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Improved prediction accuracy of biomass heating value using proximate analysis with various ANN training algorithms

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ABSTRACT

The conventional experimental methods to determine biomass heating value are laborious and costly. Numerous correlations to estimate biomass' higher heating values have been proposed using proximate analysis. Recently, the utilisation of artificial neural network (ANN) has been extensively applied to predict HHV. However, most studies of ANN to estimate the biomass' HHV only use one algorithm to train a small number of biomass datasets. The specific objective of this study is to predict the HHV of 350 samples of biomass from the proximate analysis by developing an ANN model which was trained with 11 different algorithms. This study fills a gap in the research on how to predict the HHV of biomass using numerous ANN training algorithms utilising sizeable biomass datasets. Results show that the ANN trained with Levenberg-Marquardt gave the highest accuracy. The Levenberg–Marquardt algorithm shows the best fit giving the highest R and R^2 values and the lowest MAD, MSE, RMSE and MAPE. Compared with previous biomass HHV prediction studies, the ANN model developed in this study provides improved prediction accuracy with higher R^2 and lower RMSE. Results from this study have also indicated that the Levenberg-Marquardt should be the first-choice supervised algorithm for feedforward-backpropagation.

1. Introduction

Biomass is a promising bioenergy resources due to its net-balanced CO_2 emissions [1–3]. The utilisation of biomass needs a thorough understanding of its key fuel properties. One of crucial properties to determine is the higher heating value (HHV). HHV is described as the total heat liberated when one unit fuel mass is burned entirely, including the latent heat stored in the vapourised water of liquid as the product of combustion. Therefore, fuel with greater HHV will produce relatively higher energy output.

A bomb calorimeter is normally used to determine HHVs, but this conventional method is complicated, laborious and expensive to perform. To overcome these problems, a number of correlations have been recommended to quantify higher heating values using the proximate and ultimate (elemental) analysis. In terms of proximate analysis, biomass has a higher heating value that is positively correlated with the composition of fixed carbon but negatively related to the ash content [1]. In general, the biomass comprises of greater than 50% volatile content (dry basis) with less than 50 and 30% of ash and fixed carbon, respectively as shown in Fig. 1a.

As for the elemental analysis, biomass normally has higher H/C and O/C ratios than the typical solid fossil fuels as shown in Fig. 1b. The

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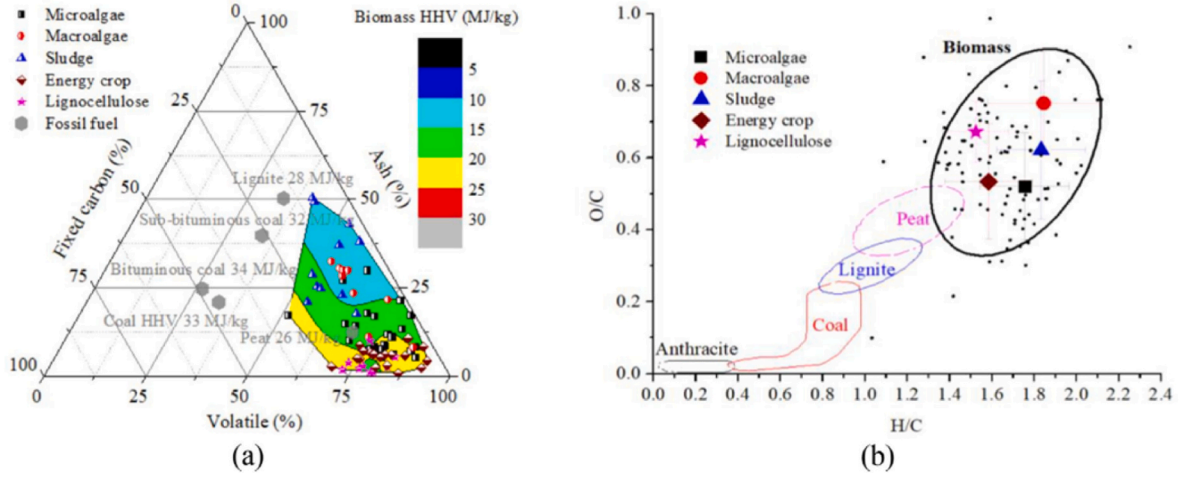

Fig. 1. (a) Proximate and (b) elemental compositions of biomass [4]. Reused with permission from Elsevier.

ultimate analysis offers an elemental composition of biomass. However, such analysis is expensive and requires specific experimentation method. The approach of proximate analysis is a more straightforward and affordable way, making it a major area of interest for HVV estimation of biomass. It determines the biomass components characterised by fixed carbon (FC), ash content and volatile matter (VM).

In addition to proximate analysis, previous studies have noted the importance of soft computation method like an artificial neural network (ANN) as the prediction tool to predict biomass' HHV. Keybondorian et al. [5], for instance, developed multi-layer perceptron (MLP) ANN to estimate the HHV based on the volatile matters, ash content and fixed carbon. In their similar study, Keybondorian et al. [6] utilised the support vector machine to predict 350 samples of biomass' HHV. The MLP ANN model was also developed by Darvishan et al. [7] to estimate the biomass' HHV according to their ultimate analysis. It was found that the MLP-ANN gave great accuracy with the coefficients of determination (R^2) for the testing and training stages being 0.999312 and 0.999986, respectively. Using iterative neural networks adapted with partial least squares (INNPLS), Hosseinpour et al. [8] successfully predicted the HHV based on their proximate investigation having the $R^2 > 0.95$, MAPE <3% and MSE <0.62.

Although several studies have indicated the promising of ANN models to estimate the HHV of biomass, little attention has been paid to investigate various ANN's training algorithm for a large number of datasets. It is remarkably challenging to determine which algorithm would give the best performance accuracy for a particular task. This study used artificial neural networks model trained with eleven different training algorithms to predict the biomass' HHV. Data comprising of 350 samples biomass' HHV in the range between 5.6 and 34.4 MJ/kg were gathered from previous studies to develop the model. This study aims to predict the HHV of 350 samples of biomass from the proximate analysis by building an ANN model trained with 11 different algorithms. This study fills a gap in the research on how to predict the HHV of biomass utilising numerous ANN training algorithms with sizeable biomass datasets.

2. Material and method

2.1. Data gathering

Data of 350 biomass's HHV along with their proximate analysis have been gathered from previous studies [8–11]. The dataset has the values of fixed carbon, volatile matter, and ash content (dry weight basis) ranging from 1.0 to 91.5%, 0.9–92.0% and 0.1–77.7%, respectively with the HHV value differs from 5.6 to 34.4 MJ/kg. The data were allocated randomly by 70% (245), 15% (52) and 15% (53) for training, validation and test, respectively. The flowchart for the overall methodology is shown in Fig. 2.

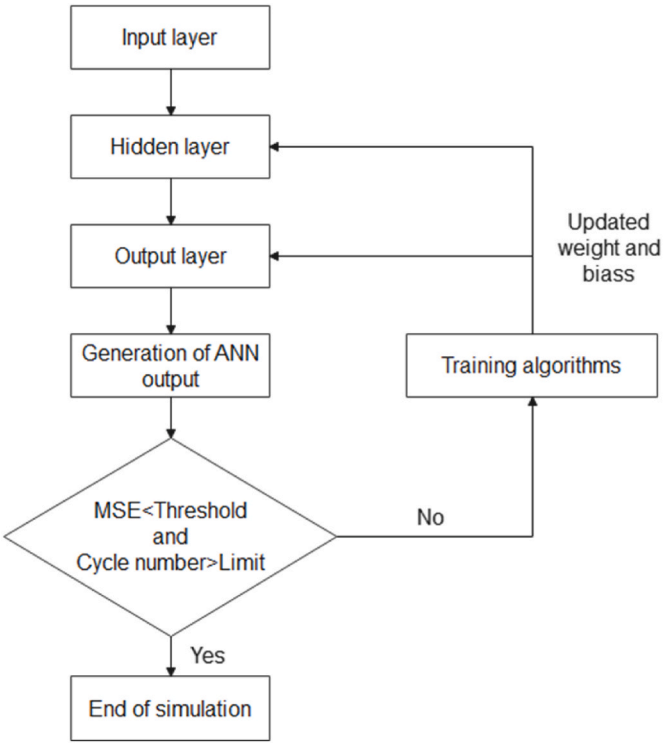

Fig. 2. Flowchart of neural network algorithm.

2.2. Artificial neural network

In this study, the feed-forward backpropagation network was used as the learning algorithm due to its effectiveness. Log-sigmoid (logsig) was set as the hidden layer transfer functions, whereas the linear (purelin) was set as the output layer. The network was trained using 11 different training algorithms as shown in Fig. 3.

The ANN's structure used in this study is illustrated in Fig. 4. The input layer consists of three neurons, while the hidden and output layers have ten and a neuron, respectively. A previous study by Veza et al. [12] showed that the ANN topology with ten hidden neurons offered the best results for various ANN's training algorithm.

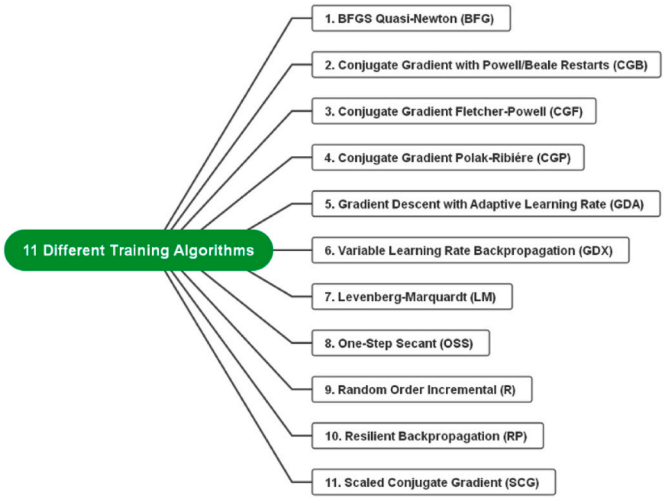

Fig. 3. Training algorithms used in this study.

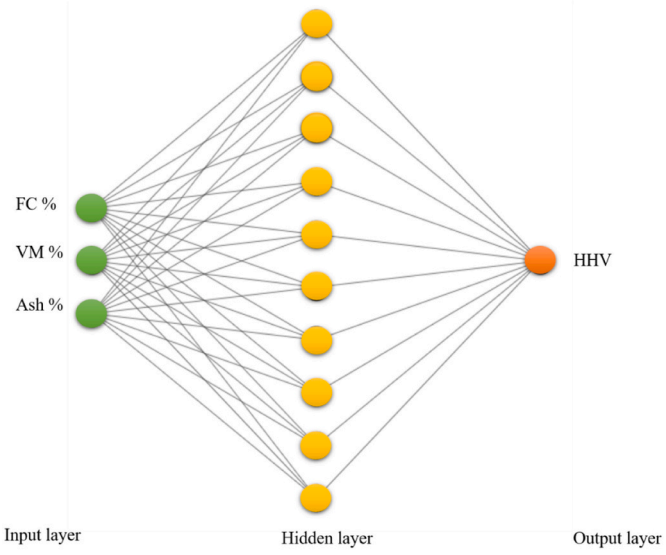

Fig. 4. The structure of ANN with 3–10-1 configuration.

2.3. Performance criteria

To evaluate the accuracy of prediction of each model, six different parameters were used; R, R^2, MAD, MSE, RMSE and MAPE. In the equations, n represents the number of samples, while M and P signify the measured (actual) and predicted values, respectively. These criteria have been used in earlier studies [13] and can be calculated using the following equations:

R is the correlation coefficient. It is used to determine how strong a relationship between data. The R value is between −1 and 1. The value of 1 signifies a solid positive relationship, while −1 suggests a clear negative relationship. An R value of 0 indicates no correlation at all. The correlation coefficient can be calculated using the following equation:

$$\text{Correlation Coefficient (R)} = \sqrt{1 - \left\{ \frac{\sum_{i=1}^{n} (M_i - P_i)^2}{\sum_{i=1}^{n} P_i^2} \right\}} \quad (1)$$

R^2 is the coefficient of determination. It provides information on how many data points fall within the results of the regression equation. A higher R^2 is an indication of a better fit. Coefficient of determination is

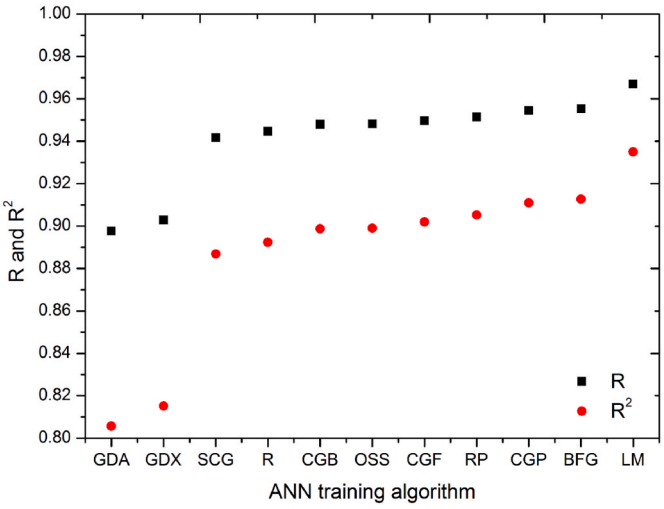

Fig. 5. R and R^2 values for the eleven ANN training algorithms.

particularly useful to find the likelihood of future cases falling within the predicted values. The determination coefficient is not sensitive to outliers. Therefore, other criteria that are sensitive to outliers are required, such as MSE and RMSE. The determination coefficient can be calculated using the following equation:

$$\text{Determination Coefficient } (R^2) = 1 - \left\{ \frac{\sum_{i=1}^{n} (M_i - P_i)^2}{\sum_{i=1}^{n} P_i^2} \right\} \quad (2)$$

MAD or Mean Absolute Deviation measures the prediction accuracy by averaging the absolute value of each error. It is particularly helpful when measuring prediction errors which have the same units. MAD can be calculated using the following equation:

$$\text{Mean Absolute Deviation (MAD)} = \frac{1}{n} \sum_{i=1}^{n} |M_i - P_i| \quad (3)$$

MSE or Mean Square Error is the average of the square of the difference between the real and predicted values. It is used to determine how close the predictions to actual values. It is sensitive to outliers and punishes larger error more. Small value signifies better prediction. MSE can be calculated using the following equation:

$$\text{Mean Squared of Error (MSE)} = \frac{1}{n} \sum_{i=1}^{n} (M_i - P_i)^2 \quad (4)$$

RMSE or Root Mean Square Error is simply the square root of the mean square error. Like MSE, RMSE is sensitive to outliers, punishes larger error more, with lower value indicating better fit. Lower the RMSE, the closer is the prediction to the actual values. RSME can be calculated using the following equation:

$$\text{Root Mean Squared of Error (RMSE)} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (M_i - P_i)^2} \quad (5)$$

MAPE or Mean Absolute Percentage Error is one of the most extensively utilised measure for checking prediction accuracy. It is scale independent and can be used to compare series on different scales. However, it can become undefined when the actual value is 0. MAPE can be calculated using the following equation:

$$\text{Mean Absolute Percentage of Error (MAPE)} = \left\{ \frac{100}{n} \sum_{i=1}^{n} \left| \left(\frac{M_i - P_i}{M_i} \right) \right| \right\} \% \quad (6)$$

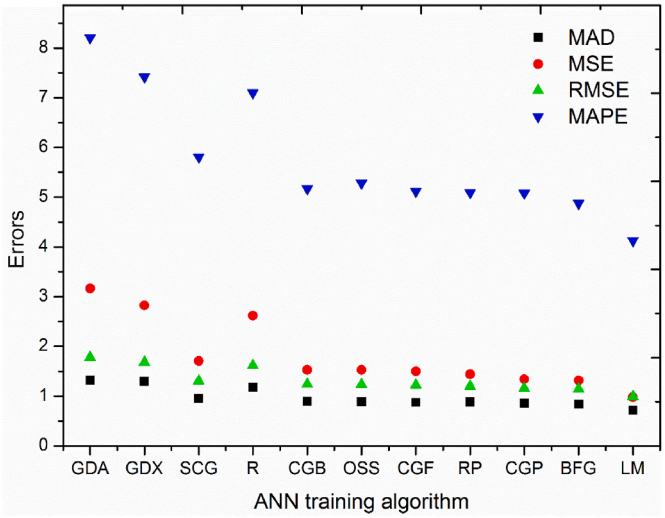

Fig. 6. Errors for the eleven ANN training algorithms.

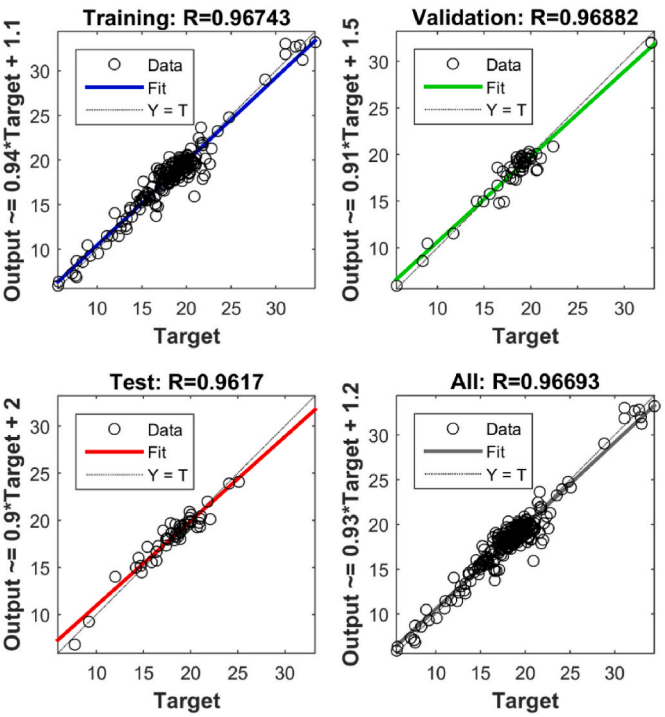

Fig. 7. Values of R of LM algorithms for the training, validation, test and all processes.

3. Results and discussions

Fig. 5 depicts the R and R^2 results of the developed eleven ANN's training algorithms for predicting the biomass' HHV using their proximate analysis. It was shown that the highest R and R^2 values close to 1 are given by the Levenberg-Marquardt algorithm, indicating a decent agreement between the predicted and real values. Furthermore, the LM algorithm also provides the least errors where it can be seen in Fig. 6 that its MAD, MSE, RMSE and MAPE are the lowest of all the examined training algorithms with 0.7153, 0.9786, 0.9892 and 4.1264, respectively.

Several factors may contribute to the highest performance accuracy of the Levenberg–Marquardt algorithm. One of the factors is the LM's capability to adjust the learning rate by itself. Also, the

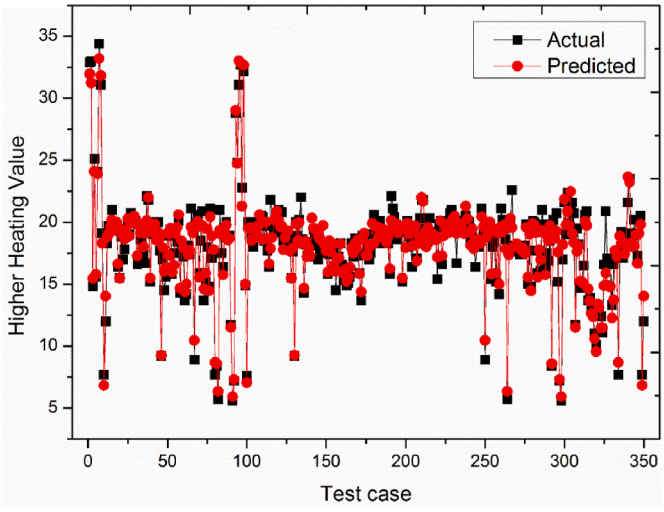

Fig. 8. Actual and predicted HHV for various test cases using ANN Levenberg-Marquardt training algorithm.

Table 1
Performance evaluation of ANN models.

ANN training algorithm	R	R^2	MAD	MSE	RMSE	MAPE
GDA	0.8976	0.8057	1.3187	3.1670	1.7796	8.2078
GDX	0.9028	0.8151	1.2914	2.8247	1.6807	7.4174
SCG	0.9417	0.8868	0.9513	1.7076	1.3067	5.8094
R	0.9446	0.8924	1.1761	2.6187	1.6183	7.0959
CGB	0.9480	0.8987	0.8927	1.5297	1.2368	5.1738
OSS	0.9482	0.8990	0.8824	1.5261	1.2353	5.2834
CGF	0.9497	0.9020	0.8737	1.4977	1.2238	5.1166
RP	0.9515	0.9053	0.8785	1.4378	1.1991	5.0920
CGP	0.9544	0.9109	0.8623	1.3396	1.1574	5.0835
BFG	0.9554	0.9127	0.8412	1.3131	1.1459	4.8755
LM	**0.9669**	**0.9350**	**0.7153**	**0.9786**	**0.9892**	**4.1264**

Levenberg–Marquardt gives a compromise between the Gauss-Newton's speed and the certain steepest descent method convergence, thus outperforming simple gradient descent and other conjugate gradient methods. Similar to the Quasi Newton techniques, the Levenberg-Marquardt approaches the speed of second order training without the necessity to calculate the matrix of Hessian. Therefore, it has the capability to accelerate the training and convergence of the algorithm. Although LM requires more memory than other algorithms, it is the fastest algorithm. Fig. 7 displays the R values of LM algorithms for four different stages.

Overall, the Levenberg–Marquardt shows the greatest performance with the highest R and R^2 values and the lowest MAD, MSE, RMSE and MAPE. This is further illustrated in Fig. 8 for 350 samples of biomass. The performance of the BFG algorithm is almost similar to that of the LM algorithm. However, it is worth noting that the computation requirement for BFG algorithm will rise geometrically with the network size as a matrix inverse equivalent need to be calculated for each iteration. It was also found that the Gradient Descent Adaptive Learning Rate (GDA) algorithm gave the worst performance accuracy where its R and R^2 are the lowest and its MAD, MSE, RMSE and MAPE are the highest of the 11 examined training algorithms in this study. GDA is a function of training which updates bias and weight values according to the gradient descent with the rate of adaptive learning. The worst prediction accuracy of GDA algorithm may be attributed to the sensitivity of the learning rate. If it was set excessively high, the algorithm would be unstable, but if it is overly small, the algorithm would be significantly longer to converge.

Table 1 summarises the six statistical parameters performance (R, R^2, MAD, MSE, RMSE and MAPE) of the eleven ANN's training algorithms to

Table 2
Performance evaluation of ANN models.

Researchers	Method	R^2	RMSE
Choi et al. [15]	Linear regression	0.0040	7.0574
Callejón-Ferre et al. [16]	Multiple/multivariate linear regression	0.0059	7.6947
Kathiravale et al. [17]	Multiple/multivariate linear regression	0.0416	10.0098
Nhuchhen and Salam [10]	Multiple/multivariate nonlinear regression	0.1935	4.4877
García et al. [18]	Nonlinear regression	0.3616	5.0950
Thipkhunthod et al. [19]	Linear regression	0.3766	4.2316
Phichai et al. [20]	Linear regression	0.3766	2.9990
Sheng and Azevedo [21]	Linear regression	0.5114	2.8574
Mohammed et al. [22]	Multiple/multivariate linear regression	0.5925	3.4597
Yin [23]	Multiple/multivariate linear regression	0.6157	2.3581
Kieseler et al. [24]	Multiple/multivariate linear regression	0.8425	3.6982
Soponpongpipat et al. [25]	Multiple/multivariate linear regression	0.8451	1.7049
Cordero et al. [26]	Multiple/multivariate linear regression	0.8470	1.6759
Parikh et al. [9]	Multiple/multivariate linear regression	0.8539	1.5843
Ghugare at al [27].	Genetic programming	0.8827	1.3058
Akkaya [28]	ANFIS-GP4	0.8780	1.3288
Akkaya [28]	ANFIS-FCM3	0.8574	1.4461
Akkaya [28]	ANFIS-SC5	0.8836	1.3006
Keybondorian et al. [5]	MLP Artificial neural network	0.9211	1.0891
Keybondorian et al. [6]	Least squares support vector machine	0.9293	1.0309
Samadi et al. [14]	Gradient boosted regression trees	0.9300	0.9460
Veza et al. (This study)	ANN-LM 3-10-1 topology	0.9350	0.9892

predict the HHV of 350 samples biomass according to their proximate analysis.

Compared to previous studies, the ANN model developed in this study provides significant improvement owing to its highest R^2 and lowest RMSE values. This indicates that the ANN-LM model with a 3-10-1 network structure model successfully predict the HHV of biomass with a decent-performance accuracy that has not yet been found in the previous studies. Keybondorian et al. in their two separate studies [5,6] also used 350 samples of biomass to estimate their HHVs using the multi layer perceptron (MLP) ANN and SVM. However, their R^2 values are slightly lower and their RMSE values are also marginally higher than the present study. The closest performance accuracy is given by Samadi et al. [14] using the gradient-boosted regression trees (GBRT) where it was reported that the fixed carbon had the most significant impact on the biomass HHV. The performance accuracy comparison of the present study with previous published works is summarised in Table 2.

4. Conclusion

The design of new systems fuelled with biomass requires fundamental knowledge of its higher heating value (HHV) due to its essential role in representing the energy output. The traditional approach to determine the heating value is difficult and expensive. In this study, an ANN model was built utilising a dataset of 350 samples of biomass. To predict the biomass' higher heating value in term of their proximate analysis (fixed carbon, volatile matter and ash content), 11 different ANN training algorithms using a 3-10-1 network structure were compared and analysed. Results revealed that the ANN trained with Levenberg-Marquardt gave the highest accuracy. This model effectively predicted the HHV with the highest R and R^2. Also, the LM algorithm gave the least errors than any of the other 11 examined algorithms with MAD, MSE, RMSE and MAPE at 0.7153, 0.9786, 0.9892 and 4.1264, respectively. Therefore, the ANN-LM model with a 3-10-1 network structure could be regarded as a promising substitute to the empirical/experimental correlations. Furthermore, comparison with previous biomass HHV prediction models proves that the developed ANN-LM gave the highest R^2 with the least RMSE. Despite its better prediction accuracy, it is recommended that further research be undertaken in investigating the optimum neuron numbers in the hidden layer. This can be done by performing numerous trial and errors. Also, network types other than feed-forward backpropagation such as the Elman and Hopfield networks are worth investigating.

Credit author statement

Ibham Veza: Conceptualization, Formal analysis, Writing – original draft, Visualization. **Irianto**: Resources, Funding acquisition, Writing-Reviewing & Editing. **Hitesh Panchal**: Investigation, Resources, Project administration. **Permana Andi Paristiawan**: Supervision, Funding acquisition. **Muhammad Idris**: Resources, Visualization. **I. M. Rizwanul Fattah**: Writing- Reviewing & Editing, Supervision. **Nicky R. Putra**: Methodology, Validation. **Rajendran Silambarasan**: Formal analysis, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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