Neural Network Algorithm Development For Ion Sensitive Field Effect Transistor (ISFET) Sensor

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Abstract— **Ion Sensitive Field-Effect Transistor, which later in this paper will refer as ISFET is a kind of sensor that able to differentiate the ion by replacing the gate of the FET with electrode and the membrane. Membrane acts as selector for the ions. The sensor detects the ions and converts it into electrical signal. However the sensor has weakness to detect main ion from the interfering ion in the mixed solution when the ions have same characteristic. For this project, potassium ion (K+) and ammonium ion (NH4+) will be used as the sample as both ions have similar size. To overcome the problem, the sensor needs to be trained for pre-calibrate and pre-process by developing a model of Artificial Neural Networks (ANN). The ANN makes the model learn the pattern by the sample of inputs and outputs to estimate results or to get more accurate data. Backpropagation is used as the learning method of ANN model. The algorithm will be developed in MATLAB. The objective of this project is to develop ANN model for ISFET sensor that able to estimate the main ion in mixed solution by learning the pattern of the input and output of the sensor. The ANN model performance can be optimized by altering certain parameters in the learning algorithm. The results show that the model is able to predict with 97% accuracy and has strong and precise estimation ability with R-factor of 91.55%.**

Keywords - ISFET; CHEMFET; Artificial Neural Network (ANN); Backpropagation; MATLAB;

I. INTRODUCTION

ISFET was invented by P. Bergveld in 1970s where it was introduced for the measurement of ionic ion [8]. ISFET sensor is a metal-oxide field-effect transistor (MOSFET) based sensor, which interfaces the electrolyte/membrane/gate in response to ionic activity [1]. The difference of ISFET and MOSFET is that the replacement of MOSFET metal gate with series combination of the reference electrode, membrane and the insulator layer [6]. ISFET is applied as a pH sensor by exposing the ion sensitive layer and the reference electrode to solution. This situation creates a gate potential and then modulates the current flow through the channel [13]. Thus, by measuring the channel current or the gate potential, we can represent the pH level of solution.

The advantage of ISFET as pH sensor is that it has smaller in size, fast response time and fabrication compatible [2]. However, the ISFET were found to have difficulties in differentiating the ions with similar charge type and number [1]. In this case, The ISFET sensor has problem in differentiating the concentration in mixed solution of potassium ion (K+) and ammonium ion (NH4+). By developing the algorithm for the pre-process model, the sensor will be able to differentiate the main ion concentration with the interfering ion. The post-process of neural network is also called as Artificial Neural Network (ANN). ANN mimics the neural structure of the brain by learning from experiences. It means that by training a neural network from past data, the model will make the network able to generate outputs based on the knowledge extracted from the data.

This project applied Supervised Backpropagation as learning algorithm. Backpropagation Neural Network (BPNN) is a network with multilayer perceptron (MLP) model which learns by updating weights and bias of the network. Back-propagation algorithm includes a forward computation and then a backward computation that propagates the error signal from the output layer to the hidden layer takes place [12]. According to P. Jeatrakul and K.W. Wong, BPNN are more robust and gives good performance results in every test case [9]. The learning algorithm will be written in MATLAB and the algorithm will be applied to the sensor.

II. METHODOLOGY

A. Structure of ISFET sensor system

ISFET sensor system includes the ISFET sensor itself than it converts to electrical signals by using the readout interface circuit (ROIC). The data will be processed by ANN model for estimation and classification of potassium and ammonium ion concentration. The data will be sent to microcontroller for data processing and cleaning to display the pH or concentration value. The project only covers for developing the ANN algorithm for pre-process stage for estimation. Fig. 1 below shows the flow of the ISFET sensor system.

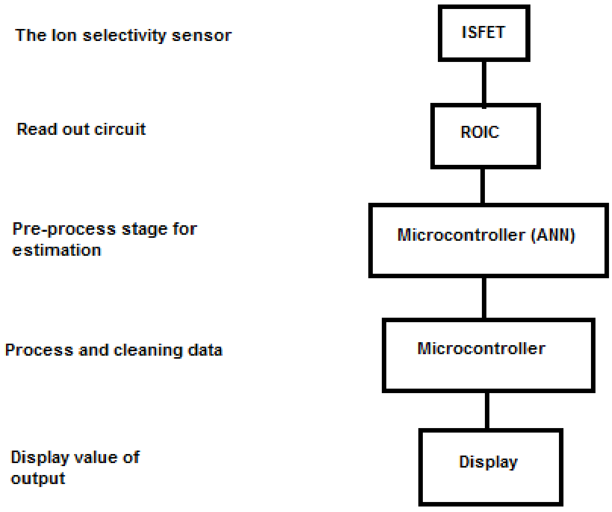


Figure 1. Block diagram of ISFET sensor system

B. *Neural Network Architecture*

Multilayer Perceptron is one of the neural network models. It has multiple layers of nodes that connected from one layer to the next. Except for the input nodes, each node is a neuron or processing element with an activation function as an output or input for the next layer of node. There will be two inputs for this model which are for potassium sensor and ammonium sensor. The outputs of this model would represent the concentration of ion for both potassium and ammonium. Fig. 2 is an illustration of the MLP model for this model.

Fig. 3 illustrates the operation of MLP. From the input, the weight will be multiplied to the input to be the parameter for the activation function. The output of the activation function would be the input of the next layer. The output of activation function and weight would be the parameter for the output function.

The activation functions used for this model are nonlinear for hidden layer because it is differentiable and easy to learn for backpropagation. The hyperbolic tangent is expected to have a better learning and activation compared to unipolar sigmoid function. Fig. 3 will show the behavior of unipolar sigmoid function and hyperbolic tangent function. For the output function, the linear function is used to match the outputs which are continuous and unbounded. Table 1 is the table for activation functions for linear (identity), unipolar sigmoid (sigmoid) and hyperbolic tangent (tanh).

TABLE 1. ACTIVATION FUNCTIONS

Activation Function	
Name	**Formula**
Identity	$F(x) = x$
Sigmoid	$F(x) = \dfrac{1}{1 + e^{-x}}$
Tanhh	$F(x) = \dfrac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$

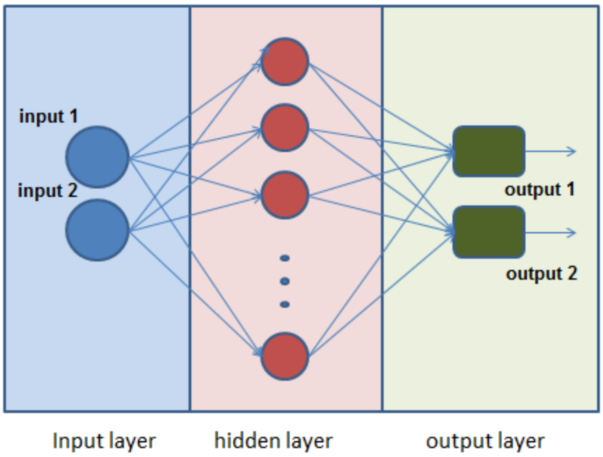


Figure 2. MLP architecture

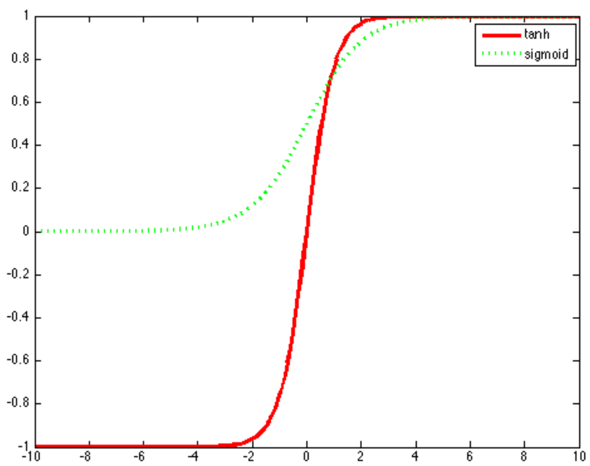


Figure 3. Sigmoid and Tanh curve.

C. *Training, and testing Neural Network*

Training a neural network is a process of learning the data so that it can form a model that is able to do data estimation and classification. It takes many repeated process of learning (epoch) before it gets to the desired model of algorithm.

Neural network can be tested by using the final model of the neural network model. The precision of the model can be obtained from the regression plot. The R value will represent the precision value. The model that has the R value closed to 1 is considered precise in estimating the data. The accuracy of the model was tested using Mean Squared Error (MSE) which is the function average of the squared errors between actual and estimated readings in a data sample. The formula of MSE is:-

$$MSE = (1/\text{number of sample data}) \times \sum(\text{error})^2 \qquad (1)$$

D. *Improve Backpropagation Design*

Backpropagation learning process is illustrated as in Fig. 4. The method used for backpropagation is gradient descent which is a method to minimize the error between the expected output and the produced output. Table 2 will show how to derive the back computation equation. Backpropagation learning performance can be improved by adjusting certain parameters. The parameters that can improve the learning performance are:-

1. Hidden neuron
2. Learning rate
3. Momentum

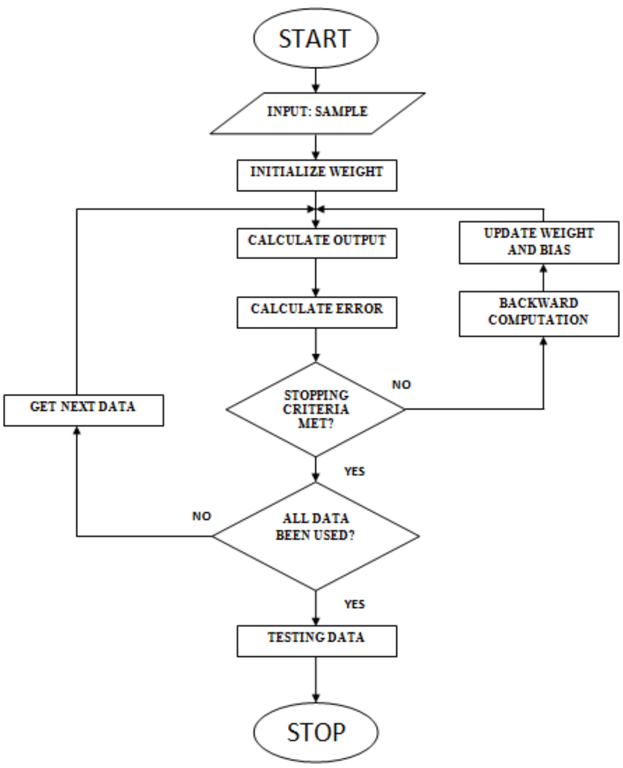


Figure 4. Backpropagation learning process flow

TABLE 2. DELTA DERIVATION FOR BACKPROPAGATION

Functions/Comments	Mathematical Equation	
Squared Error, E	$E = \frac{1}{2}(Target\ output - Actual\ Output)^2$	(2)
wi – weight xi – input	$net = \Sigma wixi$	(3)
Calculated output, y f – activation function	$y = f(net)$	(4)
The change of error when the weight is changed	$\frac{\partial E}{\partial wi} = \frac{dE}{dy} \cdot \frac{dy}{dnet} \cdot \frac{dnet}{dwi}$	(5)
Derivative of net	$\frac{dnet}{dwi} = xi$	(6)
Derivative of transfer function tanh	$\frac{dy}{dnet} = (1+y)(1-y)$	(7)
Derivative of squared error t – target output y – actual/calculatedoutput	$\frac{dE}{dy} = (t-y)$	(8)
Combine all derivatives	$\frac{\partial E}{\partial wi} = (t-y)\ (1+y)(1-y)xi$	(9)

III. RESULTS AND DISCUSSION

Fig. 5 and Fig. 6 represent the learning curve of unipolar sigmoid and hyperbolic tangent consecutively. Hyperbolic tangent shown in Fig. 6 shows its ability to learn faster compared to unipolar sigmoid in Fig. 5. The hyperbolic tangents 'learned' at the epoch of 200 while the unipolar sigmoid 'learned' later at epoch of 400. Hyperbolic tangent is also more accurate than unipolar sigmoid as it has least MSE. Hyperbolic tangent is centered on zero and anti-symmetrical rather than unipolar sigmoid where it is always in positive value. Anti-symmetric function leads to faster convergence.

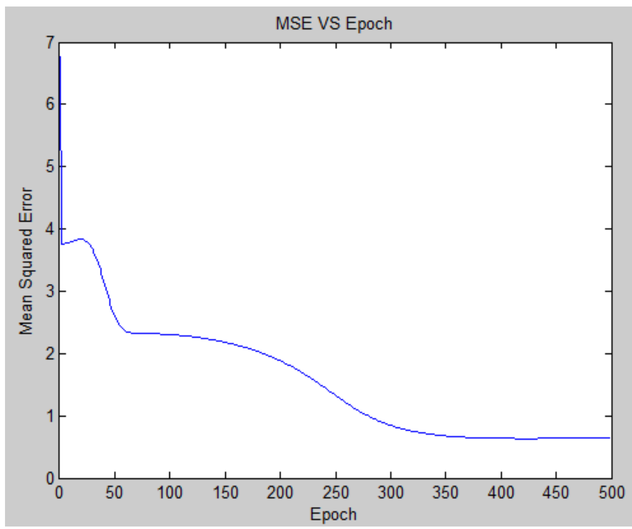


Figure 5. Unipolar Sigmoid learning curve

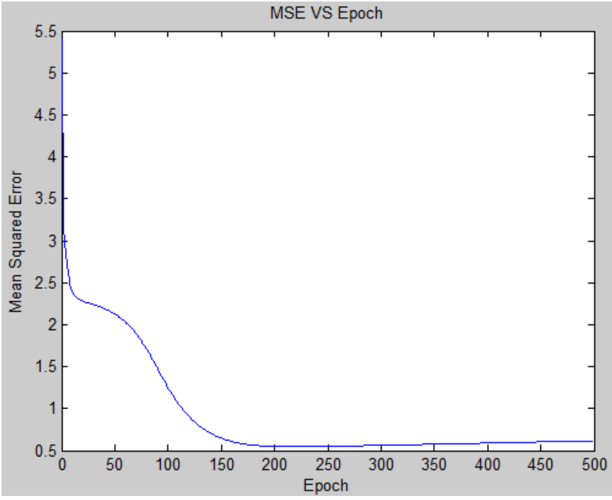


Figure 6. Hyperbolic Tangent learning curve

There are three parameters that will be altered to optimize the ANN model which are the number of hidden neuron, learning rate and momentum. The effect of number of neurons to the ANN model performance can be analyzed in Fig. 7 and Fig. 8. The value for learning rate and momentum were selected as random while the activation function used was hyperbolic tangent. The effects that it could give to the model are the estimation power which is R-factor of regression and Mean Squared Error (MSE). Minimizing the mean or total square errors between observations and model outputs is the main concern for ANN model [14]. Having least MSE indicates the low error occur in estimating the output while R-factor indicates the estimating power and accuracy of the model.

From Fig. 7, the least MSE was obtained when having 10 hidden neurons. The regression vs. hidden neuron in Fig. 8 also shows that the model is optimized when having 10 hidden neurons. The highest error occurs when having 30 hidden neurons and the lowest regression obtained when having 15 hidden neurons. Having a few hidden neurons will reduce the robustness and also reduce the processor power of the system. While having too much of it will costs the model to be slow in learning.

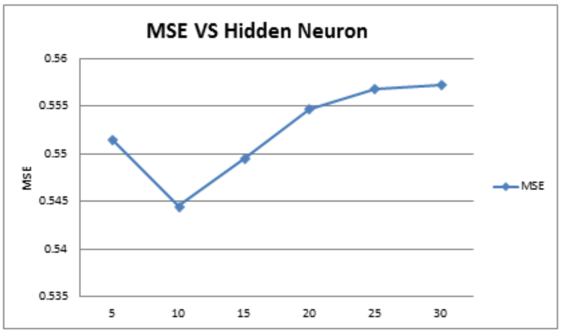


Figure 7. The effect of MSE by varying the number of hidden neuron

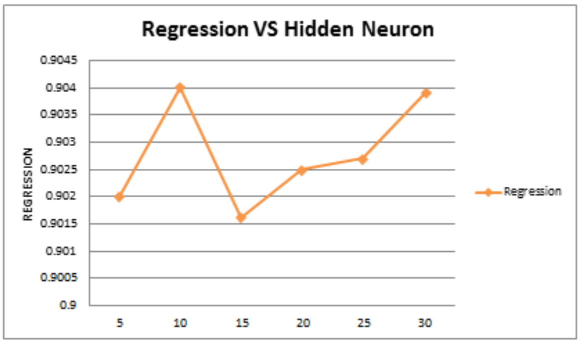


Figure 8. The effect of regression by varying the number of hidden neuron

The speed of learning of a network can be improved by increasing the learning rate. Too high of learning rate might cause the system to be unstable because the oscillation of weights. Fig. 9 and Fig. 10 are the curves of MSE and regression consecutively varying with the learning rate value. The value for momentum was selected as random and 10 neurons were used as hidden neuron.

Learning rate at its least MSE is when at 0.03 while having the best regression at 0.007. Both graphs show that a significant drop of accuracy and precision at 0.001. The most suitable learning rate is at 0.03 because it has the least error and considerably high precision.

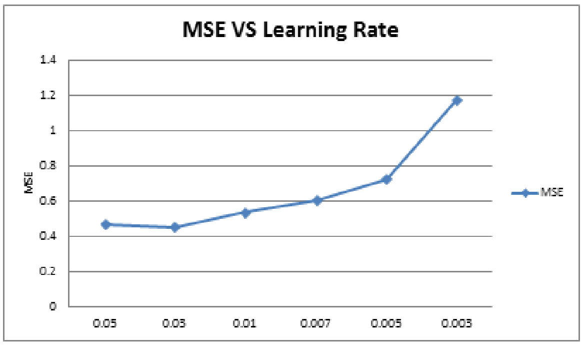


Figure 9. The effect of MSE by varying learning rate

Figure 10. The effect of regression by varying learning rate

Instead of having high learning rate to converge, momentum is more suitable and reliable to be the parameter to improve the model performance by speeding up the convergence and avoid instability. Momentum is a fraction of delta change of weights and biases. Too low of momentum might cause the learning process to be slow. Fig. 11 and Fig. 12 show the effect of momentum to the model performance.

The two curves plotted in Fig.11 and Fig.12 show that the decreasing value of momentum will increase the performance of the model. The curves start to converge as the momentum value becomes too low. From the observation of the curves above, there are not much difference in performance at the momentum of 0.01 and 0.001. The best value to fit the model is either 0.01 or 0.001.

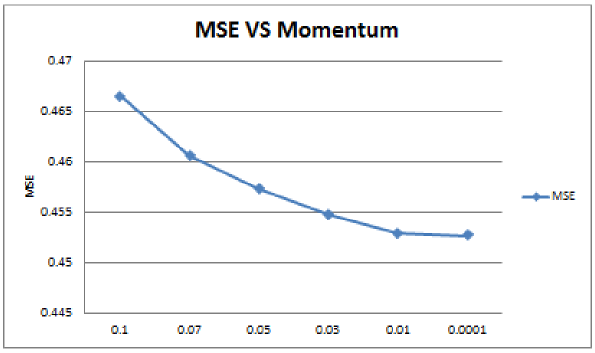


Figure 11. The effect of MSE by varying momentum

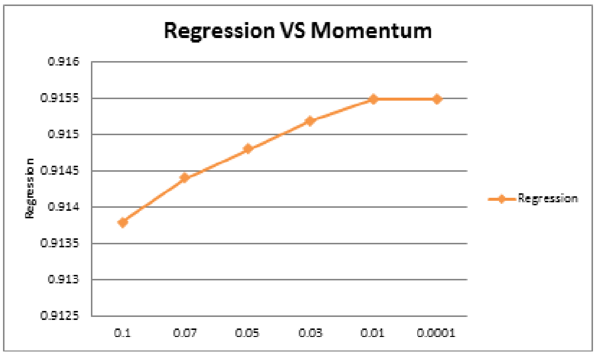


Figure 12. The effect of regression by varying momentum

The optimized parameters will be used as ANN learning model. The model will be tested for its precision and accuracy. Fig. 13 is a regression plot of the ANN. Linear regression is a scatter plot that plots the relation of expected output and calculated output to check the accuracy and precision of the estimation [14]. 'R' represents the linearity and precision of the estimation. Value of R that closing to 1 is considered strong in estimation and précised. Regression factor obtained for this model is 0.9155 which can be considered as accurate and precise in estimation.

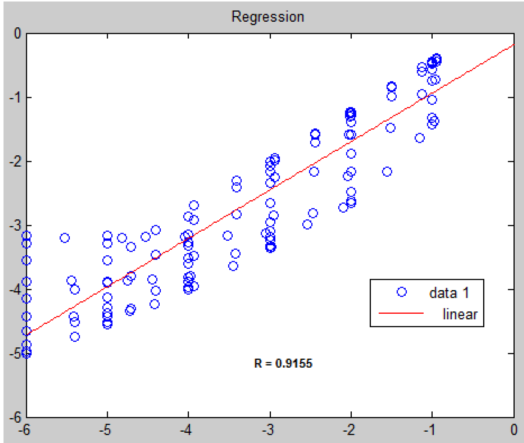
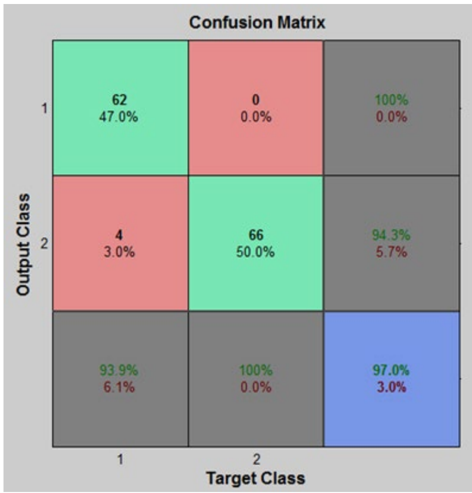


Figure 13. Regression plot

Table 3 shows a confusion matrix table. It contains information about actual and predicted classifications done by a classification system. Performance of the systems is evaluated using the data in the matrix.

The confusion table has special way to be analyzed, green boxes which are diagonal are for true/correct data reading from Neural Network testing, on the other hand, red boxes represent error data from Network tested. The green box (1,1) represents the first output that has been predicted correct. This indicates that it is able to detect the ion potassium as main ion with 93% correct. For green box (2,2), It had predicted ion ammonium for 100% correct as the main ion. The blue box (3,3) shows the overall accuracy of prediction in percentage for the network.

TABLE 3. CONFUSION MATRIX OF THE ANN MODEL



IV. CONCLUSION

The Artificial Neural Network algorithm is expected to do pre-processing so that it can estimate the main ion. Hence, it is expected to solve the selectivity complication of main ion between potassium ion and ammonium ion. By adjusting certain parameters of the backpropagation algorithm, the model performance can be improved. The parameters that had been adjusted to optimize the network are the number of hidden neurons, learning rate and momentum. This ANN model is found to be optimum when having 10 hidden neurons, 0.03 learning rate and 0.01 momentum. All these parameters are the distributing factors of improving the learning speed and accuracy. The activation function also contributes to the learning speed of ANN as the hyperbolic tangent shows a faster convergence compared to unipolar sigmoid. After optimizing the model algorithm, The ANN model can predict accurately up to 97% correct while R-factor of 91.55% shows that it has strong and precise estimation ability.

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