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Quantification of Uncertainty in Mineral Prospectivity Prediction Using Neural Network Ensembles and Interval Neutrosophic Sets

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***Abstract*— Quantification of uncertainty in mineral prospectivity prediction is an important process to support decision making in mineral exploration. Degree of uncertainty can identify level of quality in the prediction. This paper proposes an approach to predict degrees of favourability for gold deposits together with quantification of uncertainty in the prediction. Geographic Information Systems (GIS) data is applied to the integration of ensemble neural networks and interval neutrosophic sets. Three different neural network architectures are used in this paper. The prediction and its uncertainty are represented in the form of truth-membership, indeterminacy-membership, and false-membership values. Two networks are created for each network architecture to predict degrees of favourability for deposit and non deposit, which are represented by truth and false membership values respectively. Uncertainty or indeterminacy-membership values are estimated from both truth and false membership values. The results obtained using different neural network ensemble techniques are discussed in this paper.**

I. Introduction

Uncertainty estimation in mineral prospectivity prediction is an important task in order to support decision making in regional-scale mineral exploration. In this paper, we focus on uncertainty of type vagueness in which it refers to boundaries that cannot be defined precisely. In [1], vague objects are separated into vague point, vague line, and vague region. Dilo et al. [1] defined vague point as a finite set of disjoint sites with known location, but the existence of the sites may be uncertain.

This study involves gridded map layers in a GIS database, each grid cell represents a site with a known location, but uncertain existence of favourability for deposit. Hence, this study deals with vague point. Some locations have one hundred percent of favourability for deposits. Some locations have zero percent of favourability for mineral deposits. Such cells are referred to as non-deposit or barren cells. Most locations have degrees of favourability between these two extremes. Therefore, each cell contains uncertain information about the degree of favourability for deposits, degree of favourability for barrens, and degree of indeterminable information or uncertainty. In order to store these three types of information for each cell, we apply interval neutrosophic sets [2] to keep these information in the form of truth-membership, false-membership, and indeterminacy-membership values, respectively.

In recent years, neural network methods were found to give better mineral prospectivity prediction results than the conventional empirical statistically-based methods [3]. There are various types of neural network used to predict degree of favourability for mineral deposits. For example, Brown et al. [3], [4] applied backpropagation neural network for mineral prospectivity prediction. Skabar [5] used a feed-forward neural network to produce mineral potential maps. Iyer et al. [6], [7] applied a general regression neural network and a polynomial neural network to predict the favourability for gold deposits. Fung et al. [8] applied neural network ensembles to the prediction of mineral prospectivity.

Hansen and Salamon [9] suggested that ensembles of neural networks gives better results and less error than a single neural network. Ensembles of neural networks consist of two steps: training of individual components in the ensembles and combing the output from the component networks [10]. This study aims to apply neural network ensembles to predict the degrees of favourability for gold deposits and also the degrees of favourability for barrens. These two degrees are then used to estimate the degree of uncertainty in the prediction for each grid cell on a mineral prospectivity map. Each component of neural network ensembles applied in this study consists of a pair of neural networks trained to predict degree of favourability for deposits and degree of favourability for barrens, respectively. We use three components in the ensemble of neural networks. These component architectures are feed-forward backpropagation neural network, general regression neural network, and polynomial neural network. These three are selected mainly because they have successful application in the field.

A multilayer feed-forward neural network with backpropagation learning is applied in this study since it is suitable for a large variety of applications. A general regression neural network is a memory-based supervised feed-forward network based on nonlinear regression theory. This network is not necessary to define the number of hidden layers in advance and has fast training time comparing to backpropagation neural network [11]. A polynomial neural network is based on Group Method of Data Handling (GMDH) [12] which identifies the nonlinear relations between input and output variables. Similar to general regression neural network, a topology of this network is not predetermined but developed through learning [7].

In order to combine the outputs obtained from components

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of ensemble neural networks, we propose and compare six aggregation techniques which are based on majority vote, averaging, and dynamic averaging techniques. Our proposed techniques have applied the three membership values in the aggregation instead of the truth-membership only as in most conventional approaches.

The rest of this paper is organized as follows. Section II presents interval neutrosophic sets used in this study. Section III explains the proposed model for the quantification of uncertainty in the prediction of favourability for gold deposits using interval neutrosophic sets and ensemble of neural networks. Section IV explains the GIS data set used in this paper. Experimental methodologies and results are also presented in this section. Conclusions are explained in section V.

II. Interval Neutrosophic Sets

An interval neutrosophic set (INS) is an instance of neutrosophic set [13] which is generalized from the concept of a classical set, fuzzy set, interval-valued fuzzy set, intuitionistic fuzzy set, interval-valued intuitionistic fuzzy set, paraconsistent set, dialetheist set, paradoxist set, and tautological set [2]. The membership of an element to the interval neutrosophic set is expressed by three values: t, i, and f, which represent truth-membership, indeterminacy-membership, and false-membership, respectively. These three memberships are independent and can be any real sub-unitary subsets. In some special cases, they can be dependent. In this paper, the indeterminacy-membership value depends on both truth-membership and false membership values. The interval neutrosophic set can represent several kinds of imperfection such as imprecise, incomplete, inconsistent, and uncertain information [14]. In this paper, we express imperfection in the form of uncertainty of type vagueness. This research follows the definition of an interval neutrosophic set that is defined in [2]. This definition is described below.

Let X be a space of points (objects). An interval neutrosophic set in X is

$$A = \{x(T_A(x), I_A(x), F_A(x)) | x \in X \wedge \\ T_A : X \longrightarrow [0,1] \wedge \\ I_A : X \longrightarrow [0,1] \wedge \\ F_A : X \longrightarrow [0,1]\} \tag{1}$$

where

T_A is the truth-membership function,
I_A is the indeterminacy-membership function, and
F_A is the false-membership function.

The operations of interval neutrosophic sets are also applied in this paper. Details of the operations can be found in [14].

III. Uncertainty estimation using Interval Neutrosophic Sets and Ensemble Neural Networks

This paper applies GIS input data to ensemble neural networks for the prediction of favourability for gold deposits and

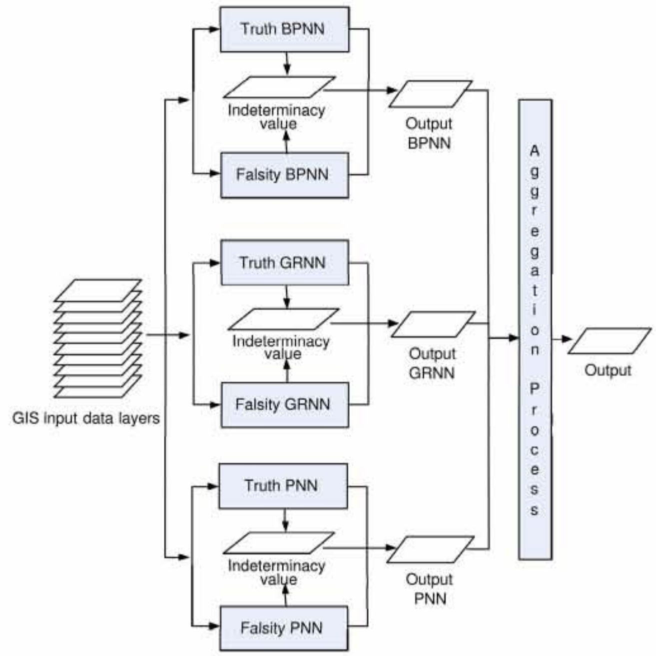

Fig. 1. Uncertainty model based on the integration of interval neutrosophic sets and ensemble neural network

utilizes the interval neutrosophic set to express uncertainties in the prediction. Fig. 1 shows our proposed model. The input feature vectors of the proposed model represent values from co-registered cells derived from GIS data layers which are collected and preprocessed from the Kalgoorlie region of Western Australia. The same input data set is used in every neural network created in this paper.

In order to predict degrees of favourability for deposits, we apply three types of neural network architecture: feed-forward backpropagation neural network (BPNN), general regression neural network (GRNN), and polynomial neural network (PNN) for training individual network in the ensembles. We create two neural networks for each neural network architecture. The first network is used to predict the degree of favourability for deposits (truth-membership values) and another network is used to predict the degree of favourability for barrens (false-membership values). Both networks have the same architecture and are applied with the same input feature data. The difference between these two networks is that the second network trained to predict degrees of favourability for barrens uses the complement of target outputs used in the first network which is trained to predict degrees of favourability for deposits. For example, if the target output used to train the first network is 0.1, its complement is 0.9. The results from these two networks are used to analyze uncertainty in the prediction. If a cell has high truth-membership value then this cell should have low false-membership value and vise versa. Otherwise, this cell contains high uncertainty. Hence, the degrees of uncertainty in the prediction or indeterminacy-membership values can be calculated as the difference between truth-membership and false-membership values. If the difference between truth-membership and false-membership is high then the uncertainty is low. In contrast, if the difference between both values is low then the uncertainty is high.

In Fig. 1, the proposed neural network ensembles contain three components which each consists of a pair of neural networks. The first pair is feed-forward backpropagation neural networks (truth BPNN and falsity BPNN). The second pair is general regression neural networks (truth GRNN and falsity GRNN). The third pair is polynomial neural networks (truth PNN and falsity PNN). Each pair of neural networks is trained to predict degrees of favourability for deposits (truth-membership values) and degrees of favourability for barrens (false-membership values). The indeterminacy-membership values are calculated from the different between truth-membership and false-membership values. Therefore, we have three interval neutrosophic sets which are outputs from those three pairs of neural networks. We can define these outputs as the following.

Let X_j be the set of outputs from the neural network. In our case, we have three sets of outputs, i.e. X_1, X_2 and X_3, representing output sets from BPNN, GRNN and PNN respectively. Each set X_j contains the outputs from each pair of the neural networks. The output set for BPNN is therefore represented as $X_1 = \{x_{11}, x_{12}, ..., x_{1i}, ..., x_{1n}\}$ where x_{1i} is a cell in the output from the BPNN at location i.

Let A_j be an interval neutrosophic set of X_j. A_j can be defined as

$$\begin{aligned} A_j = \{x(T_{A_j}(x), I_{A_j}(x), F_{A_j}(x)) | x \in X_j \wedge \\ T_{A_j} : X \longrightarrow [0,1] \wedge \\ I_{A_j} : X \longrightarrow [0,1] \wedge \\ F_{A_j} : X \longrightarrow [0,1]\}, \end{aligned}$$

$$I_{A_j}(x) = 1 - |T_{A_j}(x) - F_{A_j}(x)|$$

where T_{A_j} is the truth (deposit) membership function, I_{A_j} is the indeterminacy membership function, and F_{A_j} is the false (barren) membership function. After the individual neural network is trained and the three interval neutrosophic sets A_j are created, the next step is to combine these three sets. Instead of using only truth membership values to predict the favourability for gold deposits, the followings are our proposed aggregation techniques using truth-membership, false-membership, and indeterminacy-membership values.

1) Majority vote using $T\&F$
   For each interval neutrosophic set A_j, if a cell x has truth-membership value $T_{A_j}(x)$ greater than a threshold value then this cell is classified as deposit, otherwise it is classified as barren. In this paper, we use threshold values ranging from 0.1 to 0.9 in steps of 0.1. If a cell has false-membership value $F_{A_j}(x)$ less than a threshold value then this cell is classified as deposit, otherwise it is classified as barren. The results calculated from the best threshold for truth-membership values and the results calculated from the best threshold for false-membership values are then calculated using the logical operator *and* to provide the prediction results for each cell x in each output X_j. The degree of uncertainty for each cell is expressed by the indeterminacy-membership value, $I_{A_j}(x)$.
   After the three outputs are classified, the next step is to combine these outputs. The majority vote is then applied in order to aggregate the three outputs. For each cell, if two or more outputs are classified as deposits then the cell is deposit. Otherwise, the cell is classified as barren. The uncertainty value for each "deposit" cell is estimated from the average indeterminacy-membership value for all the neural network pairs in the ensemble that classified the input pattern as a deposit. Likewise, uncertainty values for "barren" cells are calculated as the average of indeterminacy-membership values from the members of the network pairs that gave a classification of barren.
2) Majority vote using $T > F$
   This technique is more flexible than the first technique. The threshold value is not required for the prediction. For every cell in each interval neutrosophic set A_j, if the truth-membership value is greater than the false-membership value ($T_{A_j}(x) > F_{A_j}(x)$) then the cell is classified as deposit. Otherwise it is classified as barren. The degree of uncertainty for each cell is represented by the indeterminacy-membership value, $I_{A_j}(x)$. Similar to the first technique, the majority vote is then used to combine the three outputs and the indeterminacy-membership values are calculated according to the predicted cell type for each individual output.
3) Averaging using $T\&F$
   In this technique, the three interval neutrosophic sets $A_j, j = 1,2,3$ are averaged. Let O be an averaged output map. $O = \{o_1, o_2, ..., o_n\}$ where o_i is a cell of the averaged output map at location i. Let Avg be an interval neutrosophic set of the averaged output map O. Avg can be calculated as follow

   $$Avg = \sum_{j=1}^{n}(A_j/3).$$

   If a cell has averaged truth-membership value $T_{Avg}(o)$ greater than a threshold value then this cell is classified as deposit, otherwise the cell is classified as barren. If a cell has averaged false-membership value $F_{Avg}(o)$ less than a threshold value then this cell is classified as deposit, otherwise this cell is classified as barren. Similar to the first technique, the logical operator *and* is used to calculate the prediction from the results obtained from the best threshold for both truth-membership and false-membership values. The degree of uncertainty is expressed by the averaged indeterminacy-membership value $I_{Avg}(o)$.
4) Averaging using $T > F$
   In this technique, the three interval neutrosophic sets are also averaged and the results are stored in Avg. if the averaged truth-membership value is greater than the

averaged false-membership value $T_{Avg}(o) > F_{Avg}(o)$ then the cell is classified as deposit. Otherwise the cell is classified as barren. The degree of uncertainty for each cell is represented by the averaged indeterminacy-membership value $I_{Avg}(o)$.

5) Dynamic averaging using $T\&F$

Instead of using equal weight averaging, this technique uses dynamic weight averaging in which the weight is the complement of the uncertainty value or indeterminacy-membership value for each cell. Uncertainty is integrated into truth-membership and false-membership values to support the confidence of the prediction. Let Y be a dynamic averaged output map. $Y = \{y_1, y_2, ..., y_n\}$ where y_i is a cell of dynamic averaged output at location i. Let D be an interval neutrosophic set of the dynamic averaged output Y. D can be defined as follow

$$D = \{y(T_D(y), I_D(y), F_D(y)) | y \in Y\}$$

where

$$\begin{aligned}
T_D(y_i) &= w_{1i}T_{A_1}(x_{1i}) + w_{2i}T_{A_2}(x_{2i}) + w_{3i}T_{A_3}(x_{3i}),\\
F_D(y_i) &= w_{1i}F_{A_1}(x_{1i}) + w_{2i}F_{A_2}(x_{2i}) + w_{3i}F_{A_3}(x_{3i}),\\
I_D(y_i) &= 1 - |T_D(y_i) - F_D(y_i)|,\\
w_{ji} &= \frac{1-I_{A_j}(x_{ji})}{\sum_{j=1}^{3}(1-I_{A_j}(x_{ji}))}, \; j = 1,2,3; \quad i = 1,2,...,n.
\end{aligned}$$

If a cell has truth-membership value $T_D(y)$ greater than a threshold value then this cell is classified as deposit, otherwise the cell is classified as barren. On the other hand, if a cell has false-membership value $F_D(y)$ less than a threshold value then this cell is classified as deposit, otherwise the cell is classified as barren. The results obtained from the best threshold for both truth-membership and false-membership values are then combined using the logical operator *and* to provide the prediction results. The degree of uncertainty is expressed by the indeterminacy-membership value $I_D(y)$ which is calculated as the different between truth-membership and false-membership values.

6) Dynamic averaging using $T > F$

In this technique, an interval neutrosophic set D is created using the same previous technique. In order to predict the favourability for deposits, if the truth-membership value is greater than the false-membership value $T_D(y) > F_D(y)$ then the cell is classified as deposit. Otherwise the cell is classified as barren. The degree of uncertainty for each cell is represented by the indeterminacy-membership value $I_D(y)$.

IV. Experiments

A. GIS data set

The data set used in this study was obtained from an approximately 100×100 km area of the Archaean Yilgarn Block, near Kalgoorlie, Western Australia. This data set were preprocessed and compiled into GIS layers from a variety of sources such as geology, geochemistry, and geophysics. We used ten layers in raster format to create input feature vectors for our model. These layers represent different variables such as favourability of host rocks, distance to the nearest regional-scale fault, and distance to the nearest magnetic anomaly. Each layer is divided into a grid of square cells of 100 m side. Hence, the map area contains 1,254,000 cells. Each cell stores a single attribute value which is scaled to the range $[0, 1]$. For example, a cell in a layer representing the distance to the nearest fault contains a value of distance scaled to the range $[0, 1]$. Each single grid cell is also classified into deposit or barren cell. The cells containing greater than 1,000 kg total contained gold are labeled as deposits. All other cells are classified as non-deposits or barren cells. In this paper, we use 268 cells which are separated into 120 deposit cells and 148 barren cells. These cells are divided into training and test data sets. We use 85 deposit cells and 102 barren cells for training data. For testing data, we use 35 deposit cells and 46 barren cells.

B. Experimental methodology and results

In this paper, two pairs of neural networks trained using feed-forward backpropagation neural network and general regression neural network are created using Matlab. A pair of polynomial neural networks is trained using PNN online-software developed by Tetko et al [15]. Each pair of neural networks is trained to predict degrees of favourability for deposits and degrees of favourability for barrens which are truth-membership $T_{A_j}(x)$ and false-membership $F_{A_j}(x)$, respectively. These two values are then used to calculate the indeterminacy-membership values $I_{A_j}(x)$. The three outputs obtained from these three network architectures are combined using the proposed ensemble techniques. All results shown in this paper are calculated from the test data set.

Table I and Table II show the percentage of total correct cells obtained from individual neural network architectures using a range of threshold values to the truth-membership and to the false-membership values, respectively. The best thresholds to the truth-membership for BPNN, GRNN, and PNN are 0.5, 0.6, and 0.5, respectively. The best thresholds to the false-membership for BPNN, GRNN, and PNN are 0.4, 0.4, and 0.5, respectively. Table III shows the percentage of total correct cells obtained from the comparison between truth-membership and false-membership values $T_{A_j}(x) > F_{A_j}(x)$, and obtained using the logical operator *and* to the prediction results using the best threshold for truth-membership and the best threshold for false-membership values. Table IV shows the percentage of total correct cells obtained from equal weight averaging and dynamic weight averaging using a range of threshold values to the truth-membership values ($T >$ threshold values) and to the false-membership values ($F <$ threshold values).

Table V shows the classification accuracy for the test data set using our proposed ensemble techniques including the accuracy obtained from the existing techniques that apply only truth-membership values and the accuracy obtained by applying only false-membership values. The comparison of accuracy among these techniques shows that the accuracy obtained from our proposed techniques using both truth-membership and false-membership values is similar to the accuracy obtained from the existing techniques using only truth-membership values and also similar to the accuracy obtained from the techniques using only false-membership values. In dynamic weight averaging technique, the uncertainty or indeterminacy-membership values are integrated into the truth-membership and false-membership values to support the confidence of the prediction. This proposed technique provides a slightly better accuracy than the other ensemble techniques shown in this paper. Furthermore, all our proposed techniques can represent uncertainty in the prediction for each cell location.

Table VI shows sample outputs from ensemble of neural networks using dynamic weight averaging by considering the comparison between truth-membership and false-membership values ($T_D(y) > F_D(y)$). Quantification of uncertainty can support the decision making. For example, the third row of this table contain the uncertainty value 0.2949 in which the decision maker can accept this result with more confidence. Sometimes, uncertainty for a cell is high. For example, the fourth row and the seventh row of this table contain very high uncertainty values which are 0.9475 and 0.9716, respectively. The truth-membership and false-membership for each of these cells are very close together. The cell at the fourth row is predicted to be a deposit which is correct. The cell at the seventh row is also predicted to be a deposit but it is incorrect. In this case, the decision maker can remake decision for the cells that contain high degree of uncertainty.

TABLE I
RESULTS FOR THE TEST DATA SET OBTAINED BY APPLYING A RANGE OF THRESHOLD VALUES TO THE TRUTH-MEMBERSHIP VALUES OF INDIVIDUAL NEURAL NETWORKS

Threshold value	BPNN %correct	GRNN %correct	PNN %correct
0.1	60.49	43.21	53.09
0.2	67.90	64.20	58.02
0.3	71.60	65.43	66.67
0.4	75.31	76.54	74.07
0.5	80.25	80.25	75.31
0.6	79.01	81.48	74.07
0.7	74.07	72.84	70.37
0.8	64.20	62.96	66.67
0.9	58.02	56.79	62.96

V. CONCLUSIONS

In this paper, interval neutrosophic sets are integrated into ensemble of neural networks to predict degrees of favourability for deposits and barrens. They are also used to quantify uncertainty in the prediction. Three pairs of neural networks are trained using three different neural network architectures in order to provide three interval neutrosophic sets which are then combined using our proposed aggregation techniques. The three neural network architectures used in this paper are feed-forward backpropagation neural network, general regression neural network, and polynomial neural network. The experimental results show that our proposed ensemble techniques provide similar accuracy to other existing ensemble techniques applied in this paper. Results from the experiments have not identified any approach which is able to provide a significant improvement over the others. However, the dynamic averaging approach has a slightly better performance. The key contribution in this study is that all the proposed techniques are capable of representing uncertainty in the prediction of favourability for each cell location. While this paper focuses only on the uncertainty in the prediction output, research is continued on the assessment of uncertainty in the GIS input data prior to applying to the prediction system.

TABLE II
RESULTS FOR THE TEST DATA SET OBTAINED BY APPLYING A RANGE OF THRESHOLD VALUES TO THE FALSE-MEMBERSHIP VALUES OF INDIVIDUAL NEURAL NETWORKS

Threshold value	BPNN %correct	GRNN %correct	PNN %correct
0.1	56.79	56.79	58.02
0.2	59.26	62.96	59.26
0.3	71.60	72.84	65.43
0.4	75.31	81.48	67.90
0.5	72.84	80.25	69.14
0.6	70.37	76.54	64.20
0.7	64.20	65.43	62.96
0.8	58.02	64.20	59.26
0.9	49.38	43.21	50.62

TABLE III
RESULTS FOR THE TEST DATA SET OBTAINED BY APPLYING THE PROPOSED TECHNIQUES FOR INDIVIDUAL NEURAL NETWORKS

proposed technique	BPNN %correct	GRNN %correct	PNN %correct
$T\&F$	75.31	81.48	71.61
$T > F$	81.48	80.25	75.31

TABLE IV
RESULTS FOR THE TEST DATA SET USING EQUAL WEIGHT AVERAGING AND DYNAMIC WEIGHT AVERAGING TECHNIQUES OBTAINED BY APPLYING A RANGE OF THRESHOLD VALUES TO THE TRUTH-MEMBERSHIP (T) AND FALSE-MEMBERSHIP (F) VALUES

Threshold value	averaging (%correct) (T)	averaging (%correct) (F)	Dynamic weight averaging (%correct) (T)	Dynamic weight averaging (%correct) (F)
0.1	49.38	56.79	49.38	56.79
0.2	62.96	59.26	64.20	59.26
0.3	69.14	72.84	69.14	70.37
0.4	77.78	76.54	79.01	75.31
0.5	80.25	79.01	80.25	80.25
0.6	80.25	72.84	81.48	71.60
0.7	72.84	66.67	77.78	62.96
0.8	59.26	59.26	67.90	56.79
0.9	56.79	46.91	56.79	46.91

TABLE V

CLASSIFICATION ACCURACY FOR THE TEST DATA SET USING THE PROPOSED TECHNIQUES AND THE EXISTING TECHNIQUES

Ensemble Technique	Deposit cell (%correct)	Barren cell (%correct)	Total cell (%correct)
Majority voting (T)	82.86	78.26	80.25
Majority voting (F)	71.43	86.96	80.25
Majority voting (T&F)	68.57	86.96	79.01
Majority voting (T>F)	85.71	76.09	80.25
Averaging (T)	82.86	78.26	80.25
Averaging (F)	80.00	80.43	80.25
Averaging (T&F)	80.00	80.43	80.25
Averaging (T>F)	82.86	78.26	80.25
Dynamic averaging (T)	80.00	82.61	81.48
Dynamic averaging (F)	80.00	78.26	79.01
Dynamic averaging (T&F)	80.00	82.61	81.48
Dynamic averaging (T>F)	82.86	78.26	80.25

TABLE VI

SAMPLE OUTPUTS FROM ENSEMBLE OF NEURAL NETWORKS USING DYNAMIC WEIGHT AVERAGING ($T > F$) FOR THE TEST DATA SET

Actual Cell Type	Predicted Cell Type	Truth-Membership	False-Membership	Indeterminacy Membership
Deposit	Deposit	0.8326	0.2529	0.4203
Deposit	Barren	0.4198	0.6762	0.7436
Deposit	Deposit	0.8348	0.1298	0.2949
Deposit	Deposit	0.5674	0.5149	0.9475
Barren	Barren	0.1629	0.8686	0.2943
Barren	Deposit	0.6104	0.4556	0.8452
Barren	Deposit	0.5181	0.4898	0.9716
Barren	Barren	0.3079	0.6538	0.6542

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