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Artificial Neural Network in the Development of Halal Cosmetic Formulation Containing Okara

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Abstract

The development of halal cosmetic formulations presents a challenge to obtain optimised formulations with desirable qualities as it involves many ingredients. The advancement of cosmetic technologies employs multivariate statistical techniques such as artificial neural networks (ANN) to optimise cosmetic formulation, which aims to overcome the shortcomings of traditional formulation methods, which are laborious and cumbersome. Okara is a by-product of the production of soy-based products. Okara has been found to have numerous benefits for many industries and has been discovered as a promising halal cosmetic ingredient. Okara is a plant-derived ingredient; it can be incorporated as a cosmetic ingredient if essential aspects of production are addressed, such as using permissible substances, manufacturing, storage, packaging, and delivery following Shariah requirements. This study aims to develop an optimised halal cosmetic soap formulation containing okara using ANN to achieve the desired hardness of the soap. The influential input variables were the main compositions of the okara soap formulations, containing different fatty acids and oils, and okara through a saponification process. In contrast, the hardness (N) of the soap was the response used as the output. Five different algorithms trained ANN. Generic Algorithm (GA) 6-09-1 was selected as the final optimum model to optimise the halal cosmetic soap formulation. GA modelling was further validated, and the experimentally obtained actual hardness (N) value was close to the predicted value. In conclusion, they were optimised formulating using ANN to produce a soap with desirable properties better than those of commercial ones.

***Keywords**: Artificial Neural Network, Cosmetic, Halal, Okara*

Introduction

Concerns regarding animal-derived substances in cosmetic goods, such as gelatine, collagen, lard, and tallow, are driving demand, particularly among Muslim customers. With increased awareness of cosmetics, Muslim customers are seeking cosmetic products that are ecologically friendly but also halal and safe for consumers. As a result, finding substitutes for those critical elements is essential. According to Malaysia Standard for Cosmetics-MS2634:2019 Halal Cosmetics-General Requirement, halal cosmetics refer to cosmetic products that contain ingredients permitted under Shariah law and fatwa and fulfil the

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following conditions: they must not contain substances derived from pigs, carrion, blood, or human body parts, predatory animals, reptiles, or insects, among other things. In addition, hygiene and sanitation must always be preserved during the preparation, processing, manufacturing, storage, and transportation of halal cosmetic products. The goals of halal cosmetic product certification are analogous to the goals of other quality assurance systems such as Good Manufacturing Practice (GMP), Good Hygiene Practice (GHP), and Halal Risk Management Plan (HRMP), where in halal certification itself, 30% of products must meet the Sharia requirements and 70% must meet the requirements of the quality assurance system (Nordin et al., 2021; Sugibayashi et al., 2019).

Formulating cosmetic cleansing products such as soap, shampoo, and detergent takes work. Formulating requires a skilful combination of permitted ingredient selections and scientific thought to produce good quality cosmetic formulations. However, the most challenging part of the formulation is attributed to the fact that overall stability, physicochemical properties, rheological properties, consumer requirements, and standards sometimes take work to meet. Concerning that, it is undeniable that the usage of animal-based fats contributes to the excellent quality of personal care products such as soap. However, to be deemed halal, cosmetic materials originating from acceptable animals must be slaughtered following Islamic law, and cosmetic constituents originating from prohibited animals must be avoided. Plant-based fats and oil can be alternative and substitute for those animal-based ingredients. Recently, a study revealed that okara oil has a high level of functional lipids, can be used as a new source of essential oil, and is suitable for cosmetic applications. Okara showed high potency as a functional cosmetic ingredient, mainly to improve skin conditions, skin whitening agent and exhibited sun protective effect against UV rays (Borhan, 2021)

At the moment, developments of halal cosmetic formulations are often carried out by a trial-and-error method with one variable at a time, which is time-consuming, laborious and sometimes misleading (Masoumi et al., 2011). This problem can be overcome using optimisation techniques such as experimental design and mathematical modelling. In addition, mathematical modelling does not solely minimise the number of experiments but provides a better understanding of the effect of different variables on the response (Abd Gani et al., 2018). Artificial neural network (ANN) has lately emerged as one of the most prominent methodologies for empirical modelling and prediction in bioprocess, chemical, pharmaceutical, and cosmetic formulation (Yang et al.,2019; Simões et al.,2020;Rodriguez-Granrose et al.,2021; Pomeroy et al.,2022).

In the present study, ANN was used to predict the influence of individual factors, such as the different compositions of oil or fatty acids and their interactive effects, and to obtain an optimal formulation with desirable physical characteristics, especially regarding the hardness of soap. Halal cosmetic products must have halalan-toyyiban and be economically attractive and physically stable along the supply chain to avoid product damage and changing appearance during storage, owing to melting at high temperatures before it reaches the consumer.

Methodology

Plant material

Okara was prepared and extracted using as described by Borhan et al. (2014) & Borhan (2021).

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Soap containing okara

Soap samples were prepared according to ingredients formulated from the design matrix. The okara soap was formulated using a mixture of oils and fatty acids (olive oil, palm oil, castor oil, cocoa butter, and virgin coconut oil) and okara oil (superfatted) with additional ingredients for the saponification process. The fats and oils were weighed and transferred into a 500 mL beaker and heated at 82°C with continuous stirring, using an overhead stirrer (IKA® RW 20 Digital, Nara, Japan). The temperature of the soap mixture was not allowed to exceed 82°C or to fall below 71°C. The saponification reaction was initiated by adding half of the NaOH, and the other half was added after 5 min, along with EDTA. The mixture was stirred until it turned into a pudding-like consistency, indicating the saponification process's completion. Next, the temperature of the mixture was cooled to 65–60°C, and no other ingredients were added; the temperature was then further cooled to 40°C, at which point the okara was added to the mixture. Then, 50 g of the soap paste was moulded using a wooden mould and allowed to cool in a refrigerator (to 4°C) overnight before de-moulding. The finished, moulded soap samples were each cut to dimensions of 7.5 cm wide, 4.0 cm long, and 1.0 cm high. The finished soap samples were air-dried on the plastic trays and conditioned at ambient temperature (25±2°C) for three weeks before they were analysed. The hardness of the okara soap was measured using a TA HD-plus texture analyser (Stable Micro System Ltd., Surrey, UK) with a cell load of 500 N and using needle geometry. The probe used was a stainless-steel P/2:2 diameter needle cylinder. The hardness was reported as the maximum penetrating force (N) required for the needle to penetrate through a sample (70.5 mm × 40 mm, depth 10 mm) at 25°C, over a distance of 8 mm at a constant speed of 10 mm/s.

Experimental design

In modelling the okara soap formulation, NeuralPower version 2.5 (CPC-X Software) was employed. To design the experiments, the blend of oils (X1–X4), fatty acid (X5), and (okara, X6) were selected as the influential independent variables or inputs. In contrast, the hardness (N) of the soap was chosen as the dependent variable (output). The variables and their levels are listed in Table 1. The design and all experimental procedures were performed in the laboratory to obtain actual responses. The actual experimental values were then used for ANN modelling. The designated data were divided into two different sets, namely, the training and test data, as shown in Table 2. A total of 25 experiments containing training and testing data were used to compute and ensure the effectiveness and robustness of the selected network parameters. Training data were established through experimental data using experimental run design by Design of Experiments software. Training data were trained using a different algorithm. A total of 6 runs were set as testing data.

Table 1: Summary of causal factor variables for ANN

	Causal factor variables	Coded level of variables (%)	
		Low	High
X_1	Virgin coconut oil	24.00	28.00
X_2	Olive oil	15.00	20.00
X_3	Palm oil	6.00	10.00
X_4	Castor oil	15.00	20.00
X_5	Cocoa butter	6.00	10.00
X_6	Okara	2.00	7.00

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Table 2. The actual and predicted value of the ANN is based on the GA model of Okara soap formulation.

Run No.	X_1	X_2	X_3	X_4	X_5	X_6	Hardness (N)	
							Actual	**Predicted**
Training Set								
1	28.00	20.00	9.99	19.16	6.00	4.25	506.2	526.0
2	27.98	20.00	6.00	20.00	8.29	5.13	507.5	491.08
3	28.00	20.00	9.99	19.16	6.00	4.25	504.0	526.0
4	27.18	19.45	9.02	19.78	9.97	2.00	469.4	446.46
5	27.18	19.45	9.02	19.78	9.97	2.00	418.1	446.46
6	24.02	20.00	9.90	16.49	10.00	7.00	523.6	549.05
7	28.00	20.00	6.06	18.49	7.85	7.00	494.0	511.37
8	26.54	19.99	10.00	16.24	7.63	7.00	593.1	555.71
9	28.00	20.00	10.00	15.65	10.00	3.76	544.1	535.98
10	28.00	20.00	8.29	16.77	8.39	5.95	563.6	536.36
11	25.07	20.00	10.00	18.17	8.88	5.28	530.2	537.27
12	28.00	20.00	6.43	15.98	10.00	7.00	510.2	521.36
13	28.00	19.79	7.21	18.07	10.00	4.33	497.8	483.12
14	24.82	18.87	6.71	20.00	10.00	7.00	402.3	368.71
15	24.02	20.00	9.90	16.49	10.00	7.00	573.4	549.05
16	27.17	17.91	10.00	17.89	9.06	5.37	258.7	250.87
17	27.03	18.54	8.19	20.00	9.07	4.58	326.7	321.25
18	28.00	17.69	6.54	18.96	10.00	6.21	239.8	201.59
19	26.35	18.45	10.00	19.57	6.06	6.96	305.2	283.95
Test Set								
1	26.70	17.30	9.50	19.30	9.40	5.20	190.83	190.83
2	25.90	18.80	8.50	19.30	8.50	6.40	368.2	368.2
3	25.70	19.30	7.90	18.50	9.70	6.30	444.46	444.46
4	24.80	19.30	9.40	18.80	8.10	7.00	441.34	441.34
5	27.60	17.00	7.80	18.70	9.50	6.80	152.45	152.45
6	27.50	19.30	9.30	15.00	9.80	6.50	473.42	473.42

Artificial neural network (ANN) modelling

ANN is an inter-discipline between biology and computer science that simulates the microstructure of a biological neuron system. ANN is also one of the computational systems that mimic the learning process of a natural brain, which operates and applies knowledge from given examples to resolve a given problem (Hasson et al., 2020). It operates like water, which follows the flow irrespective of shape or depth; it only cares about the input and output data to run the system.

ANN systems consist of a myriad of neurons in different layers, in which each unit performs a basic information process. ANN systems recognise simple artificial neurons as nodes. Each unit of nodes is interconnected by weight values, which aid explicitly and express knowledge. Every input is then multiplied by a connection bridge of weight and summed. The presented values are then passed through the transfer function to generate a result, and finally, an output is gained.

In summary, the generated data from another design utilised as the input data is transmitted through the network system layer by layer, and a set of outputs is

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gained. Figure 1 vividly explains the artificial neuron architecture. The multilayer feed-forward (MLFF) network is the most used network, which generally consists of three or more layers for the architecture: an input, an output, and at least one hidden layer (Huang, 2021). The layers include a first layer of input data (x_n), which transmits the data through the weights to the nodes of the second layer (hidden layer, w_n) and then to the third layer (y, output). Figure 2 clearly illustrates the schematic diagram of an MLFF network. The perceptron of the multilayer consists of multiple layers of computational units, which are primarily interconnected in an indirect way, such as in a feed-forward neural network. The hidden layer of the feed-forward neural network can be more than one layer, but one single layer is frequently and commonly suggested.

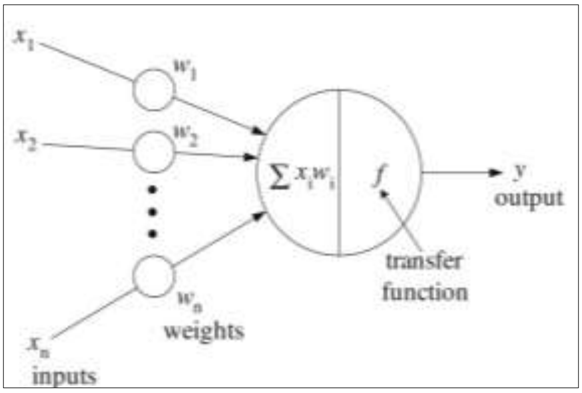

Figure 1: An Artificial neuron model

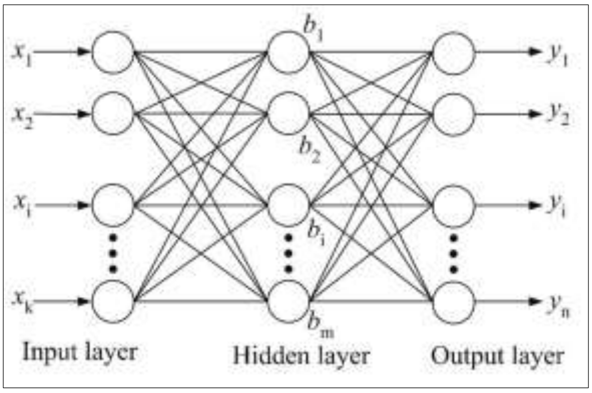

Figure 2: Schematic diagram of a multilayer feed-forward neural network

Learning process

In the learning process, the number of hidden nodes is calculated and obtained by a trial-and-error method by changing the node's value, which can be from 1 to n nodes, to disclose the architecture of the minimum RMSE value. After obtaining the output of the hidden nodes, it undergoes a similar or other transformation algorithms. In other words, learning an ANN is a process or procedure of modifying the weights (Bernasconi, 1990). In the present study, the ANN was trained by five different algorithm programs, which included Levenberg–Marquardt (LM), batch back-propagation (BBP), quick propagation (QP), incremental back-propagation (IBP), and the generic algorithm (GA), using multilayer feed-forward as the connection types. In the learning process, the input layer acts as a distributor for the hidden layer, and the inputs and output of the hidden layer are multiplied by the weighted summation as follows:

$$\mathrm{S} = \sum_{i=1}^{n}(b - W_i I_i) \quad (1)$$

Where S is the summation, b is a bias, I_i is the i^{th} input to the hidden neuron, and W_i is the weight associated with I_i. The bias shifts the space of the nonlinear properties. Thus, this makes the outputs of the hidden layer act as inputs to the final layer (output), which undergoes a transfer function. The most common and popular transfer function is the logarithmic sigmoid for both hidden and output layers, which are bounded from 0 to 1. The bounded sigmoid area is used to standardise and regularise the input and output data that is provided by software scaling. The scaled data are passed into the first layer and propagated to the hidden

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layer before finally meeting the output layer of the network by an utterance procedure. The utterance or iteration is repeating a process to approach a desired result. Therefore, the iteration results are used as a starting point for the subsequent iteration. For example, when the results of the last iteration become almost equal to those of the previous iteration, the process will be terminated. It can be done step-by-step or automatically. The iteration process is maintained by a self-similarity method as follows:

$$S(B) = \sum_{I=1}^{m} [y_{\mathrm{i}} - f(x_i\beta)^2] \quad (2)$$

Where m is an actual empirical data pair of independent and dependent variables such as x_i, x_i, and $f\ (x_i, \beta)$ is the model curve. In a self-similarity process, the β parameter of $f\ (x_i, \beta)$ is optimised by minimising the sum of the squares. As a result, the main aim of the learning process is to find the weights to minimise the root mean square error (RMSE), which is obtained from the total value through the subtraction of the actual responses and network predictions as follows:

$$\mathrm{RMSE} = \left(\frac{1}{n}\sum_{i=1}^{n}(y_i - y_{di})^2\right)^{1/2} \quad (3)$$

Where n is the number of points, y_i is the predicted value, and y_{di} is the actual value. To avoid random correlation, owing to the random initialisation of the weights, the examination of each node is repeated several times. During the repeated examinations, the architecture with the lowest RMSE is selected for each node. Then, the architectures' RMSE values are compared to find the best topology for the particular algorithm. The topology is the architecture with minimum relative RMSE. For more certainty, R^2 [see Equation (4)] and average absolute percentage deviation (AAD) values [see Equation (5) are calculated from the performance of the topology in the training and testing data sets:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - y_{di})^2}{\sum_{i=1}^{n}(y_{di} - y_m)^2} \quad (4)$$

$$\mathrm{AAD} = \left(\frac{1}{n}\sum_{i=1}^{n}\frac{|y_i - y_{di}|}{y_{di}}\right) \times 100 \quad (5)$$

Where n is the number of points, y_i is the predicted value, y_{di} is the actual value, and y_m is the average of the actual values. The learning process is carried out for different algorithms to obtain the best topology. Then, the topologies' RMSE, AAD, and R^2 are compared to find the optimised topology, which is selected as a provisional model for the process. Finally, the model is evaluated by the validation data set. After that, it is used for navigation of the process that determines the optimum and importance of the input variables to maximise the yield.

Genetic algorithm (GA)

The GA is a hypothetical global search that stimulates natural biological evolution based on the theory of genetics. In addition to GA are also parallel, efficient, and global randomised searching algorithms in handling amalgamation optimisation problems (Venkateshwar, 2022). According to the theory of GA, there are plausible ways to solve the field of a problem that is considered to be an individual or a chromosome of the colony, and all the individuals are then coded to be a sequence of characters or a symbol string.

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By imitating the evolutionary processes of organisms, such as natural selection and elimination, a colony is iteratively selected, inter-crossed between each other, and mutated. Based on the evolutionary rules of "survival of the fittest" and "elimination of the incompetent or least fit", as well as the adaptive estimation of every individual, an increasingly better colony is gradually evolved (Ramezanpour & Farajpour,2022). At the same time, the best adaptive individuals in the optimised colony are also searched for by global and parallel methods. As the processed objects of GA are individual genes coded with parameter strings, GA can directly and precisely operate the structures of these objects. In particular, as GA simultaneously evaluates multiple ways in the search space, it has a strong ability for global searching and can easily be parallelised. For example, the input data of hidden nodes were calculated by weighted summation Eq. (1). Then, the output data of the hidden layer were transferred to the output layer (hardness) using a log-sigmoid function Eq. (6).

$$f(x) = \frac{1}{1+\exp(-x)} \qquad (6)$$

Where *f(x)* is the hidden output neuron. As a result, GA-6-09-1 was utilised to determine the optimum and importance values of the input variables of the soybean-waste-based bar-soap formulation in order to achieve the desired hardness.

Results and Discussion

Modelling process

The okara soap formulation optimisation network contains input, hidden, and output layers, each of which consists of one or more nodes. For this experiment, there are six essential nodes, virgin coconut oil, olive oil, castor oil, palm oil, cocoa butter, and okara, in the input layer, whereas the hardness of soap was the only node in the output layer; the number of influential variables determined these. The hidden layer was obtained by modelling.

The structure of the hidden layer was obtained by scrutinising a series of topologies containing 15 architectures that contained varying numbers (1–15) of nodes for each algorithm. Five algorithms were examined for the construction of the hidden layer: LM, BBP, QP, IBP, and GA. To avoid random correlations, owing to the random initialisation of weight, the examination process was repeated ten times for each node by testing the data set, and the RMSE reading was recorded. The training was carried out identically for all algorithms to generate the optimised topology for each algorithm. Among the ten repetitions for the learning data, the smallest RMSE was selected for each algorithm. Figure 3 plots the value of the RMSE versus the node number for LM, IBP, BBP, QP, and GA. As shown, one node of 15 topologies for each algorithm presented the smallest RMSE, which was selected as the best topology for comparison purposes. The selected topologies were 6-09-1, 6-12-1, 6-05-1, 6-15-1, and 6-15-1 for GA, BBP, QP, IBP, and LM algorithms. Figure 3 shows the topology of GA-6-09-1, where 6 indicates the input number, 9 (node number) and 1 (output), which presented the lowest RMSE among other topologies. It was selected as the provisional and temporary model for the okara-based formulation optimisation. However, the results of the topologies as

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temporary models were compared for

greater certainty.

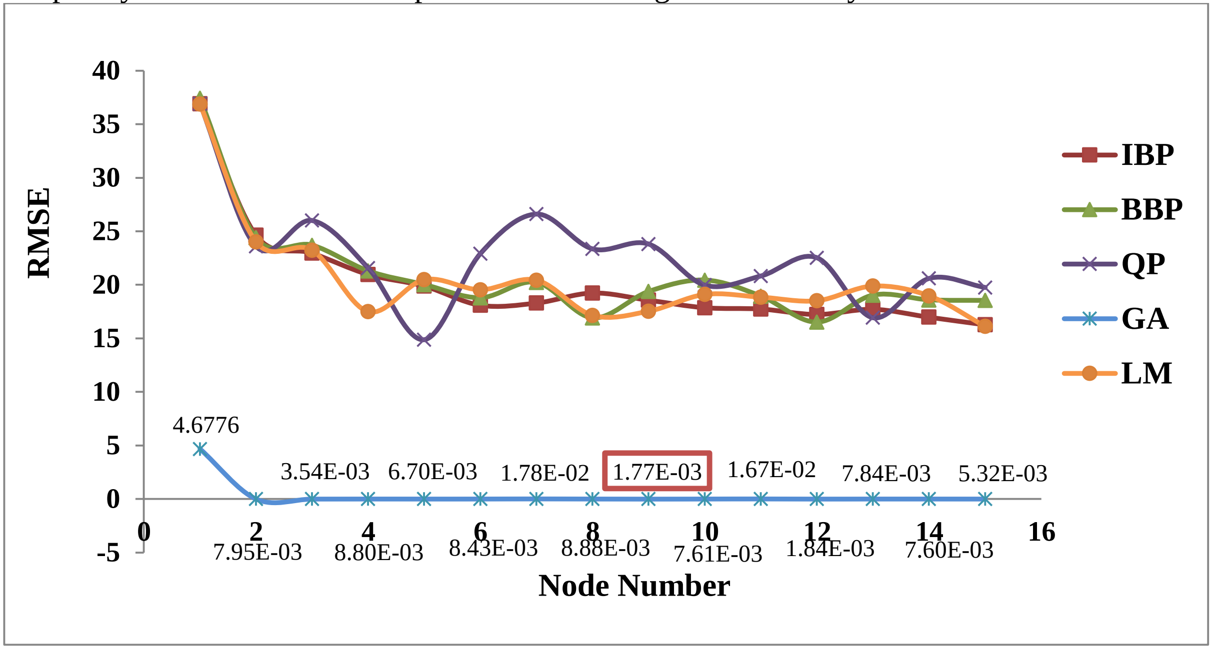

Figure 3. The network performance at different hidden nodes using five algorithms (IBP, BBP, QP, GA, and LM).

Model selection

To select the final model for the optimised okara soap formulation, the RMSE, AAD, and R^2 values were studied and compared for GA-6-09-1, BBP-6-12-1, and QP-6-05-1, respectively IBP-6-15-1, and LM-6-15-1. To calculate R^2, the predicted topologies and the actual values of the hardness were plotted for training the data set, as shown in Figure 5. As can be observed, GA-6-09-1 also shows the lowest AAD value. As a result, GA-6-09-1 pioneered with minimum RMSE and AAD values and the maximum R^2 value among the topologies of all five algorithm testing and training data sets. Therefore, after statistically comparing the topologies and considering all aspects, GA-6-09-1 was selected as the optimum model for optimising okara soap formulation.

Model validation

The GA -6-09-1 network

Figure 4 shows the GA-6-09-1 network as the final model for the formulation mixture, which consists of input, hidden, and output layers. The input layer, with six nodes (virgin coconut oil, olive oil, castor oil, palm oil, cocoa butter, and okara, is the distributor for the hidden layer, with nine nodes that were determined by the learning process. As a result, GA-6-09-1 was utilised to determine the optimum and importance values of the okara bar soap formulation's input variables to achieve the desired hardness.

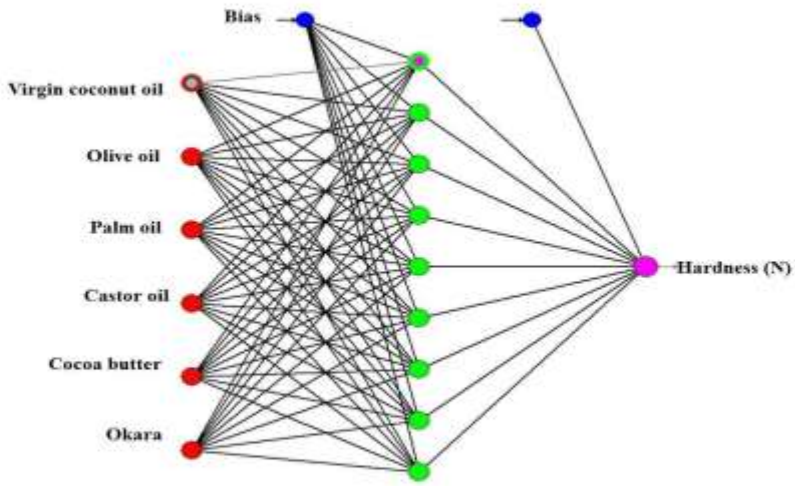

Figure 4. Schematic representation of a multilayer perceptron feed-forward network of ANN based on GA consisting of 6 inputs, one hidden layer with 9 nodes and 1 node in the output layer as the response.

The navigation of blended ingredients

The optimised topologies for different learning algorithms were determined by training and testing data set in the modelling process. The comparison was carried out to explain the best relative topology with optimum R^2, RMSE and AAD values which were selected as the provisional model for more evaluation. The adequacy of the chosen model (GA - 6-09-1) was further determined by testing the data set. As a result of the process, the network of GA -6-09-1 was selected to navigate the blended solution. The navigation contained graphical optimisation of the influential variables and analysed the importance of each variable. The predicted optimum importance of virgin coconut oil, olive oil, palm oil, castor oil, cocoa butter, and okara, used in the experiment to determine the actual hardness (556.347 N), is shown in Table 3. The actual hardness value (N) was quite close to the value of the predicted model.

Table 3. Optimum conditions derived by ANN based on GA model Okara soap formulation

Method	**Independent Variables**						**Hardness** (N)		
	Virgin coconut oil	Olive oil	Palm oil	Castor oil	Cocoa butter	Okara	**Actual Value**	**Predicted Value**	**RMSE (%)**
ANN-GA	26.537	19.999	9.998	16.241	7.633	7.000	556.347	553.30	0.5639

Importance of the Effective Variables

The model determined the relative importance of the influential variables in the optimum levels, as presented in Figure 5. As demonstrated, the most significant importance belonged to olive oil (27.89%), followed by cocoa butter (19.1%). However, the effects of other variables such as palm oil (16.58 %), castor oil (14.4%), okara (12.44%) and virgin coconut oil (9.54 %) were also crucial for

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the hardness of the soap. As a result, the selected variables were influential, and all were addressed in this formulation.

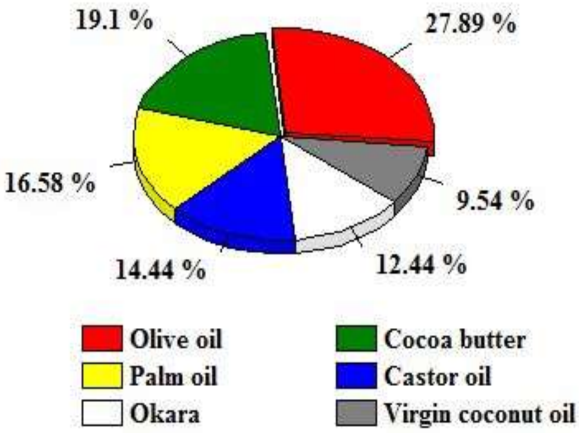

Figure 6. The relative influence of the main compositions of okara soap containing different fatty acids and oils

Conclusion

The compositions of the soap formulation, including olive oil, cocoa butter, palm oil, castor oil, okara, and virgin coconut oil as influential independent variables, were modelled with different configurations by an ANN to define the desired hardness of the soap. Five different algorithms, namely, GA, BBP, QP, IBP, and LM, were utilised and learned using testing and training data sets to gain the qualified network. The results of the ANN learning program were five topologies: GA-6-09-1, BBP-6-12-1, QP-6-05-1, IBP-6-15-1, and LM-6-15-1. RMSE, R2, and AAD optimised the performance of the topologies. The GA-6-09-1 topology, with the minimum RMSE and AAD and the highest R^2 value, was chosen as a temporary, or provisional, network of the soap formulation for the testing set. The importance of the variables followed the order of olive oil (27.89%), cocoa butter (19.1%), palm oil (16.58 %), castor oil (14.4%), okara (12.44%), and virgin coconut oil (9.54%). This shows that all of the variables could be addressed in this work. The predicted optimum points were olive oil (19.999%) followed by cocoa butter (7.633%), palm oil (9.998%), castor oil (16.241%), okara (7.000%), and virgin coconut oil (26.537%), which performed experimentally to obtain actual hardness (553.30 N). The RMSE data obtained from the ANN-GA shows R^2=1.000 which is the highest in comparison with other algorithms. In future work, testing data should be added to provide higher predictability in optimising the okara soap formulation. The ANN is a powerful and efficient quantitative tool that can model the influential input variables to predict the desired hardness of okara soap.

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