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Ultrasound–assisted extraction optimization of phenolic compounds from *Psidium guajava* L. using artificial neural network-genetic algorithm

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Abstract.Artificial Neural Network-Genetic Algorithm (ANN-GA) was used in this work to model the extraction parameters using Ultrasound Assisted Extraction (UAE) in producing phenolic compounds of guava (*Psidium guajava* L.) leaves. The ANN-GA model was used to evaluate and predict the effect of frequency, temperature, time, and their interaction under optimum conditions. The controlled parameters were frequency (20-40 kHz), temperature (25-35 ^{0}C), and sonication time (20-40 minutes). Furthermore, the input and output parameters were modeled by LM-back propagation ANN. The optimization variable was then determined by GA. ANN trial and error method was used to determine the bias, weight, and number of hidden layer nodes. The fitness function for optimization with GA used the bias and weight which were obtained from ANN. The prediction of total phenolic on guava leaves using the ANN model showsthe mean absolute precentage error value is 13.07. Based on the experiment the optimum conditions were obtained at 40 kHz, 35^{0}C,30 minutes and resulted 589.02 ppm. While ANN-GA model obtained optimum results at 39.79 kHz, 34.83^{0}C, 20 min, then the mean absolute error optimization was 3.46.It can be concluded that ANN-GA model can be usedfor optimizing the phenolicyields of guava leaves.

1. Introduction

Nowadays, food is required to have substances that can improve both health and prevent disease[1]. The food's materials that are present in plants is phenolic compounds, a secondary metabolite in plants. Phenolics are known as antioxidants with positive effects on various diseases such as cancer, neurodegenerative or cardiovascular disease [2,3]. One of the plants that can be used as a source of drug is guava (*Psidium guajava* L.). Some research showed that guava contains phenolic compounds that can be used as antioxidants, anti-hyperglycemic, and medicine for diarrhea, dysentery. Guava leaves are also used for diabetics militus because it can inhibit amylase and glucosidase[4,5].

The method, which is used to know the content in the plant is the extraction method. However, the conventional method usually used for extraction process are masceration and soxhlet extraction. In the masceration process needs higher solvent consumption and longer extraction time which is influence the economic factor. Besides that, the length of heating time in soxhlet extraction leads to a decrease of the main function of the substance due to oxidation, ionization, and hydrolysis during the extraction process[6-8]. Therefore, we should find a technology, which does not only maintain the quality of the plants, but also the quality of the substances[1]. The physical technologies that have been used in solid and liquid material extraction processes are ultrasound assisted extraction, microwave assisted extraction, and electric field pulse.

Of these three methods, ultrasonic power is currently being used to assist the extraction. The application of ultrasonic irradiation accelerates chemical processes through acoustic cavities in materials with wave propagation through liquid[8,9]. From the food's quality side, ultrasound assisted extraction (UAE) not only can maintain the quality of foodstuffs, but also it can improve the function of food[1]. In addition, UAE is used because it has advantages such as the relatively cheap price, easy to do, environmentally friendly, reduce energy consumption, shorten the extraction time, and reduce the use of chemicals[9-11].

To improve the extraction process, we need a model which can predict the optimum value for improving efficiency of the extraction process, reducing time and operational costs. The use of prediction techniques such as artificial neural network (ANN), fuzzy inference system (FIS), genetic programming (GP), and response surface methodology (RSM) were highlighted[11]. Several studies have attempted to compare an ANN and RSM model for evaluating, predicting, modeling, and simulating extraction using UAE on phenolic substances from safranin O (SO) substances[11] and *P lenticus* L. leaves[12]. ANN has high accuracy, generalization capability for the extraction model, and able to solve non-linearityform compared with RSM. ANN optimization can be improved using Genetic Algoritm (GA). Because of the advantages, the aim of this work is to predict and optimize the extraction parameters (frequency, temperature, and sonication time) with UAE on guava leaves (*Psidium guajava* L.) to obtain phenolic compounds using the hybrid ANN-GA model.

2. Methods
Sound waves with frequencies above 20 kHz are calledultrasonic. The mechanism of UAE is the firing of ultrasonic waves on a material, propagation of the intensity of ultrasonic waves in the material resulting in cavitation phenomena[13]. Ultrasonic waves are generated by ultrasonic transducers which has adjustable frequency at 20-60 kHz and power at 120 W. The ultrasonic transducers contain piezoelectric crystals that have the ability to convert mechanical energy into electrical energy, and vice versa. When the piezoelectric crystal is given a voltage pulse then the wave oscillates from every surface of the crystal element [14]. The UAE system diagram, which we developed, consists of hardware (Figure 1) and software.

The extraction tank (15 cm diameter) is equipped by the heater (AC 220 volt) which was controlled by thermocontroller (0^0-1372^0C range for K-type thermocouple). The thermocouple (K-type) was monitored the temperature for switching the heater through relay (DC 12 volt) when the temperature suitable with set point on thermocontroller. An ATSAM3X8E microcontroller performs data acquisition from the temperature sensor (LM35, -55^0-150^0C temperature range), which is read by microcontroller ATSAM3X8E and sent directly to the computer. Data obtained from the microcontroller is displayed through the program interface computer usung a software algorithm that was developed using Delphy and Arduino. Subsequently, the temperature, time, and frequency of sonication were monitored.

The material used for extraction was fresh guava leaves (*Psidium guajava* L.) which were obtained from Temanggung, Central Java, Indonesia. Every 0.5 gram of guava leaves were blended and mixed in15 mL of ethanol (pro analysis). After that, the solvent was put in the extraction tank (15 cm diameter) for sonication. During the ultrasonic firing process, variations in frequency, temperature,and

timeof sonication were performed, respectively 20-40 kHz, 25-35 ^{0}C, and 20-40 minutes. Then, the sample of guava leaves extract was analized by spectrophotometer UV-vis (751,5 nm).
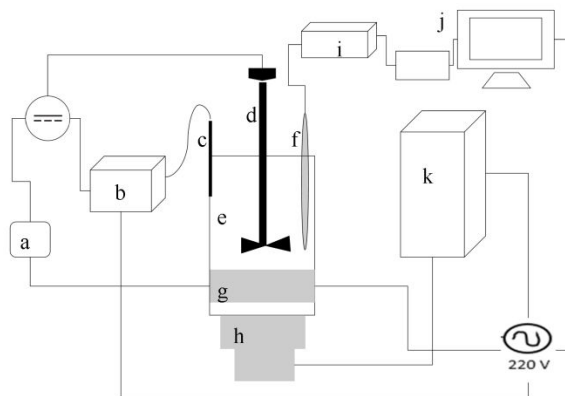
Figure 1. Experimental set up of extraction system using UAE. a: relay, b: thermocontroller, c: thermocouple, d: mixer, e: tank, f: LM35, g: heater, h: tranducers, i: microcontroller, j: mini PC, k: ultrasound power supply.

Artificial Neural Network (ANN) was used to predict nonlinear relationships between input parameters (X_1, X_2, and X_3) and output parameters (Y). The input parameters X_1, X_2, and X_3 were frequency, temperature, and timeof sonication, while the output parameter Y was the phenolic compounds. ANN has input layer, hidden layer, and output layer. The input layer used 3 nodes and the output layer used 1 node. The trial-and-error method was used to determine the bias, weight, and number of nodes whichshows the best fit with the hidden layer to model the extraction process. The schematic diagram of modelling and optimization using ANN-GA is shown in Figure 2.
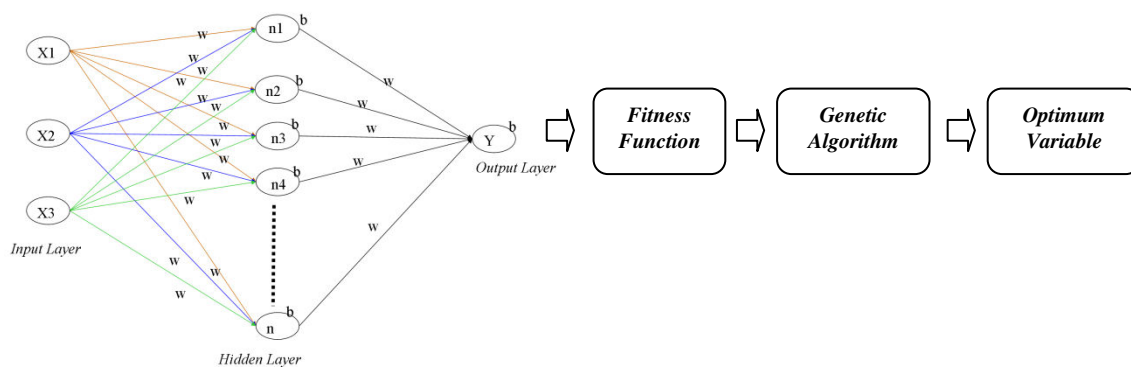
Figure 2. Schematic diagram of modeling. x: input variable, y: output variable, w: weight, b: bias, n: hidden layer nodes

MATLAB Neural Network Toolbox^{TM}and Genetic Algorithm toolbox were used as the software. ANN used the Levenberg-Marquardt algorithm which was divided into 2 parts, 80% data training and 20% data validation. The optimum value of each variable was determined by the Genetic Algorithm (GA). GA calculates the value of variable optimization based on the weight and the bias values of ANN. The flowchart of optimization using ANN-GAis shown in Figure 3.

To evaluate the fitness and prediction accuracy of the ANN-GA model, Root Mean Square Error (RMSE), Mean Absolute Precentage Error (MAPE), and Mean Absolute Error (MAE) were carried out between experimental and predicted data. The lowest value of RMSE, MAPE, and MAE, as calculated using the equation bellow (Eq. 1,2,and 3), indicated the best condition of the model.

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Y_{i,exp} - Y_{i,pred})^2} \qquad (1)$$

$$MAPE = \left(\frac{1}{N}\sum_{i=1}^{N}\left|\frac{Y_{i,pred}-Y_{i,exp}}{Y_{i,exp}}\right|\right)x100 \qquad (2)$$

$$MAE = \frac{1}{N}\sum_{i=1}^{N}\left|Y_{i,pred} - Y_{i,exp}\right| \qquad (3)$$
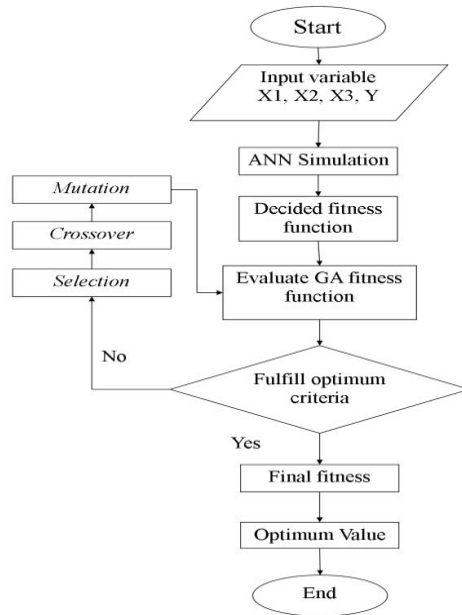
**Figure 3**. Flowchart optimization of ANN-GA and optimization using ANN-GA

3. Results and discussion

3.1 Artificial Neural Network (ANN) Model

ANN is a computational system for nonlinear multivariate modeling, which is able to estimate the response based on train data [16]. In this study, the phenolic compounds of guava leaves (*Psidium guajava* L.) has been successfully predicted using ANN through LM-backpropagation. In the ANN model, determination of the number hidden layer nodes was very important. The upper limit of the hidden layer nodes was specified by the rule:

$$N \leq \frac{N^{tr}}{N^{input}+1} \qquad (4)$$

where N^{tr} is the number of training data and N^{input} is the number of input nodes. The total data were 15 data, where 80% data were used as training data and 20% data as validation data. We used 2 hidden layer and the first hidden layer had 3 nodes. Based on the amount of training data, we then used the variation of the number of sedond hidden layer nodes as much as 1 to 3 nodes. The reason of choosing 80% data for training was the more artificial intelligence trained, it would record the relation of variables and could predict the suitable output data when the input variables were varied. The RMSE, MAPE, and MAE values were increase with the number of hidden layer nodes as shown Figure 4. The number of nodes in the hidden layer with the lowest RMSE, MAPE, and MAE was 1 nodes in epoch 4. The RMSE, MAPE, and MAE data training in 1 hidden layer node was respectively 7.91; 0.87; and 3.04. Therefore, the ANN architecture was used 1 node in the second hidden layer for validation data of ANN model.
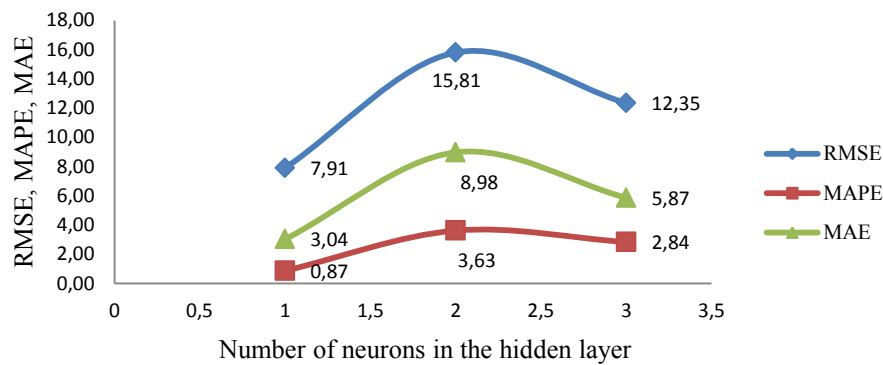
Figure 4. Heuristic determination of the optimum number of neuron of the second hidden layer

To prove the ANN model architecture, 3 data were used for validation data as shown in Figure 5. Based on statistical analysis, the mean absolute precentage error value was13.07. From these data, the ANN model could predict the phenolic compounds of guava leaves (*Psidium guajava* L.) with relatively low error value.
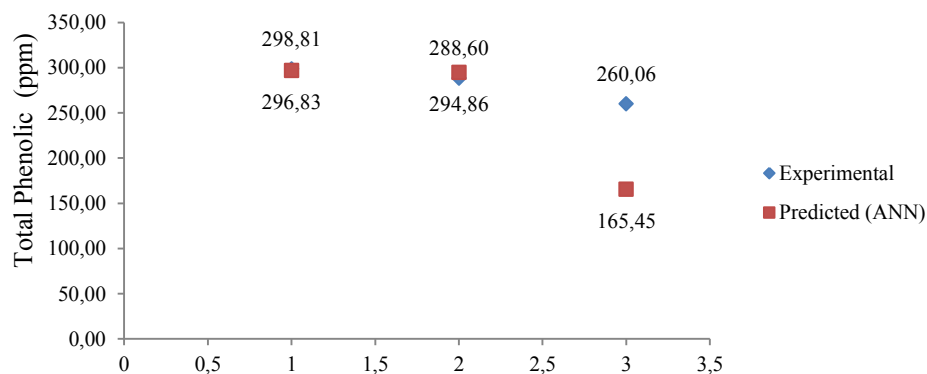
Figure 5. Comparison the phenolic compounds between experimental and predicted value using ANN

*3.2 Optimization using the hybridArtificial Neural Network-Genetic Algorihm (ANN-GA)*
After the ANN model was established, in this study, GA was used to optimize the input variables for the maximizing the total phenolic content. GA is an optimization algorithm based on the law of biological evolution [17]. The GA parameters in this study were 20 population size, 51 generations, scattered crossover, and proportional fitness scalling. The optimization process run several times to avoid local optimum. The trained ANN model, both the weights and bias, was applied as the fitness function. The weights used in this function were the weights that connected the *i*-th neuron on the input layer with the neuron on the hidden layer. While the bias was based on the bias in the neuron's hidden layer. The fitness function of GA was determined by the Eq. 5 :

$$f = 1 / \{1+\exp[((-4.7593*x)+3.2197)+((1.2357*y)+3.2197)+((0.055315*z)+3.2197)]\} \quad (5)$$

Best individual for each generation are shown in Figure 6. The 50 generations were sufficient for GA to achieve optimum accurate conditions. The optimum condition of phenolic compounds guava extraction (*Psidium guajava* L.) determined by ANN-GA result in frequency, temperature, and optimum time respectively at 39.79 kHz, 34.83^{0}C, and 20 min. Based on the experiment, the result

shows that the optimum value of phenolic was obtained at 40 kHz, 35^0C, 30 minutes and resulted 589.02 ppm of total phenolic compound. The mean absolute error optimization is 3.46 by comparing the experimental value of phenolic yield to the the values obtained by ANN-GA.

Optimization process of phenolic compounds using hybrid ANN-GA through the weight and bias which get from ANN trial and error, makes it become flexible and easy to exploit. Besides that, ANNdoes not require standard experimental design to build a model like RSM model [12]. So, ANN-GA approach is more trustable, flexible and permits to add new experimental data. It can be concluded that the data of UAE of guava leaves' phenolic compounds are reliable to model using hybrid ANN-GA.
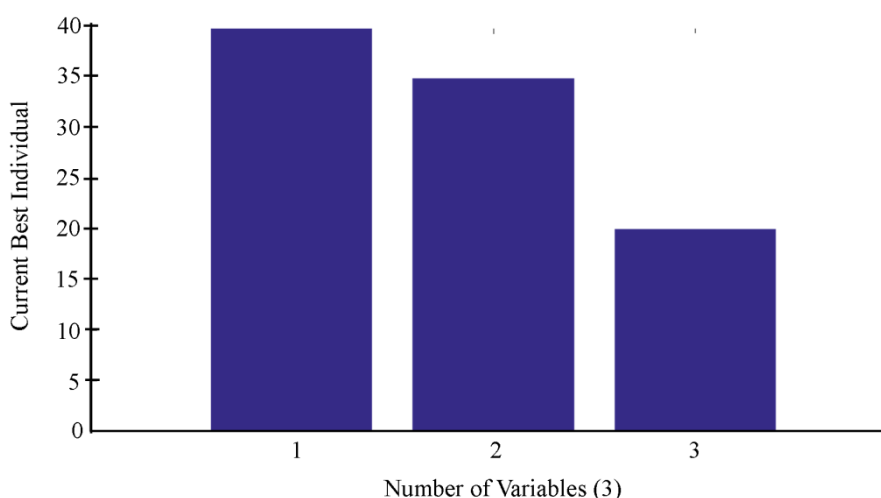
Figure 6. The best individual as optimum value from f, T, and t parameters

4. Conclusion

The prediction ofphenolic compounds on guava leaves (*Psidium guajava* L.) using ANN model, and 1hidden layer node at second hidden layershowed thethe mean absolute precentage errorvalues between experimental and predicted data was 13.07. Based on the experiment the optimum conditions were obtained at 40 kHz, 35^0C, 30 minutes and resulted 589.02 ppm. While ANN-GA model obtained optimum results at 39.79 kHz, 34.83^0C, 20 min, then the mean absolute error optimization was 3.46. So, it can be concluded that ANN-GA model can be usedfor optimizing the phenolicyields of guava leaves.

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