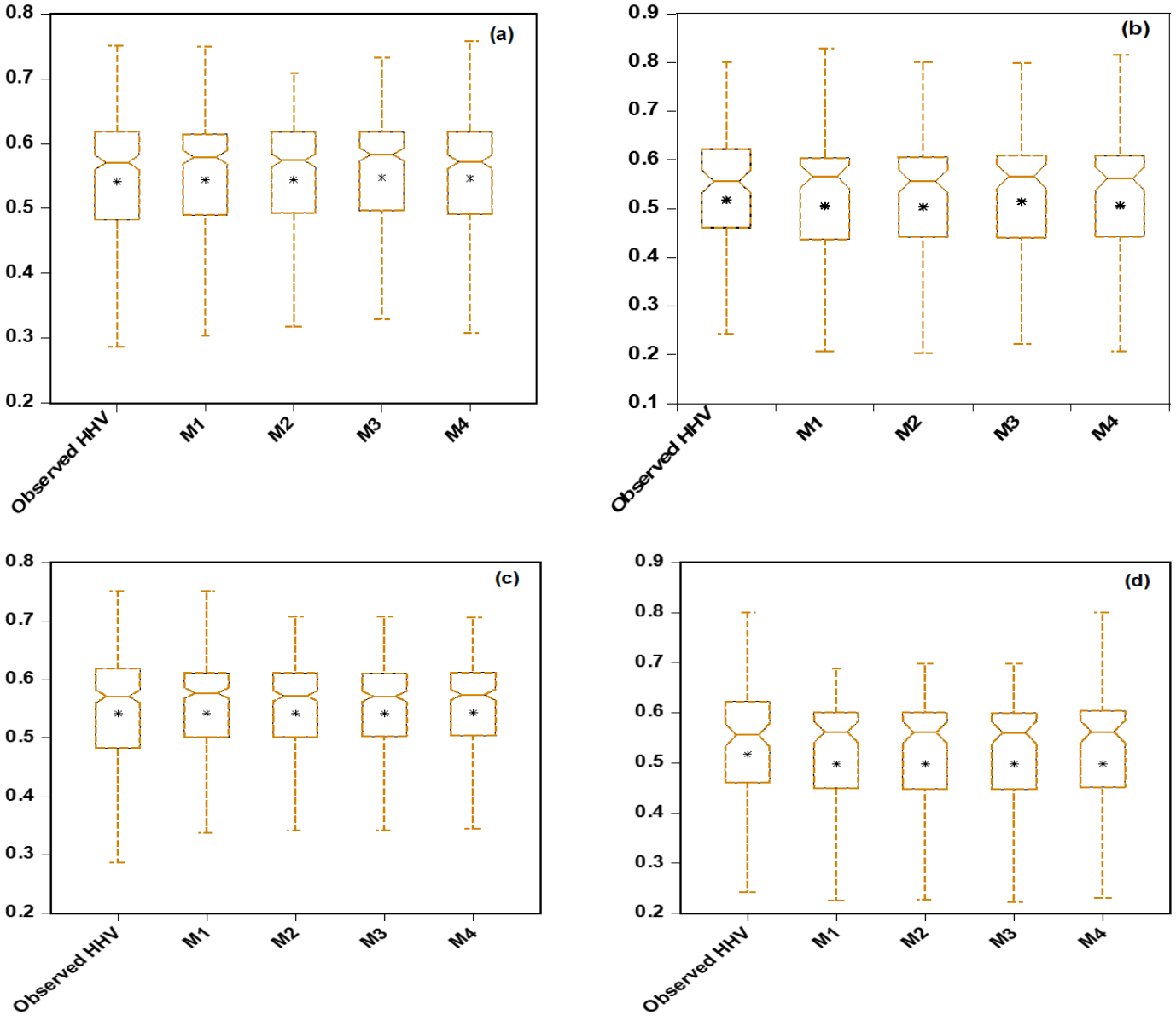


Fig. 4: Box plots: (a) ANN-Training phase, (b) ANN-Testing phase, (c) SVM-Training phase, (d) SVM-Testing phase

of correlations and coefficient of determinations in both phases of training and testing. The closer these metrics are to unity the better the prediction models' performances. The input combination comprising ash and VM (i.e. M1) in both the ANN and SVM formalisms provided the least impressive prediction capability followed by M2 and M3. Meanwhile, outstanding performances were seen when the VM and FC served as the prediction models' input combinations.

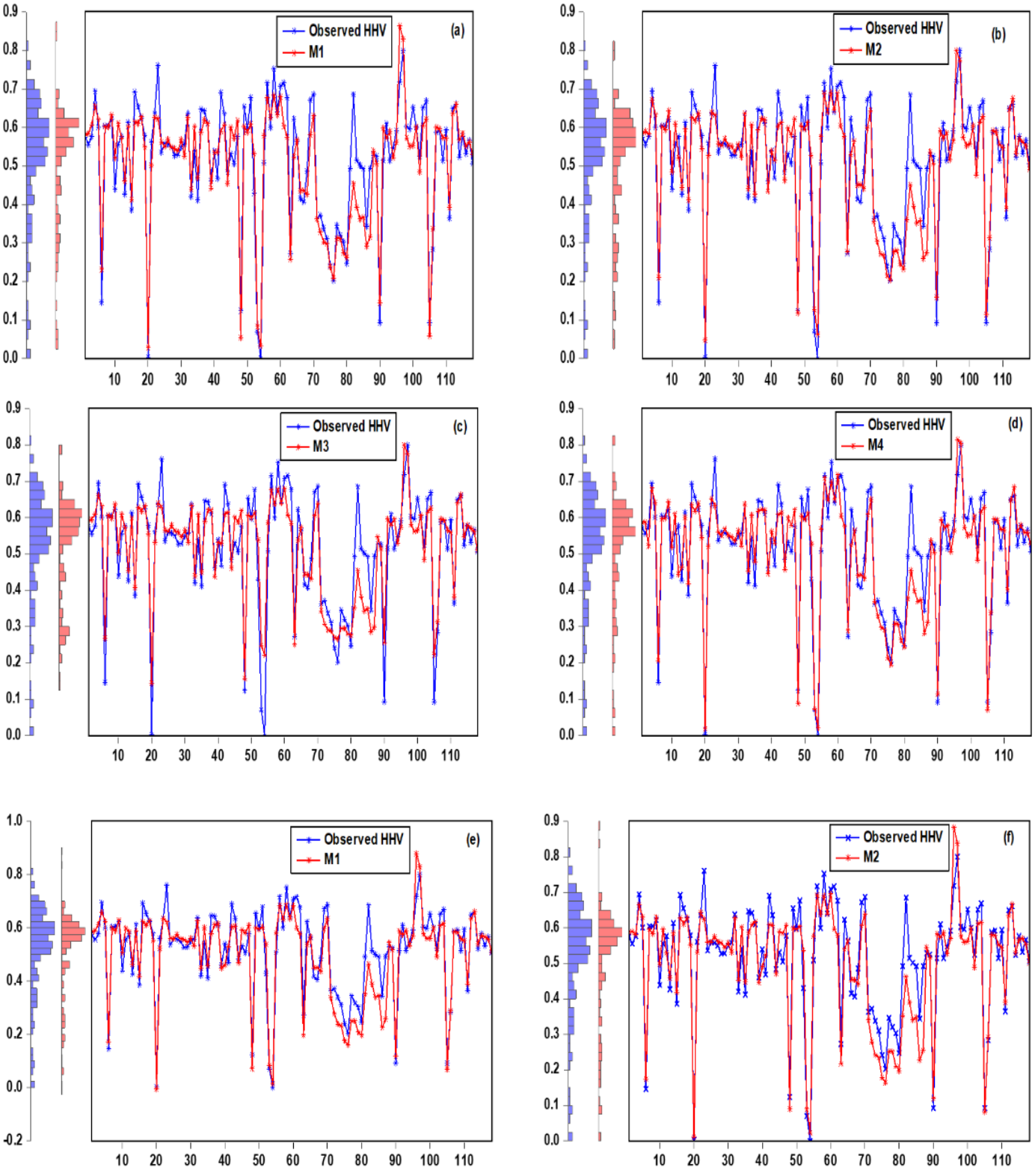
The boxplots shown in Figure 4 provide a visual summary of the predicted HHV and experimental HHV data in both phases of training and testing. The spread of data and the whiskers for M4 using ANN and SVM correlated with their respective experimental HHV in both phases of training and

testing followed by M3, M2, and M1 in descending order of prediction performance respectively.

Furthermore, as depicted in the time series plots of Figure 5 using the testing dataset, the predicted HHV pattern closely follows the experimental HHV. These are indications of strong correlations between the experimental HHV and predicted using ANN and SVM models. Thus, the implemented models are consistent and accurate at making predictions.

B. Performance comparison of ANN and SVM models

The spider plots in Figure 6 provide a quick overview of the prediction performance comparison of ANN and SMV using the RMSE and R. In the spider plots, each input combination (M1, M2, M3, and M4) has an axis that runs from the center to parity. With the correlation coefficient (i.e. Fig. 6 (a)), the data point nearest to the outermost gridline in the model is considered the best predictive performance.



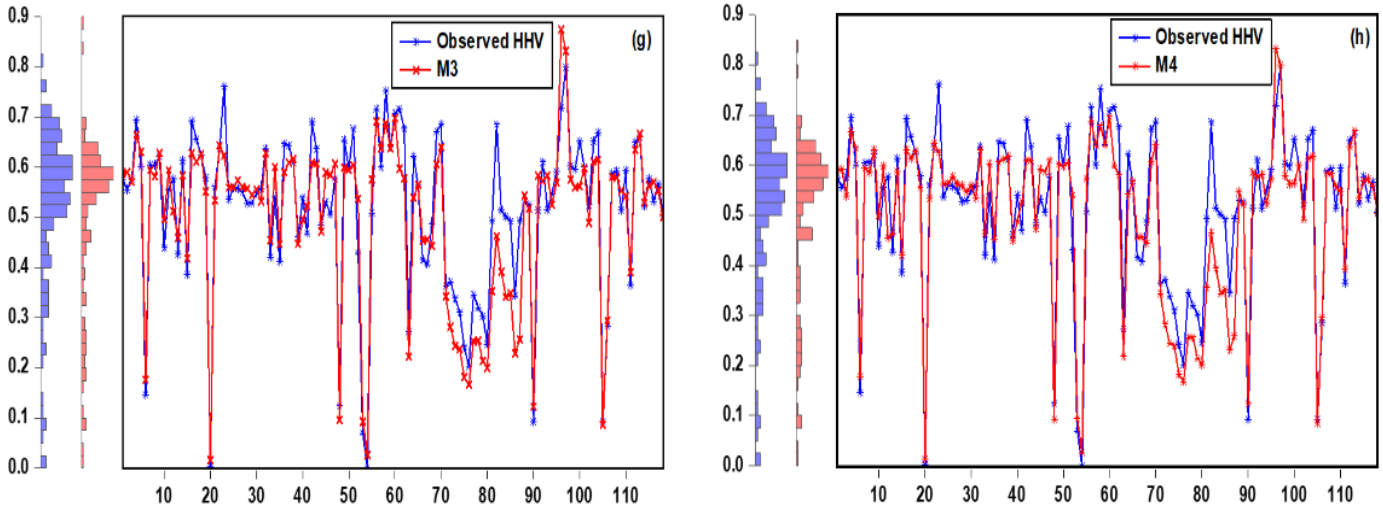


Fig. 5: Time series plots of the combinations M1-M4: (a)-(d) SVM, (e)-(h) ANN

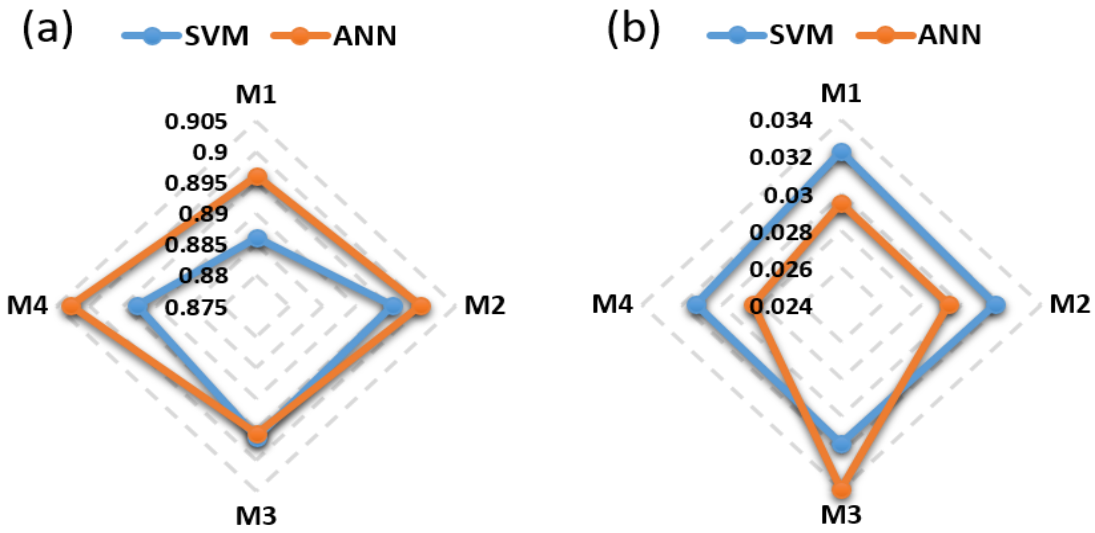


Fig. 6: Spider plots using performance evaluation metrics: (a) R (b) RMSE

As for the root mean square error of Fig. 6 (b), the model with the best prediction accuracy is whose data point is closest to the center. As shown in Fig. 6, the ANN demonstrated the strongest capability to predict the HHV of biomass compared to the SVM for all the input combinations except M3 (FC, VM, ash) in which the SVM presented better performance. Thus, in M3, the SVM has a lower RMSE of 0.0315 and a higher R of 0.9224 compared to RMSE of 0.0340 and an R of 0.9087 in ANN.

C. Prediction models validation

The computational intelligence models implemented by Yaka *et al.* (2022) which included random forest regression, genetic programming, polynomial regression, decision tree regression, multilinear regression, and support vector regression had mean squared errors up to 1.7932. Hence, they cannot guarantee better performance compared to all the models of this study. More so, Nhuchhen and Salam (2012) developed 24 empirical models that had mean squared errors and determination coefficients ranging from 8.72 to 19.28 and 0.0005 to 0.2398, respectively. This places the models developed in this study as superior alternatives to empirical models for biomass HHV prediction. Although the prediction models created by Uzun *et al.* (2017) and Akkaya (2016) have shown competing prediction capabilities, they employ more input parameters in comparison to the optimal models of M1, M2, and M4 of this study. From the viewpoint of economy, a model that utilizes more input parameters has the downsides of increasing the budget and labour and may not attract the interest of the energy audience especially if the model with fewer input parameters is also capable of delivering better performance.

IV. CONCLUSION

In this study, two heterogeneous AI-based models, namely, SVM and ANN were applied to develop biomass HHV prediction models based on the proximate analysis– ash, VM, and FC. These proximate analysis variables were paired to form four distinct inputs to the implemented models. The overall results demonstrated the preciseness of both the ANN

and SVM to predict the biomass HHV. Meanwhile, the ANN proved to be superior in predictive precision having presented the least RMSE of 0.0008 and the highest R of 0.9274 when FC and VM were employed as the input combination. It is recommended that further studies be conducted to investigate the capabilities of ANN types other than the feed-forward neural network and other AI techniques such as the gaussian process regression and a neuro-fuzzy system to predict the HHV of biomass feedstock.

AUTHOR CONTRIBUTIONS

U. A. Dodo: Conceptualization, Methodology, Software, Validation, Writing – original draft, Writing – review & editing. **M. A. Dodo**: Methodology, Writing – original draft, Writing – review & editing. **Y. A. Badamasi**: Methodology, Writing – review & editing. **A. F. Shehu**: Validation, Writing – review & editing.

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