Adaptive neuro-fuzzy inference system classifier with interpretability for cancer diagnostic

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Received 12 Sep 2022; Revised 6 Dec 2022; Accepted 15 Dec 2022; Published 30 Dec 2022.
DOI: https://doi.org/10.54939/1859-1043.j.mst.CSCE6.2022.56-64

ABSTRACT

Clinical outcome analysis using patient medical data facilitates clinical decision-making and increases prognostic accuracy. Recently, deep learning (DL) with learning big data features has shown expert-level accuracy in predicting clinical outcomes. Many of these sophisticated machine learning models, however, lack interpretability, creating significant trust-related healthcare issues. This necessarily requires the need for interpretable AI systems capable of explaining their decisions. In this respect, the paper proposes an interpretable classifier of the adaptive neuro-fuzzy inference method (iANFIS), which combines the fuzzy inference system with critical rule selection by attention mechanism. The rule-based processing of ANFIS helps the user to understand the behavior of the proposed model. The essential activated rule and the most important input features that predict the outcome are identified by the attention-based rule selector. We conducted two experiments with two cancer diagnostic datasets to verify the performance of the proposed iANFIS. By using recursive rule elimination (RRE) to prune fuzzy rules, the model's complexity is significantly reduced while preserving system efficiency that makes it more interpretable.

Keywords: Neuro-fuzzy network; Attention; iANFIS; Interpretable AI; Cancer diagnostic.

1. INTRODUCTION

Recent advances in medicine have allowed a large amount of patient medical data to be accessible to medical practitioners. Predicting clinical results from this data is one of the most challenging tasks. Because early detection and prognosis of cancer can improve treatment decisions and promote subsequent clinical management of patients, there has been a surge of work on predictive models for early prediction of cancer. A majority of them used machine learning (ML) methods to identify critical features from complex data in artificial intelligence (AI) applications, resulting in efficient and precise decision making [1]. Nevertheless, conventional ML algorithms used pre-engineered features to create predictions, which has limited their usefulness in clinical practice.

With recent advances in deep learning, there has been a surge of research on AI applications in medicine to improve diagnosis [2], classification, and prediction [3]. Predicting clinical outcomes using machine learning has been attempted in [3]. Identification of biomarkers useful for cancer diagnosis using stacked denoising autoencoder (SDAE) was attempted in [2]. Another model was proposed by Al-Bahrani et al. in [4] based on deep neural networks (DNNs) [5] combines convolutional and recurrent architectures to train a deep network to predict CRC outcome based on images of tumor tissue samples. Unfortunately, most of those models are hard to interpret, making it hard for medical practitioners to trust the result.

The extraction of rules is an approach that reveals the hidden behavior of the network. Simple rule-based approaches, such as decision lists, decision trees, or simple IF-THEN rules, provide a more intelligible explanation of decision-making processes. Fuzzy Inference Systems (FIS) makes the decision process more humanely interpretable by utilizing the fuzzy rule-based reasoning [6]. Adaptive neuro-fuzzy inference system (ANFIS) [7] uses neural networks to tune fuzzy rule-based systems by automatically learning the fuzzy membership functions and, as a result, deriving fuzzy rules from a large amount of training data. While ANFIS has shown significant improvements in classification accuracy, it remains challenging to interpret thousands of fuzzy rules and criteria for high dimensional application problems. Therefore, there are two contradictory standards concerning the optimization of fuzzy structures, i.e., interpretability and accuracy. It is assumed that the simultaneous optimization of both would improve device performance.

For compromising between model interpretability and predictive efficiency, this paper proposes an interpretable ANFIS (iANFIS) classifier. The proposed system benefits from the FIS's rules-based structure that helps explain why a classification category has been chosen. The system of attention is based dynamically on more specific rules to enhance interpretability. The proposed iANFIS is tested on two diagnostic cancer problems: the prediction of colorectal cancer recurrence (CRC) and the classification of breast cancer. After the model has been conditioned, we can further decrease the size of the ruleset using recursive rule elimination (RRE), which reduces the model's complexity.

The paper is structured as follows: In the next section, we describe the proposed architecture of the iANFIS model. Section 3 addresses the experiment and results. We summarize our findings in the last section and present our future plans.

2. INTERPRETABLE ANFIS (IANFIS)

As one of the most commonly used fuzzy classifiers, the ANFIS takes its fuzzy rules in the following form [8]:

Rule k: If $x_1$is μ_{k1} And x_2 is μ_{k2} And, ..., And x_n is μ_{kd} then y_k = f_k(x), $k = 1,2,\ldots,K$

where μ_{ki} is a fuzzy set subscribed by the input variable x_i for the kth rule, K is the number of fuzzy rules, and And is a fuzzy conjunction operator. Each rule is premised on the input vector $x = [x_1, x_2, \ldots, x_n]^T$ and maps the fuzzy sets into the input space $\mu_k \subset R^d$ to a function $f_k(x)$ as its output.

The operation of an ANFIS is described in Fig. 1. Each node of the input layer corresponds to one input feature. If necessary, the node scales the input to the range as the universe of discourse and forwards it to the layer 1. In layer 1, each node is a fuzzy transformation node which calculates a membership value corresponding to its fuzzy set μ_{kj}, with Gaussian membership function given by Eq. (1) as:

$$\mu_{kj}(x_j) = exp(-(\frac{(x_j - m_{kj})^2}{\sigma_{kj}^2})) \tag{1}$$

where m and σ denote the mean and variant of the Gaussian fuzzy set, respectively. m and σ are antecedent parameters of ANFIS. The number of fuzzy sets in each node is equal to the number of antecedent values of the fuzzy rules. In layer 2, each node represents a fuzzy logic rule and performs antecedent matching of this rule using the following AND operation:

$$w_k(\tilde{x}) = \prod_{j=1}^{n} \mu_{kj}(x_j) \tag{2}$$

where $x = [x_1, \ldots, x_n]$. The number of nodes in this layer is equal to the number of rules K. Layer 3 includes normalizing nodes. The ith node calculates the ratio of ith rule's firing strength to the sum of all rule's firing strengths using:

$$\overline{w}_i = \frac{w_i}{\sum_{j=1}^{R} w_j}, i = 1, \ldots, K \tag{3}$$

Consequently nodes in layer 4 are linear functions of inputs as shown in Eq.5. Combination of layer 4 and layer 5 works as a defuzzifier which uses the weighted average operation in Eq. (4)

$$\hat{y} = \sum_{i=1}^{K} \overline{w}_i f_i = \sum_{i=1}^{K} \overline{w}_i \left(\sum_{j=1}^{K} p_{ij} x_j + q_i\right) \tag{4}$$

where p, q are consequent parameters of the ANFIS. Fig. 2 shows the proposed iANFIS. The attention-based fusion operator first weighs and then sums multiple input rules into a single representation. The rules-specific attention weights are computed by neural networks integrated into an end-to-end model such that a single back-propagation learning process is sufficient. This attention mechanism allows the model to tune its attention towards more task-informative rules dynamically.

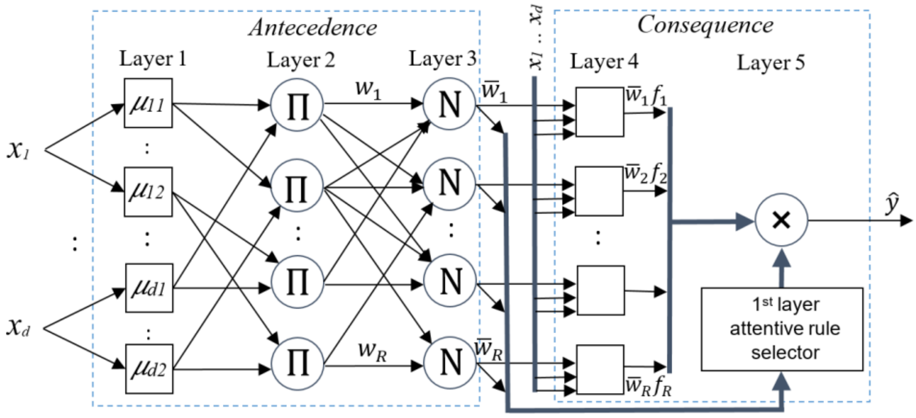

Figure 1. *iANFIS with attentive rule selector.*

For all the iANFIS component units, we choose three membership functions corresponding to three partitions with respective linguistic values as low, $medium$, $high$. The output of the attentive rule selector is a scoring vector of size R with near-zero value for all the elements except for the selected rule with a value near-one. By multiplying the ANFIS output of layer 4 with the scoring vector, only the selected rule's activation value is passed to the output, as shown in Eq. 5

$$\hat{y} = ratt(\mathbf{H}, \mathbf{w}) \sum_{i=1}^{R} \overline{w}_i f_i = ratt(\mathbf{H}, \mathbf{w}) \sum_{i=1}^{R} \overline{w}_i \left(\sum_{j=1}^{R} p_{ij} x_j + q_i\right) \tag{5}$$

where $\overline{w}_i$ is normalized firing strength of $i - th$ rule. p and q are consequent parameters of the ANFIS, and $ratt(.)$ is an attention module based on multilayer perceptron (MLP) [9]. Eq. 6 describes the working of the attentive rule selector unit.

$$ratt(\mathbf{H}, \mathbf{w}) = softmax(S)\mathbf{w} \tag{6}$$

where S is computed by Eq. 7, and v_0 and H_w are learned attention parameters.

$$S_{ij} = v_0^T tanh(H_w w_j) \quad (7)$$

2.1. ANFIS classify layer

The last layer of the proposed iANFIS is a classified layer. As shown in Fig. 2, the ANFIS classifier is the integration of the ANFIS's consequence layers and a softmax layer. The consequence part of the ANFIS includes multiple consequence units. Each unit receives the same output from the premise part and computes output value corresponding to one class. Thus, the number of units is corelative with the number of classes that model classifies. The softmax layer is a normalized exponential function that calculates the probabilities for each class in a multi-class problem. By integrating with a softmax layer, the ANFIS classifier can be a multi-class classifier so that the iANFIS can also be applied to any multi-class classifier problem.

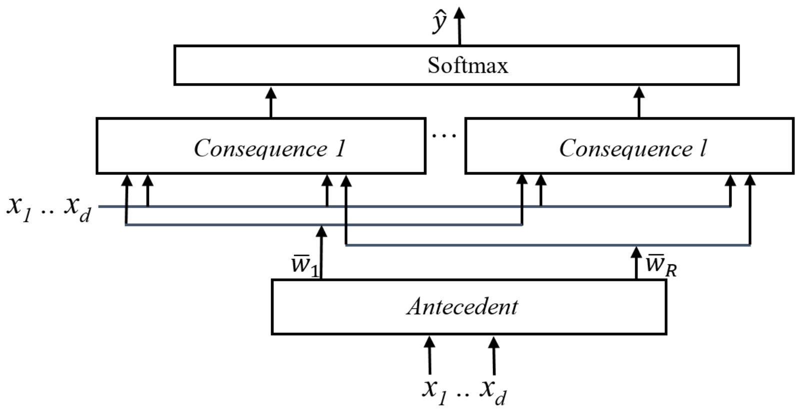

Figure 2. *ANFIS classify layer.*

2.2. iANFIS training

```
Input          : Training samples X and corresponding
                 labels y, hyper-parameters (learning
                 rates α_ant and α_cons; batch number B;
                 dropout rate; training epoch number N)
Output         : Trained parameters of iANFIS (m, σ, p,
                 q)
Initialization: Randomly initialize antecedent
                 parameters m, σ and consequence
                 parameters p, q
for e=1 to N do
    for b=1 to B do
        X^b ← iANFIS(X^b);
        ŷ^b = clfANFIS(X^b);
        E^b ← crossentropy(y^b, ŷ^b);
        (m^(t+1), σ^(t+1), p^(t+1), q^(t+1)) ←
          update(E^b, m^(t), σ^(t), p^(t), q^(t));
    end
end
```

Algorithm1. *Training procedure of the proposed iANFIS.*

The iANFIS model is first initialized by setting initial parameters for all component units. Each component iANFIS is initialized with M Gaussian membership functions corresponding to the range of its input value. The fuzzy rule set is randomly assigned a number of rules, which is ten times the number of antecedents.

The parameters of the model are trained by Adam algorithm [10] with the cross-entropy loss function. For a given training dataset with feature set X and target y, we apply mini-batch training procedure to gain the best parameters of the iANFIS. The mini-batch training also helps reduce the computation complexity because of the large number of initial rules of the iANFIS model. The hyper-parameters, such as learning rates, batch size, and dropout rate, are chosen by a hyperparameter optimization framework called Optuna [11]. The antecedent and consequence parameters have unique learning rates while updating. The training process for iANFIS with back-propagation strategy is summarized in Algorithm 1.

3. EXPERIMENTS AND RESULTS

We verify the performance of the proposed iANFIS on two cancer diagnostic problems: colorectal cancer recurrence prediction problem and breast cancer diagnostic problem.

3.1. Colorectal cancer recurrence prediction

3.1.1. Dataset and data preprocessing

CRC dataset is a medical data of patients, including information of 5,376 patients (non-recurrence: 4,399, recurrence: 977) who had undergone CRC surgery. Each sample has 30 variables recorded from an operation. Based on the data, we want to predict the postoperative recurrence of cancer in patients. We separate the dataset to training data of 5,176 samples (non-recurrence: 4,299, recurrence: 877), 100 validation data samples 100 test samples with 50% recurrence, respectively.

To overcome the imbalance in training data, we employ the Synthetic Minority Oversampling Technique with Edited Nearest-Neighbours (SMOTEENN) method [12]. Firstly, we apply SMOTE, which does over-sampling by generating new samples by interpolating with some of the original samples of the minority class. Then, a cleaning method called edited nearest-neighbors (ENN) is used to obtain a cleaner space [12]. Thus, we get 6,185 samples of a balanced training set.

3.1.2. Model configuration

Table 1. *iANFIS Model Hyper-Parameters for CRC recurrence prediction.*

Hyper-Parameter	**Value**
Number of Epochs	2,000
Learning rate	Antecedent: 0.006
	Consequence: 0.08
	Others: 0.00002
Weight decay	2.5e-6

We use a multi-layer neural perceptron (MLP), support vector machine (SVM), and ANFIS as three traditional machine learning models for comparing the performance with the proposed model. The structure and the detailed settings of the hyperparameters for training the iANFIS model for the CRC experiment are illustrated in table 1. The optimal hyper-parameters of the SVM were selected by grid search, which are: kernel = ‘poly’; degree = 3; C = 0.35; coef0 = 0.125, gamma = 0.0625. We also choose MLP parameters by empirical with standard setting. ANFIS and iANFIS have the same parameter sets.

For iANFIS, we use Optuna [11] to find the optimal hyper-parameters as shown in table 1. We initialize the rule set for both models (ANFIS and iANFIS) using training samples, and the number of rules is 1,813. Our implementation uses the PyTorch framework on Ubuntu 16.04 system. The training process for iANFIS takes approximately 14 minutes on Titan V GPU.

3.1.3. Results

We train and test the prediction models by repeating the experiment 10 times. The average test accuracy and variances are then calculated, as summarized in table 2. As the result shows, the average F-scores of the classification models are 0.7548, 0.7664, 0.7721, and 0.7832 for the MLP, SVM, ANFIS, and iANFIS, respectively. The results show that the ANFIS related models perform better than the traditional models. The attention mechanism helps iANFIS to get a higher F-score than ANFIS.

Table 2. *Comparison of average classification F-score of SVM, ANFIS, and iANFIS for CRC dataset.*

	MLP	**SVM**	**ANFIS**	**iANFIS**
Average	0.7548	0.7664	0.7721	0.7832
STD	0.0093	0.0115	0.0168	0.0195

3.2. Breast cancer diagnostic

The second dataset we use for the experiment is Wisconsin Diagnostic Breast Cancer (WDBC) [13]. This dataset contains a record of 569 subjects with 32 tumor features, which has been obtained from a digital image of breast Fine Needle Aspirates (FNA). There are 30 actual tumor features, and the other two represent the subject ID and the class label, respectively. The binary class label determines whether the subject belongs to the benign or the malignant tumor class. From the digital image of breast FNA, ten attributes of cell nuclei, which include radius, texture, points, fractal dimension, perimeter, area, concavity, symmetry, smoothness, and compactness, are recorded for each subject. In table 3, the calculations (values of mean, standard deviation, and maximum) for deriving the 30 features from these ten attributes have been presented.

Table 3. *Wisconsin Diagnostic Breast Cancer dataset description.*

Index	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
Feature	**Radius mean**	**Texture mean**	**Perimeter mean**	**Area mean**	**Smoothness mean**	**Compactness mean**	**Concavity mean**	**Concave points mean**	**Symmetry mean**	**Fractal dimension mean**	**Radius SE**	**Texture SE**	**Perimeter SE**	**Area SE**	**Smoothness SE**
Abbr.	**RdM**	**TM**	**PM**	**AM**	**SmM**	**CmM**	**CnM**	**CpM**	**SM**	**FdM**	**RSE**	**TSE**	**PSE**	**ASE**	**SmSE**

Index	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
Feature	**Compactness SE**	**Concavity SE**	**Concave points SE**	**Symmetry SE**	**Fractal dimension SE**	**Radius max**	**Texture max**	**Perimeter max**	**Area max**	**Smoothness max**	**Compactness max**	**Concavity max**	**Concave points max**	**Symmetry max**	**Fractal dimension max**
Abbr.	**CmSE**	**CSE**	**CpSE**	**SSE**	**FSE**	**RMx**	**TMx**	**PMx**	**AMx**	**SmMx**	**CmMx**	**CnMx**	**CpMx**	**SMx**	**FMx**

3.2.1. Model configuration

The parameter sets of SVM, ANFIS and iANFIS are inherited from CRC dataset experiment.

The optimal hyper-parameters of iANFIS obtained by Optuna are showed in table 4.

The rule set for all three neural-fuzzy models is initialized by using training samples. ANFIS and iANFIS have the same ruleset with 2,531 rules.

Table 4. *iANFIS Model Hyper-Parameters for breast cancer diagnostic.*

Hyper-Parameter	**Value**
Number of Epochs	1,000
Learning rate	Antecedent: 0.0232
	Consequence: 1.6358
	Others: 0.00047
Weight decay	4e-7
Dropout rate	0.23

3.2.2. Results

We train and test the prediction models by repeating the experiment 10 times. The average of test accuracy and variances are then calculated, as summarized in table 5. As the result shows, the average F-scores of breast cancer classification is 0.965, 0.969, 0.9760, and 0.9813 for the MLP, SVM, ANFIS, and iANFIS, respectively. The results show that the ANFIS related models perform better than the traditional models. Attention mechanism helps iANFIS get a higher f-score than ANFIS, and the iANFIS can get the best performance among all the comparison models.

Table 5. *Comparison of average classification F-score of SVM, ANFIS, and iANFIS for breast cancer diagnostic dataset.*

	MLP	**SVM**	**ANFIS**	**iANFIS**
Average	0.965	0.969	0.9760	**0.9813**
STD	0.0095	0.0126	0.0186	0.0235

After training the ANFIS regressions and the ANFIS classifier, we get the insight into its behavior by extracting their fuzzy rule set. To extract the rule set for negative and positive classes, we use the train dataset corresponding to each class and obtain the rules related to that class. From this fuzzy rule set extracted, we can interpret which antecedents contribute more to the classification of cancer.

The extracted fuzzy rule sets can be used to interpret the behavior of the model. But the number of rules is still high. Therefore, it makes the high complexity and lowers the interpretability of the model. To reduce the number of rules while retaining the performance of the model, we propose a new rule reduction method called recursive rule elimination (RRE). In this method, we recursively remove rules and analyze the change in model performance. If the performance does not decrease, the rules can be removed permanently. The RRE extracts 216 critical rules from a total of 1,813 original rules of iANFIS for CRC dataset and 308 out of 2,531 rules from video modality. Thus, the number of rules is dramatically reduced to about ten percent of the original rule sets.

Fig. 3 illustrates the final ruleset's antecedents of iANFIS for breast cancer diagnostic problems. The ruleset is separated into negative and positive set. Positive and negative rulesets are represented in upper and lower parts, respectively. Each row represents the antecedents of a rule in the ruleset, each cell of a row is an antecedent of the rule. The red, white, and blue cells denote the low, $medium$, and $high$ value of membership functions. By analyzing this ruleset, we can understand the critical variables and their contribution to the classification performance.

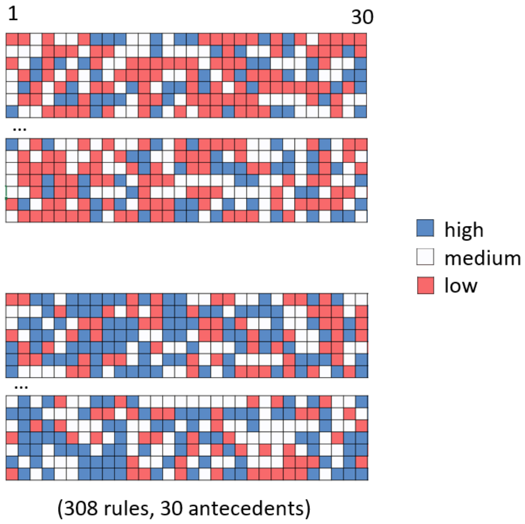

Figure 3. *Critical rule sets selected from breast cancer diagnostic dataset.*

Deriving from Fig.3 and table 3, the first rule (corresponding the first row in Fig.3) can be interpreted as a fuzzy rule as follows:

IF ***RdM*** *is* ***low*** *and* ***TM*** *is* ***low*** *and* ***PM*** *is* ***medium*** *and ... and* ***CpM*** *is* ***high*** *and ... and* ***FMx*** *is* ***low*** THEN ***tumor*** *is* ***benign***

4. CONCLUSIONS

Fuzzy modeling has many advantages over non-fuzzy methods, such as robustness against uncertainties, less sensitivity to the varying dynamics of nonlinear systems, and transparency of the decision processes. This paper takes advantage of fuzzy modeling, attention mechanism, and proposes a hybrid learning based neuro-fuzzy model, called iANFIS, which integrates fuzzy inference system attention mechanism, for cancer diagnostic datasets. The results show that iANFIS can achieve better classification accuracy on cancer data than conventional approaches such as MLP, SVM, and ANFIS. The proposed iANFIS can interpret the inference process for diagnostic using fuzzy if-then rules and their contribution to the prediction performance. We intend to develop a higher hierarchical structure that utilizes the deep learning method with more interpretability in the future.

Acknowledgement: *This work was supported by Thainguyen University of Technology.*

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TÓM TẮT

Bộ phân lớp dựa trên suy diễn nơ-ron mờ thích nghi với tính diễn giải được cho chẩn đoán bệnh ung thư

Phân tích kết quả lâm sàng sử dụng dữ liệu y tế của bệnh nhân tạo điều kiện thuận lợi cho việc ra quyết định lâm sàng và tăng độ chính xác của tiên lượng. Gần đây, học sâu (DL) với tính năng học tập dữ liệu lớn đã cho thấy độ chính xác cấp chuyên gia trong việc dự đoán kết quả lâm sàng. Tuy nhiên, nhiều mô hình học máy tinh vi này thiếu khả năng diễn giải, tạo ra các vấn đề liên quan đến chăm sóc sức khỏe đáng tin cậy. Điều này đòi hỏi sự cần thiết của các hệ thống AI có thể diễn giải có khả năng giải thích các quyết định của chúng. Về mặt này, bài báo đề xuất một bộ phân loại có thể diễn giải của phương pháp suy luận nơ-ron mờ thích nghi (iANFIS), kết hợp hệ thống suy luận mờ với trich chọn luật mờ bằng cơ chế attention. Quá trình xử lý dựa trên luật của ANFIS giúp người dùng hiểu được hành vi của mô hình được đề xuất. Luật mờ được kích hoạt và các tính năng đầu vào quan trọng nhất giúp dự đoán kết quả được xác định bởi bộ chọn luật mờ dựa trên attention. Chúng tôi tiến hành hai thử nghiệm với hai bộ dữ liệu chẩn đoán ung thư để xác minh hiệu suất của iANFIS được đề xuất. Bằng cách sử dụng phương pháp loại bỏ quy tắc đệ quy (RRE) để loại bỏ các quy tắc mờ, độ phức tạp của mô hình được giảm đáng kể trong khi vẫn duy trì hiệu năng của hệ thống khiến nó dễ diễn giải hơn.

Từ khoá: Mạng nơ-ron mờ; Attention; iANFIS; AI diễn giải được; Chẩn đoán ung thư.