ARTIFICIAL NEURAL NETWORK (ANN) MODELLING USING DIFFERENT ALGORITHMS FOR PREDICTING THE TOTAL PHENOLIC CONTAIN IN COCOA SHELL EXTRACT.

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ABSTRACT - *In this study, three algorithm networks, Increment Back Propagation (IBP), Batch Back Propagation (BBP), and Genetic Algorithm (GA) for ANN model were used to predict the total phenolic content from cocoa shell extract. The data were divided into two sections, 75% training set and 15% the test set. All algorithms were training, testing, and calculating its Root Mean Square Error (RMSE), Average Absolute Deviation (AAD), and Coefficient of Determination (R^2). The model result was compared and show a high correlation of coefficient (R^2 IBP 0.9997, R^2 BBP 0.9997, R^2 GA 0.9996). This showed the ANN using three different network algorithms was able to predict the total phenolic content. The ANN model with BBP shows better prediction data with a higher R^2 value and smaller RMSE (IBP 0.3131, BBP 0.0622, GA 0.3068) and ADD (IBP 1.1987, BBP 0.2989, GA 1.2048). This finding suggests that the ANN with algorithm BBP showed a better prediction and fitting ability compared to the BBP and GA.*

Key words: Artificial neural network, cocoa shell, phenolic content

INTRODUCTION

Artificial neural networks (ANN) were a type of virtual computing method based on the behavior of the biological brain system (Ghaffari et al. 2006). It can deal with complicated, complex, and incomplete problems and use mathematical modeling to quickly produce forecasts of data (Ziolkowski and Niedostatkiewicz 2019). In business and industry (manufacturing, process control, quality control, etc), artificial neural networks were commonly used to build a complex relationship between the inputs and outputs of a manufacturing or commercial process. Although some users believe that neural networks were "black boxes" with no method for clearly defining the learned input-output connections, there were several metrics of variable effect that may be used to define network activity (Zobel and Cook 2011). Due to their capacity to use learning algorithms and detect input-output correlations for complicated, nonlinear systems, artificial neural networks (ANN) were increasingly being used as prediction tools in a wide range of fields, including engineering. One of the most used neural networks was the backpropagation (BP) neural network, which was a multilayer feedforward network trained using the error inverse propagation method. The essential principle behind the BP algorithm was that the learning process involves both forward and backward propagation of signals and mistakes (Fu, Hsu, and Principe 1996). The input layer, hidden layer, and output layer were the three geometric topologies of the BP neural network. The same topologies were applied to the learning algorithm such as the Genetic algorithm (GA) and Levenberg–Marquardt (LM) backpropagation (Zhu et al. 2019).

. The objective of this study was to present a method to process control and decision-making based on a selective interpretation and combining of neural network variable influence measurement. By providing a quick review of the usage of neural network models for decision-making in extraction process control, as well as a description of their identified flaws. Next, go over the research on variable influence measures for describing the behaviour of a trained neural network model and provide recommendations on how to utilize them most effectively to aid decision-making. Finally,

this paper will demonstrate how the selected measurements may be used to improve process control in total phenolic content from Malaysian cocoa shells (MSC).

MATERIAL AND METHODS

Materials and chemicals

The dried cocoa bean was collected from Pusat Penyelidikan Dan Pembangunan Koko (PPPK), Jengka, Pahang, Malaysia. The dried bean was washed and dried with a clean towel. All the dried bean was then freeze-dried to remove moisture. Next, the Malaysian cocoa shell (MCS) was manually removed from the bean and crushed in the mechanical grinder (IKA, German) with a 1.0mm blade. The crushed MCS were stored in a desiccator for further process. Other chemicals used in this study are Folin-Ciocalteu phenol reagent (FC), sodium carbonate, gallic acid, and ethanol. All chemicals were analytical grade.

Ultrasound-assisted extraction

Each sample containing 1g of MCS was weighed and mixed with a 50mL various concentration of solvent as in table 1. The mixture was extracted by using a sonication bath machine (Wiseclean 40kHz, Korea). The sonicator was connected to the chiller and the temperature was adjusted to the desired temperature. The extraction process duration was conducted according to Table 1. The extract was filtered by using Watman filter paper number 4 to remove debris. Next, the aqueous extract was removed from its solvent by using a rotary evaporator (IKA, German) and dried by using freeze-dried (Labconco, USA) to get the crude extract. The crude extract was stored at -40 °C in the sample bottle until further analysis.

Experimental design

ANNs consist of several factors such as a number of inputs, hidden layer, output, and type of network model. It can be used to determine the best topological model for the process as in figure 1 by connecting the link between the entrance (input) to the exit signal (output) through certain layers and nodes. It is often considered as human neuron between brain and muscle (Kamairudin et al. 2015). The network was labeled as chosen algorithm-3-10-1, where the chosen algorithm was either IBP, BBP, and GA, where number 3 was the number of inputs, number 10 was the number of layers and number 1 was the number of outputs. The input for this study was an independent variable while the output was the response. Two separated data need to be considered in the ANN, the training data set, and the testing data set. The data sets were chosen randomly by the software and separating them into 70% training data, and 30% testing data. The training data was trained the network by controlling errors and weights while the testing data was simulating the process obtained from the training data (Selvan et al. 2018). The weights were calculated by the weight summation of the received data from the hidden layer in the learning process. All calculation was done by the neural power professional trial version 2.5 software. The number of hidden layers was set into default and the network algorithm was changed between IBP, BBP, and GA. To select the best network, three-factor should be observed and taken into consideration which was The value of average deviation (AAD) as in equation 1, the root of mean square (RMSE) as in equation 2, and to observe the determination of coefficient (R^2), on each algorithm. The smaller AAD and RMSE and the bigger R^2 between of these three algorithms were chosen as the best network to predict the future observation between the design range.

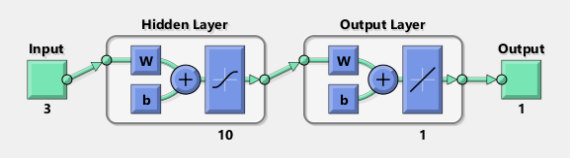

Figure 1. The illustration of topological of the developed artificial neural network (ANN) created using MATLAB.

$$AAD = \left(\frac{1}{n}\sum_{i=1}^{n}\left(\frac{R_{pred} - R_{exp}}{R_{exp}}\right)\right) \times 100 \quad (1)$$

$$RMSE = \left(\frac{1}{n}\sum_{i=1}^{n}\left(Y_{pred} - Y_{exp}\right)^2\right)^{\frac{1}{2}} \quad (2)$$

Where Y_{pred} is the predicted data obtained from ANN, Y_{exp} is the experimental data, and n is the number of the experimental run (n = 20)

Determination of total phenolic content

The total phenolic content (TPC) of the Malaysian Cocoa Shell Extract (MCSE) was determined spectrophotometrically using the Folin- Ciocalteu phenol reagent mentioned by Karim et al (2014)

Table 1. Actual and predicted values of the ANN based on the IBP, BBP and GA model of Total Phenolic Content

Run	Ethanol concentration, X_1(%)	Temperature, X_2(°C)	Ultrasound irradiation time, X_3(minutes)	TPC Experiment (mg RE/g DW)	TPC $_{IBP}$ Prediction (mg RE/g DW)	TPC $_{BBP}$ Prediction (mg RE/g DW)	TPC $_{GA}$ Prediction (mg RE/g DW)
1	70.00	45.00	60.00	31.13±0.05	31.133	31.094	31.077
2	70.00	65.00	60.00	33.42±0.33	33.401	33.418	33.354
3	80.00	38.18	45.00	19.58±0.42	19.392	19.616	19.47
4	96.82	55.00	45.00	12.85±0.16	13.459	12.933	13.238
5	70.00	65.00	30.00	33.81±0.17	33.814	33.791	33.751
6	90.00	65.00	30.00	19.58±0.07	19.683	19.611	19.732
7	80.00	55.00	45.00	22.13±0.12	21.768	21.739	21.742
8	80.00	55.00	45.00	21.78±0.08	21.768	21.752	21.742
9	80.00	55.00	70.23	20.04±0.13	20.069	20.112	20.168
10	80.00	71.82	45.00	24.94±0.13	24.977	24.955	25.054
11	90.00	45.00	60.00	15.04±0.04	14.728	15.003	14.898
12	90.00	45.00	30.00	14.44±0.08	14.187	14.397	14.235
13	80.00	55.00	19.77	20.60±0.32	20.675	20.596	20.739
14	80.00	55.00	45.00	21.12±0.21	21.768	21.774	21.742
15	90.00	65.00	60.00	18.92±0.06	18.856	18.827	18.776
16	80.00	55.00	45.00	21.19±0.21	21.768	21.758	21.742
17	70.00	45.00	30.00	27.87±0.17	27.842	27.876	27.781
18	80.00	55.00	45.00	22.89±0.19	21.768	21.74	21.742
19	80.00	55.00	45.00	21.46±0.38	21.768	21.764	21.742
20	63.18	55.00	45.00	40.09±0.07	40.095	40.148	40.371

and Azizah Othman et al (2007) with several modifications. Approximately 0.5mL of diluted samples (500ppm) was added to the 2.5mL of 10% FC reagent. The mixture was then vortex for 10 seconds. Next, added with 1.8mL of 7.5% sodium carbonate and vortex again for 10 seconds. The mixture was incubated for 60 minutes in the dark at a temperature of 40 °C. The total phenolic content was determined by absorbance at wavelength 765nm (Karim et al. 2014; Othman et al. 2007) visible spectrophotometer (Cary 60, Agilent, USA). The TPC was expressed as milligrams of gallic acid equivalent per gram of sample [(mg GAE/g DW (dry weight)]. The standard gallic acid (0-1000ug/mL) was used as a standard.

RESULTS AND DISCUSSIONS

Modeling Process

The neural network model was trained and tested using an experimental data set with the varied condition of the extract process. As input layers, the network was set to ethanol concentration, temperature, and ultrasound irradiation time. The output was set to the total phenolic content as the only node for the output layer. To establish the structure of the hidden layers, a set of topologies with default nodes (10 nodes) were used and test it with a chosen algorithm. For the test data set, model learning was used to establish the RMSE function's minimal value. The process was repeated with a different algorithm. To find the optimum topology for each algorithm, the IBP, BBP, and, GA, algorithms were all trained in the same way. From the learning repetition data values for each algorithm, the least value of the RMSE was picked and displayed as in table 2. From table 2, BBP-3-10-1 was selected preliminary as the best topology network as it shows the smallest RMSE compared to another network. The AAD of the topologies for the testing and training sets was shown in Table 2. For the test data set, BBP-3-10-1 has the lowest AAD value, compared to another algorithm. Next, the value of R^2 was studied, comparatively, for the final selection of the TPC model. To determine the R^2 value, the prediction, and the actual values of the TPC model were plotted for each algorithm as in

figure 2. IBP-3-10-1 and BBP-3-10-1 have similar R^2 values compared to the GA-3-10-1 as seen in the scatter graphs. BBP-3-10-1 was the pioneering topology with the lowest RMSE and ADD values as well as the highest R^2 value. As a result, BBP-3-10-1 was chosen as the best model for the TPC.

Table 2: The performance results of the optimized topologies of the TPC: IBP-3-10-1, BBP-3-10-1, and GA-3-10-1.

Algorithm	Learning		Testing	
	RMSE	AAD	RMSE	AAD
IBP	0.6981	1.2525	0.3131	1.1987
BBP	0.3424	0.8435	0.0622	0.2989
GA	0.3852	1.2304	0.3068	1.2048

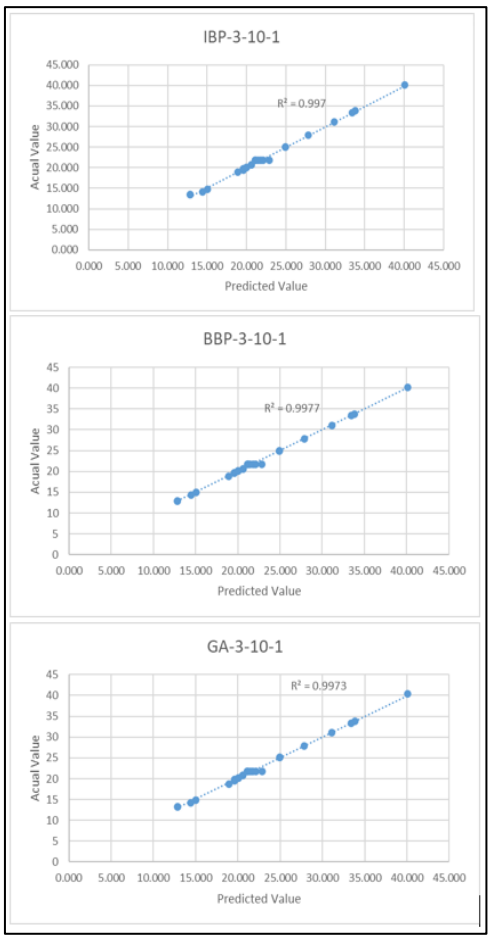

Figure 2: Plot of actual value and predicted value of different learning algorithms.

Model Vadilation.

The selected model for the extract condition of the TPC was the BBP-3-10-1 network. Table 3 was showing the optimal condition derived from the selected model by using software neural power professional trial version 2.5. The TPC value experimental was compared with the predicted value obtained from each algorithm by comparing its P-value as shown in table 4. Based on the observation, the TPC value was quite close to the value predicted by the model. The higher P-value shows the data between experimental and predicted was close to each other. Therefore, the ANN model (BBP-3-10-1) predicted more accurately compared to other learning algorithms. Hence the model validation was a success and support the data obtained for the selecting TPC model in this study.

Table 3. Optimum conditions derived by an ANN-based on BBP for TPC.

Method	Ethanol Concentration (%)	Temperature (°C)	Ultrasound Irradiation Time (minutes)
ANN-BBP	63.59	60.00	37.41

Table 4. The actual and predicted value of TPC at a different learning algorithm.

Learning Algorithm	TPC_{actual}	TPC_{pred}	p-value
IBP	39.81	40.22	0.40
BBP	39.81	39.73	0.85
GA	39.81	39.51	0.67

CONCLUSIONS

Using an ANN approach, the impacts of several extract conditions such as ethanol concentration, temperature, and ultrasound irradiation time on TPC value were studied. Using training and test data sets, several algorithms such as IBP, BBP, and GM, were evaluated to create the learning network. The learning program produced the following topologies: IBP-3-10-1, BBP-3-10-1, and GA-3-10-1. The RMSE, ADD, and R^2 values were used to select the best model among the three-model studied, and the validation model was used to support the data. The model's ability to forecast the TPC value was confirmed by the test and learning data set's through RMSE, R^2, and ADD values. The optimal values and relative relevance of the effective factors were found using ANN. Thus, the ANN model (BBP-3-10-1) could be a better alternative in data fitting to determine the TPC value in MSCE.

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REFERENCES

Fu, Li Min, Hui Huang Hsu, and Jose C. Principe. 1996. "Incremental Backpropagation Learning Networks." *IEEE Transactions on Neural Networks* **7(3)**: 757–761.

Ghaffari, A. et al. 2006. "Performance Comparison of Neural Network Training Algorithms in Modeling of Bimodal Drug Delivery." *International Journal of Pharmaceutics* **327(1–2)**: 126–138.

Kamairudin, Norsuhaili et al. 2015. "Modeling of a Natural Lipstick Formulation Using an Artificial Neural Network." *RSC Advances* **5(84)**: 68632–68638.

Karim, Azila Abdul et al. 2014. "Antioxidant Properties of Cocoa Pods and Shells." *Malaysian Cocoa Journal* **8**: 49-56

Othman, Azizah, Amin Ismail, Nawalyah Abdul Ghani, and Ilham Adenan. 2007. "Antioxidant Capacity and Phenolic Content of Cocoa Beans." *Food Chemistry* **100(4)**: 1523–1530.

Selvan, S. Sindhanai, P. Saravana Pandian, A. Subathira, and S. Saravanan. 2018. "Comparison of Response Surface Methodology (RSM) and Artificial Neural Network (ANN) in Optimization of Aegle Marmelos Oil Extraction for Biodiesel Production." *Arabian Journal for Science and Engineering* **43(11)**: 6119–6136.

Zhu, Chonghao et al. 2019. Natural Hazards *Comparison of GA - BP and PSO - BP Neural Network Models with Initial BP Model for Rainfall - Induced Landslides Risk Assessment in Regional Scale : A Case Study in Sichuan , China*. Springer Netherlands. **100**: 173-204

Ziolkowski, Patryk, and Maciej Niedostatkiewicz. 2019. "Machine Learning Techniques in Concrete Mix Design." *Materials* **12(8)**.1256

Zobel, Christopher W., and Deborah F. Cook. 2011. "Evaluation of Neural Network Variable Influence Measures for Process Control." *Engineering Applications of Artificial Intelligence* **24(5)**: 803–812.