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Optimization of Neural Network using Nelder Mead in Breast Cancer Classification

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Abstract: Classification is one of the data mining techniques which considered as supervised learning. Classification technique such as Backpropagation Neural Network (BPNN) has been utilized in several fields to increase human productivity. BPNN can give better results (more natural) compared with other statistical techniques. However, the learning process of BPNN could give an inefficient synapse weight of each hidden layer. This ineffective weight can affect the performance of the network. In this research, BPNN optimization using Nelder Mead to identifying the appearance of breast cancer is proposed. The datasets used are Breast Cancer Coimbra Dataset (BCCD), and Wisconsin Breast Cancer Dataset (WBCD). The testing result using accuracy and k-fold validation presents better performance compared with the original BPNN. Best average performance can be seen in the fifth fold of BCCD with 76.5217% of accuracy. Moreover, the highest average result of WBCD presented in the fourth fold with 91.1765% of average accuracy.

Keywords: BPNN, Breast cancer, Classification, Nelder mead, Optimization.

1. Introduction

Classification is one of the supervised learning methods that can be used to determine the class of data based on the characteristics of the previous data [1]. By utilizing the development of information technology, the process of implementing classification methods can simplify human activities. The implementation of classification methods such as the maturity classification of tomatoes [2], classification of textual information [3], fingerprint classification [4] has been proposed to help increase human productivity. Moreover, classification techniques also can be used for medical purposes, such as cancer identification.

Breast cancer is one common cancer type that appears in the human body, especially the female body. This type of cancer is threatening human life because of the invasive, and among other cancer types, breast cancer has a high mortality rate in women. In 2018, there are estimated 2.088,849 or 11.6% of new cases of breast cancer have appeared in Indonesia. About 626,679 cases or 6.6% were predicted to end up in mortality caused by this disease [5]. Moreover, the high mortality rate in Indonesia is caused by 60% to 70% of patients who were identified with advanced-stage breast cancer.

Therefore, early detection of breast cancer can help in determining the right treatment for the patient and also decreasing the possibility of patient mortality level. Many researchers have been researched breast cancer classification through several types of data such as image [6] and laboratory test results [7, 8].

In research proposed by Mohammed et al. [6] implemented multi-fractal dimensional features as an extraction feature of ultrasound breast cancer images, and use Artificial Neural Network (ANN) as its classifier. From the test results, it generated a precision value of 82.04%, then a sensitivity value of 79.3991%, and a specificity value of 84.7559%.

Other research conducted by [7] tried to combining age, BMI, glucose, and Resistin as features to predict the breast cancer appearance.

These features were classified using Logistic Regression, Random Forest, and Support Vector Machine (SVM) to observe the performance of each method. The result of the study shows that SVM can give better performance compared to other methods with the sensitivity range between 82% and 88%, then the specificity range between 85% and 90%, moreover the confidence percentage reaches 95%. Moreover, Silva Araújo et al. [8] reconstruct the previous method, which used age, BMI, glucose, and Resistin as the predictor with Pruning Fuzzy Neural Network. The result of the proposed method denoted that Fuzzy Neural Network gives the best overall result.

The use of ANN as a classification method, especially in the study related to breast cancer classification, is because of its capability in providing better (more non-linear) and general alternative function when compared to the other statistical approaches [9]. One of the ANN training models that are easy in computational and often used is back-propagation. This technique utilizes the reverse propagation process in determining the weights used in each node on ANN. Bhattacherjee et al. [10] proposed the use of BPNN in classifying breast cancer datasets compiled from the Wisconsin Breast Cancer Dataset (WBCD). From the testing result, BPNN can achieve 99.27% of accuracy in detecting breast cancer based on nine predictors.

However, the implementation of back-propagation has a weakness where the resulting model can experience overfitting. Overfitting is a condition where the accuracy results of the training process get significant values. However, when the trained model is tested on data testing, it will produce a lower accuracy result [11]. To prevent this condition, many researchers tried to apply the optimization method into ANN. Hassan et al. [12] proposed the use of the Nelder Mead algorithm to optimize the Radial Basis Function (RBF) neural network. NM is used to optimize the parameters of the activation function in the design of the RBF. The advantage of using NM in this research is the fact that NM provides a simple and effective approach in numerical based optimization of scalar variables. From these studies, it was found that NM can reduce the error value of MSE from several problems in the engineering field.

Therefore, this research proposes the used of Nelder Mead to optimize the Backpropagation Neural Network (NM-BPNN), especially in classifying the appearance of breast cancer. Nelder Mead algorithm is used as a training function on the neural network's weights at each synapse in BPNN. The use of Nelder Mead in this research is expected to be able to reduce or prevent over-fitting during the training process of the Neural Network as well as increasing the performance in predicting the appearance of breast cancer. This research will use two public datasets, which are Breast Cancer Coimbra Dataset (BCCD) and Wisconsin Breast Cancer Dataset (WBCD), to compare the robustness of NM-BPNN in classifying breast cancer based on different variables.

Besides, this study will also perform the K-fold validation and confusion matrix in both datasets to evaluate the performance of the proposed method and compare the evaluation result with several classification methods in predicting breast cancer.

2. Literature review

2.1 Backpropagation neural network

ANN is computational systems inspired by the knowledge of biological nerve cells in the human body. The artificial neural network is portrayed as human nerve cells that always try to stimulate the learning process of every sense in the body. Artificial neural networks can be described as mathematical and computational models for non-linear approximation functions, classification or cluster data and non-parametric regression or a simulation of a biological neural network collection models.

ANN can be defined as a collection of several neurons. Each neuron has an internal state called the activation level or activity level, which is described as an input function. Typically, a neuron sends its activities to several other neurons as a signal. Therefore, ANN also can be called as multilayer Perceptron.

Back-propagation is one of the training methods in an Artificial Neural Network (ANN). This method proposed by Rumelhart in 1985 [13]. The objective function of this method is to train the weight of each perceptron by calculating the gradient and tried to propagate the temporary result to generates a new solution from the neural network structure. Like most of the multilayer perceptron, the topology of back-propagation also consisted of three-part, which are the input layer, hidden layer, and output layer [14]. The structure of the Backpropagation Neural Network with three hidden layers can be seen in Fig.1 below [15].

To calculate the activation function can be used Eq. (1) [16].

$$y = f(x) = \frac{1}{1+e^{-\sigma x}} \tag{1}$$

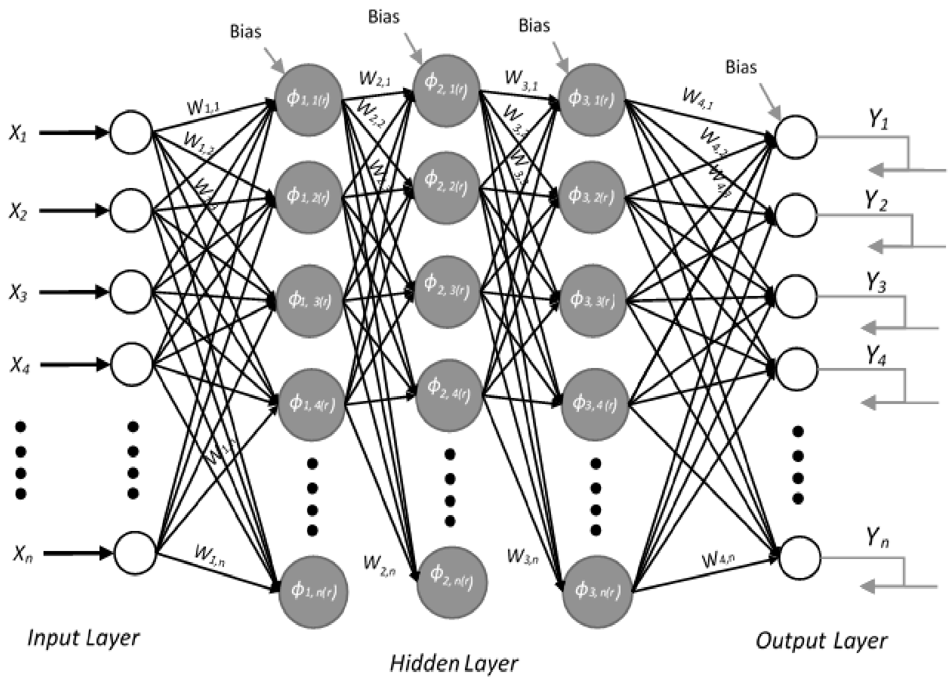

Figure. 1 The structure of backpropagation neural network with three hidden layers

In the Eq. (1) show an activation function called Sigmoid activation. *y* or (*f(x)*) is the function result, and *x* is the value from the input layer. The characteristics that the activation functions must have are continuous, differentiable, and not monotonically decreasing [17].

2.2 Nelder mead optimization

Nelder Mead (NM) is one of the heuristic optimization methods proposed by Nelder and Mead in 1965 [18]. This method is a non-derivative optimization method that is usually used to deal with non-linear and multi-dimensional problems [19]. This method is useful for finding extreme values of a function that has many variables, especially if the derived value of a function is tough to find using the calculus approach.

Nelder Mead utilizes 4 operations, namely expansion (expansion (χ)), reflection (reflection (ρ)), contraction (contraction (γ)), and shrinkage (α). Where some studies were used the fixed value in each operation $\chi = 2$, $\rho = 1$, $\gamma = ½$, and $\alpha = ½$.
Following are the details of each optimization step using Nelder Mead [20]:

- Step 1: Determine objective function (*f*) in vertices n+1, therefore $f(x_1) \le f(x_2) \le f(x_3) \le \ldots \le f(x_{n+1})$ where the value of x_{n+1} describes the simplex value for the next iteration and *n* is the number of simplexes produced.
- Step 2: **Reflection**: Find the reflection point of reflection simplex (x_{ref}) from (2):

$$x_{ref} = (1+\rho)x' - x_{n+1} \tag{2}$$

Where in Eq. (2), the value of *x'* is obtained using the formula below:

$$x' = \sum_{i=1}^{n} \frac{x_i}{n} \tag{3}$$

The value of x_i from Eq. (3) described the centroid value at the *n* best point. Then evaluate x_{ref} using the objective function of reflection phase $f(x_{ref})$.

- Step 3: ***Expansion***: if the value of $f(x_{ref}) < f(x_n)$, then determine the expansion value (x_{exp}) from formula below:

$$x_{exp} = x' + \chi(x_{ref} - x') \tag{4}$$

If the evaluation value of objective function in $f(x_{exp}) < f(x_{ref})$ then switch the value $x_{new} = x_{exp}$ and terminate the iteration. If it doesn't affect the condition, then denoted the value $x_{new} = x_{ref}$.

- Step 4: ***Contraction***: if the value $f(x_{ref}) < f(x_n)$ then:

Outside : if the value $f(x_n) < f(x_{ref}) < f(x_{n+1})$, determine contraction value (x_{con}) using formula below:

$$x_{con} = \gamma(x_{ref} - x') + x' \tag{5}$$

From the calculation result using Eq. (5) execute the contraction function $f(x_{con})$. if $f(x_{con}) < f(x_{ref})$ then accept x_{con} as x_{new} and stop the searching process. if it is not, do the next step.

Inside : if the objective value of $f(x_{ref}) \geq f(x_{n+1})$, then calculate x_{con} using formula below:

$$x_{con} = \gamma(x_{n+1} - x') + x' \tag{6}$$

After that, determine the objective function ($f(x_{con})$), if the value of $f(x_{con}) < f(x_{n+1})$ then consider x_{con} as the best solution (x_{new}) and terminate the iteration. If it is not, then continue the next step.

- Step 5: ***Shrinkage***: if the objective function results equal with $f(x_{new}) \geq f(x_{n+1})$, then evaluate the new value of v_i using:

$$v_i = x_1 + \alpha(x_i - x_1) \tag{7}$$

Where i is the iteration start from $i = 2, 3, \ldots, n+1$. On the next iteration, vertex from new simplex will consisted as $x_1, v_2, v_3, \ldots, v_{n+1}$ then stop the iteration.

- Step 6: If the conditions stop being met, then stop the Nelder Mead search process. If not, then repeat step 1.

3. Dataset

There are two datasets used in this study, which consist of Breast Cancer Coimbra Dataset (BCCD) and Wisconsin Breast Cancer Dataset (WBCD). Both datasets can be accessed through these links https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Coimbra and https://archive.ics.uci.edu/ml/datasets/breast+cancer+wisconsin+(original).

Breast Cancer Coimbra Dataset consists of 116 instances with ten variables for each sample. The predictor attributes (independent) are BMI, Age, glucose, Insulin, HOMA, Leptin, Resistin, adiponectin, and MCP1. However, previous studies [7] [8] have been conducted attributes comparison to evaluate the best attributes combination. These studies result specified that Glucose, Resistin, Age, BMI, and HOMA can give better performance. Thus, this research will use those attributes as predictors for breast cancer classification. Moreover, the dependent variable is a classification, which consists of 1 and 2, where 1 represents healthy controls, and 2 represents the patient.

Moreover, the Wisconsin Breast Cancer Dataset (WBCD) has 699 samples. This dataset contains ten columns, such as uniformity of cell size, marginal adhesion, clump thickness, uniformity of cell shape, single epithelial cell size, bland chromatin, bare nuclei, normal nucleoli, and mitoses as independent variables, and also a class for the dependent variable. All of the variables presented by an integer value, where independent variables have a value between 1 to 10, and for the dependent variable, it has value 2 for Benign appearance and 4 for Malignant presence. There are 16 missing values in the WBCD dataset, and it will be deleted since it does not give any benefit in predicting the appearance of breast cancer. Therefore, the total of WBCD samples used in this research is 683 samples.

4. Proposed method

In this study, the proposed method will be implemented in both BCCD and WBCD datasets. The proposed method is processed by splitting the dataset using the K-Fold Validation technique into two parts, namely trainset (training data) and test set (testing data).

From Fig. 2 can be seen that the next step of the proposed method is to declare a Back-propagation Neural Network along with some supporting parameters. These supporting parameters consist of epochs, learning rates, goals, training models, number of validations, and the type of sigmoid activation that were used in the hidden layer. Then the declaration result is configured. In the Nelder Mead optimization process, define the objective function, wherein this case was using MSE as the error analyses and determine the parameters such as the number of iterations, and the minimum limit value of the objective function.

The objective function in Nelder Mead is a Neural Network Model with MSE evaluation, where the target value is to train and find the best possible weight. This network will be tested using the testing set obtained from the K-Fold Validation process. The test is performed using a confusion matrix to determine the value of accuracy, precision, and recall of each test set. Then, these results will be compared with the BPNN model that is not optimized.

5. Result and discussion

In this research, an optimized BP neural network based on Nelder Mead in classifying breast cancer dataset has been proposed. This research used two different datasets, which are the Coimbra dataset (BCCD) and Wisconsin dataset (WBCD). Both datasets were evaluated using K-Fold Validation to understand the performance of NM-BPNN.

From Table 1, most of the validation result shows that NM-BPNN gives better outcome compared with original BPNN when using Breast Cancer Coimbra Dataset (BCCD) especially in sixth fold validation which offers five times improvement out of six times of fold validation.

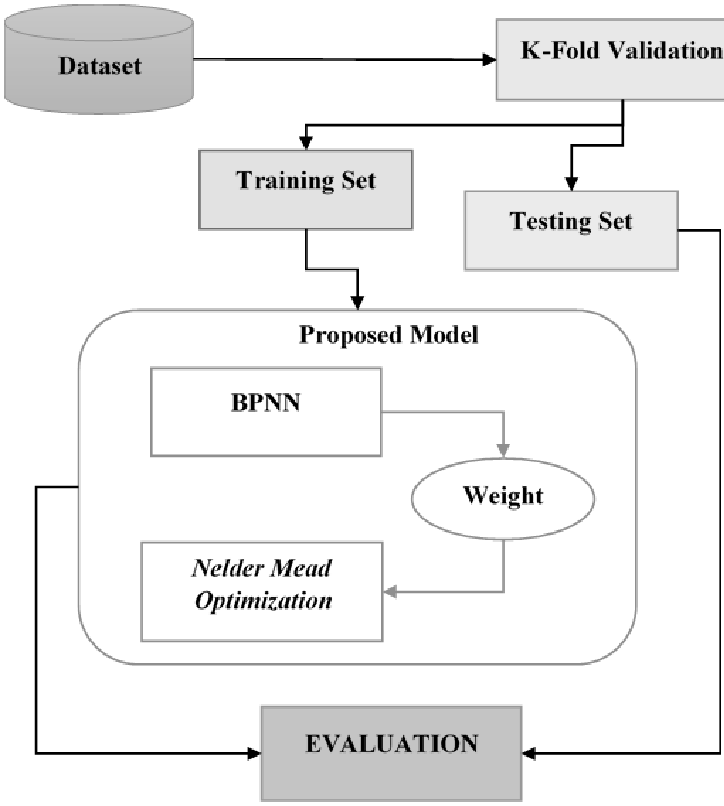

Figure. 2 Proposed method flow chart

Table 1. Evaluation result of NM-BPNN using BCCD

Method	K-Fold Validation								
	2	3	4	5	6	7	8	9	10
BPNN	67.2414	71.0526	79.3103	73.913	52.6316	**75**	**64.2857**	66.6667	72.7273
NM-BPNN	**70.6897**	71.0526	79.3103	**78.2609**	**68.4211**	68.75	57.1429	**75**	**81.8182**
BPNN	60.3448	60.5263	**79.3103**	82.6087	78.9474	81.25	71.4286	58.3333	72.7273
NM-BPNN	**63.7931**	**71.0526**	68.9655	**91.3043**	78.9474	**87.5**	71.4286	58.3333	**81.8182**
BPNN		73.6842	65.5172	**60.8696**	47.3684	68.75	71.4286	83.3333	**81.8182**
NM-BPNN		**81.5789**	**72.4138**	56.5217	**63.1579**	68.75	**92.8571**	83.3333	72.7273
BPNN			65.5172	82.6087	63.1579	68.75	42.8571	91.6667	36.3636
NM-BPNN			**68.9655**	82.6087	**68.4211**	68.75	**57.1429**	91.6667	36.3636
BPNN				**78.2609**	52.6316	81.25	**71.4286**	75	**81.8182**
NM-BPNN				73.913	**68.4211**	81.25	64.2857	75	72.7273
BPNN					73.6842	50	71.4286	58.3333	81.8182
NM-BPNN					**78.9474**	**56.25**	71.4286	**75**	81.8182
BPNN						87.5	42.8571	66.6667	72.7273
NM-BPNN						**93.75**	**78.5714**	66.6667	72.7273
BPNN							85.7143	58.3333	90.9091
NM-BPNN							**92.8571**	58.3333	90.9091
BPNN								91.6667	90.9091
NM-BPNN								91.6667	90.9091
BPNN									72.7273
NM-BPNN									72.7273

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Table 2. Evaluation result of NM-BPNN using WBCD

Method	K-Fold Validation								
	2	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
BPNN	88.2698	89.8678	92.9412	83.8235	85.8407	94.8454	84.7059	88	82.3529
NM-BPNN	**89.1496**	**91.63**	**93.5294**	**84.5588**	85.8407	94.8454	84.7059	88	82.3529
BPNN	87.9765	82.8194	87.0588	94.1176	84.9558	77.3196	85.8824	89.3333	88.2353
NM-BPNN	87.9765	**85.9031**	87.0588	94.1176	**85.8407**	**86.5979**	**87.0588**	**90.6667**	**89.7059**
BPNN		87.6652	91.7647	88.9706	92.9204	87.6289	91.7647	**88**	92.6471
NM-BPNN		**88.1057**	**92.9412**	88.9706	**95.5752**	**89.6907**	91.7647	86.6667	92.6471
BPNN			91.1765	85.2941	94.6903	**89.6907**	92.9412	89.3333	97.0588
NM-BPNN			91.1765	**86.7647**	**95.5752**	87.6289	92.9412	**90.6667**	97.0588
BPNN				84.5588	89.3805	**95.8763**	92.9412	90.6667	89.7059
NM-BPNN				**86.0294**	**90.2655**	94.8454	92.9412	90.6667	89.7059
BPNN					85.8407	**85.567**	**96.4706**	94.6667	91.1765
NM-BPNN					**86.7257**	84.5361	95.2941	94.6667	91.1765
BPNN						92.7835	88.2353	90.6667	92.6471
NM-BPNN						92.7835	**90.5882**	**92**	92.6471
BPNN							89.4118	92	86.7647
NM-BPNN							89.4118	92	**88.2353**
BPNN								86.6667	91.1765
NM-BPNN								86.6667	91.1765
BPNN									95.5882
NM-BPNN									95.5882

Table 3. Average value of each fold validation in BCCD

Fold	Dataset	BPNN	NM-BPNN
2	Coimbra	63.7931	**67.2414**
3	Coimbra	68.4211	**74.5614**
4	Coimbra	**72.4138**	**72.4138**
5	Coimbra	75.6522	**76.5217**
6	Coimbra	61.4035	**71.0526**
7	Coimbra	73.2143	**75**
8	Coimbra	65.1786	**73.2143**
9	Coimbra	72.2222	**75**
10	Coimbra	**75.4545**	**75.4545**
Average		**69.7503**	**73.3844**

Moreover, in Table 2, the proposed method was tested using WBCD. The result shows that several-fold present decrement results such as in seventh and ninth folds, but the overall result shows that the proposed Nelder method can increase the accuracy of BPNN.

Furthermore, the average result of each fold validation is presented in Table 3, in which all of the average fold results give better performance compared with original BPNN, except in 10 folds, which gives the same effect in both methods.

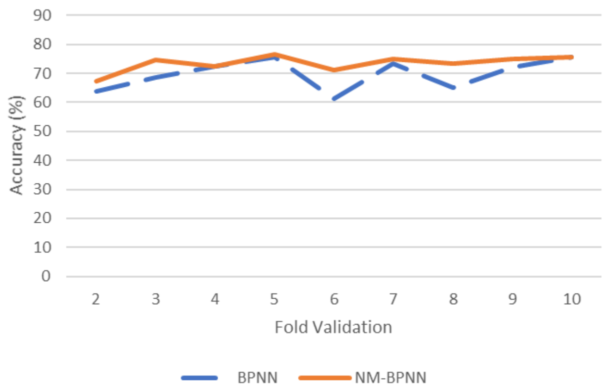

Figure. 3 Comparison between BPNN and proposed method in BCCD

Moreover, in Fig. 3 shows that the proposed method has a consistent classification result when applied in BCCD.

Table 4 shows that the proposed model outperforms the original BPNN in all fold evaluation. It also described in Fig. 3 that our proposed method can increase the performance of BPNN.

Moreover, the result of our proposed method was also compared to several classification techniques, as shown below:

From Table 5 can be seen that when using BCCD,

Table 4. Average value of each fold validation in WBCD

Fold	Dataset	BPNN	NM-BPNN
2	Wisconsin	88.1232	**88.563**
3	Wisconsin	86.7841	**88.5463**
4	Wisconsin	90.7353	**91.1765**
5	Wisconsin	87.3529	**88.0882**
6	Wisconsin	88.9381	**89.9705**
7	Wisconsin	89.1016	**90.1325**
8	Wisconsin	90.2941	**90.5882**
9	Wisconsin	89.9259	**90.2222**
10	Wisconsin	90.7353	**91.0294**
Average		**89.1100**	**89.8129**

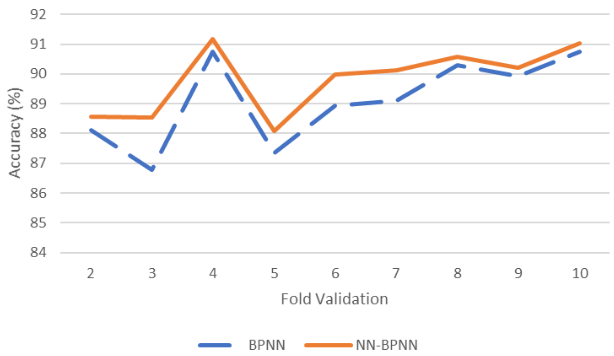

Figure. 4 Comparison between BPNN and proposed method in WBCD

Table 5. Comparison between the proposed result with several classification methods

Method	BCCD	WBCD
Decision Tree [21]	68.6	96.1
Support Vector Machine [21]	71.4	95.1
BPNN [10]	69.8	89.1
Proposed Method	73.4	89.8

our proposed result achieves higher accuracy compared to other methods. Meanwhile, when using WBCD, the decision tree method can outperformother methods. However, our method can achieve other methods. However, our method can achieve higher accuracy compared to the original BPNN.

From the evaluation, the result can be seen that the proposed optimization method using Nelder Mead in BPNN can give better performance compared with the original BPNN, especially in BCCD. The result in BCCD presents a significant increment in accuracy result; however, in WBCD, the accuracy was increased but insignificantly.

6. Conclusion

This study has been implemented the optimization of Backpropagation Neural Network based on Neldermead in classifying the presence of breast cancer. The proposed method was tested using two datasets, which are Breast Cancer Coimbra Dataset (BCCD) and Wisconsin Breast Cancer Dataset (WBCD). Both datasets were randomly separated using 10-Fold validation to produce training dan testing sets. From the testing result using the confusion matrix to obtain the accuracy result, the optimization of BPNN using Nelder Mead can give better accuracy compared to other methods, especially in BCCD, with 73.4% of average accuracy. While in WBCD, the proposed method can outperform the original BPNN. Therefore, it can be concluded that Nelder Mead can increase the performance of BPNN.

In the future study, Nelder Mead optimization can be combined with other optimization method especially from meta-heuristic method to increase the performance of Neural Network.

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Conflicts of Interest

The authors declare that they have no conflicts of interest.

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