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Addressing class imbalance with FSVM and interpreting key determinants in thyroid diagnosis through Explainable AI

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***Abstract*—Thyroid disease is recognized as one of the most prevalent medical diseases, disrupting the ability of the thyroid gland to function properly. Several machine learning algorithms like DT, KNN, LR, SVM, Random Forest, and XGBoost have been utilized to predict thyroid conditions. However, these models suffer from class imbalance and operate as black-box systems with restricted interpretability. This study aims to offer an efficient method named Fuzzy Support Vector Machine (FSVM) to address the class imbalance problem and reduce false positives in thyroid diagnosis. In addition, explainable AI approaches such as LIME and SHAP are used to increase the model interpretability and elucidate the predictive nature of the model. Linear and exponential FSVM have been applied to a thyroid dataset from Kaggle by assigning fuzzy memberships based on the distances from feature thresholds. The findings indicate that the FSVM enhances accuracy, with linear FSVM obtaining 96.65% and exponential FSVM achieving 97.22%, beating the standard SVM and other existing methods. Key clinical measurements such as TSH, FTI, and T4 are crucial for an accurate thyroid diagnosis. Moreover, pregnant women are at an increased risk of thyroid illness. Notably, the thyroxine dosage has been discovered as an essential treatment for thyroid patients.**

***Index Terms*—Fuzzy Support Vector Machine (FSVM), Class Imbalance Problem, Thyroid Disease, LIME, SHAP.**

I. Introduction

Thyroid disease is a medical condition that harms the function of the thyroid gland. It prevents the gland from producing the right amount of hormones, leading to problems such as weakness, weight gain, etc [1]. Due to the high prevalence of thyroid disorder, medical professionals and researchers have always shown interest in it. Chinese ancient literature from as far back as 2700 BC contains references to goitre. Considerable contributions to medicine were made by Greek, Byzantine, Egyptian, Chinese, and Indian systems [2]. However, these traditional methods are time-consuming and lack precise detection for diagnosing a huge population.

Supervised machine learning algorithms can be beneficial in detecting thyroid disease. The existing machine learning models, such as Support Vector Machine, Decision Tree, Logistic Regression, Naive Bayes, K-nearest neighbors, Random Forest, and XGBoost, have obtained excellent accuracy but faced difficulty classifying imbalanced datasets [3].

Various methods have been adopted to address the issue of class imbalance in recent years. The SMOTE method balances datasets using synthetic samples [4]. Nevertheless, it is not an optimal solution as the new data are synthetic and lack rationality. Ensemble techniques give better predictive performance by combining the predictions of multiple weak learners [5]. However, output forecasting is difficult due to its complexity, making it less interpretable.

The existing works have struggled with imbalanced datasets. Besides, complex machine learning algorithms are regarded as black boxes due to their insufficient clarity. This limitation leads to problems in critical fields like disease diagnosis, where understanding the reasoning of a prediction is crucial. FSVM has been applied in this study with a fuzzy membership function that is based on the distance of data from the significant feature threshold. Additionally, explainable AI techniques are proposed to explain the prediction of the FSVM model. The key contributions are stated as follows:

1) The proposed approach of applying FSVM has boosted the performance of the imbalanced thyroid diagnosis by assigning feature-based fuzzy membership.
2) The LIME method has interpreted individual thyroid predictions and provided insights into the model.
3) The SHAP technique has provided a global interpretation of the FSVM model while demonstrating the contribution of the risk factors in thyroid disease.

The structure of this work is as follows: Past research results are presented in section II, methodology is covered in section III, findings are explained in section IV, and the conclusion is included in section V.

II. Related Works

Previous work shows that H. Kumar et al. [6] applied an SVM model to the UCI thyroid dataset, which was imbalanced, reaching an accuracy of 83.37%, but the f1 scores were below average due to class imbalance. Then A. M. Ali et al. [7] employed Logistic Regression, SVM, and Random Forest on an imbalanced thyroid dataset, with Random Forest gaining a 95% accuracy rate. However, the performance of the minority

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class was not inspected or mentioned. Agarwal et al. [8] used SMOTE to balance an imbalanced thyroid disease dataset and then compared machine learning algorithms, where the RF outperformed the other methods. Similarly, W. Chaipanha et al. [9] applied SMOTE and random under-sampling strategies to balance an imbalanced car ownership dataset. Though the KNN model achieved TPR ranges from 54.4% to 63.5%, multiclass had affected the minority class prediction. P. Kumari et al. [10] employed RF, SVM, and XGBoost models on an imbalanced thyroid dataset, where the ensemble method reached 99% accuracy. G. Obaido et al. [11] offered the stacking ensemble technique for thyroid illness detection using clinical datasets, which achieved 99.9% ROC-AUC and outperformed single-model results. Regardless, ensemble methods require high computational resources. Alyas et al. [12] proposed some ML methods in the thyroid dataset. The RF achieved 84.4% of sensitivity, indicating poor performance because of the class imbalance in the positive class.

Contrasting these approaches, the proposed FSVM classifies thyroid illness to handle class imbalance. Beside, the explainable AI (LIME and SHAP) techniques improve model interpretability, overcoming the black box limitation.

III. Methodology

The methodology of the Fuzzy SVM model is represented in Fig. 1, including data preprocessing, implementation of the FSVM, evaluation and interpretation using LIME and SHAP.

A. Data Collection:

The Thyroid Disease Patient dataset obtained from Kaggle contains 3770 instances and 30 attributes, including demographic data (age, sex), medical history, patient's health status, laboratory test outcomes such as TSH, T4, FTI, etc. [13].

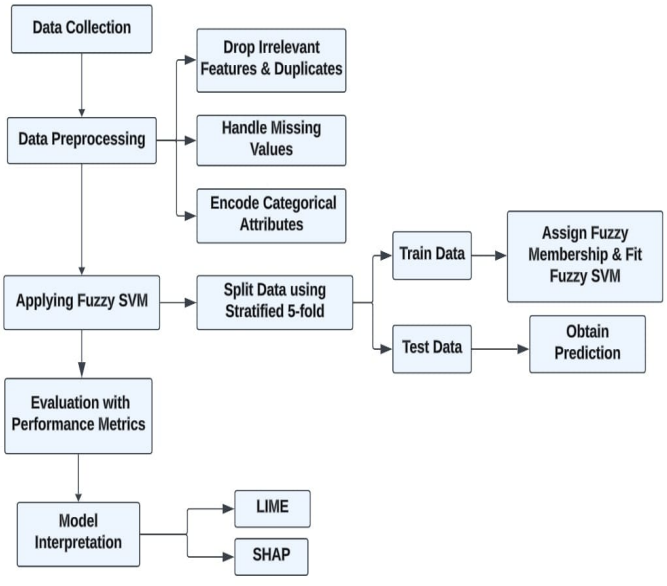


Fig. 1: Workflow diagram of the proposed method.

B. Feature Threshold:

Two key attributes are selected using Pearson, Spearman, and Kendall correlation methods, which measure coefficients to quantify the association between two variables [14]. The mean values, representing the central tendency of the dataset, act as effective thresholds to identify critical data.

C. Fuzzy SVM using Feature-Based Fuzzy Membership:

The optimal hyperplane of the SVM model can be found by solving the soft-margin optimization problem:

$$\begin{aligned} &\text{Min}\left(\frac{1}{2}w\cdot w + C\sum_{i=1}^{l}\varepsilon_i\right) \\ &\text{s.t. } y_i\left(w\cdot\phi\left(x_i\right)+b\right)\geq 1-\varepsilon_i \\ &\varepsilon_i > 0, i=1,\ldots,l \end{aligned} \tag{1}$$

C represents the misclassification cost of data. Incorporating fuzzy membership [15], the optimization problem is revised as:

$$\begin{aligned} &\text{Min}\left(\frac{1}{2}w\cdot w + C\sum_{i=1}^{l}m_i\varepsilon_i\right) \\ &\text{s.t. } y_i\left(w\cdot\phi\left(x_i\right)+b\right)\geq 1-\varepsilon_i \\ &\varepsilon_i > 0, i=1,\ldots,l \end{aligned} \tag{2}$$

Where, the membership function m_i is formulated as:

$$\begin{aligned} m_i^+ &= f\left(x_i^+\right)r^+ \\ m_i^- &= f\left(x_i^-\right)r^- \end{aligned} \tag{3}$$

$r^- = 1$ and $r^+ =$ minority to majority ratio, which assigns higher membership to the minority (negative) class data. $f\left(x_i\right)$ is the fuzzy membership function for x_i data denoted as:

$$f\left(x_i\right) = \alpha\cdot f_1\left(x_i\right) + \beta\cdot f_2\left(x_i\right) \tag{4}$$

Here, $f_1\left(x_i\right)$ and $f_2\left(x_i\right)$ are the feature-based memberships of two most significant features. $\alpha = 1$ and $\beta =$ average coefficient ratio of f_2 and f_1, which adjust the contribution of both features. Two functions are used to calculate the fuzzy membership. Firstly, the linear function is stated below, where a small positive value Δ is added to avoid zero:

$$f_{\text{lin}}\left(x\right) = 1 - \frac{f_{\text{distance}}\left(i\right)}{\max\left(f_{\text{distance}}\right)+\Delta} \tag{5}$$

The following is the exponential function with the γ parameter controlling the function's steepness:

$$f_{\exp}(x) = \frac{2}{1+\exp\left(\gamma f_{\text{distance}}\left(i\right)\right)} \tag{6}$$

The distance is calculated from the feature threshold T:

$$f_{\text{distance}}\left(i\right) = \left|T - X_{fi}\right| \tag{7}$$

The FSVM model has been implemented using the RBF kernel with $C = 100$. In order to keep the class ratio constant, stratified 5-fold cross-validation has been utilized.

D. Evaluation Metrics:

Accuracy, sensitivity, specificity, and FPR [16] are utilized as performance metrics for the evaluation of the Fuzzy SVM model, along with Gmean [17] and ROC curve [18].

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} \tag{8}$$

Here, TP and TN are accurate diagnoses, whereas FP and FN are misclassified thyroid disorders.

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}} \tag{9}$$

$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}} \tag{10}$$

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}} \tag{11}$$

$$\text{G-Mean} = \sqrt{\text{Sensitivity} \cdot \text{Specificity}} \tag{12}$$

The ROC curve compares the TPR and FPR at different thresholds, while the AUC assesses the model's overall performance ranges from 0 to 1 [18].

E. LIME and SHAP Explanation:

a) LIME: LIME is an explainable AI technique that is used to grasp the decision-making process of the Fuzzy SVM. The method approximates the complex model with a linear interpretable model in the locality of the explained instance [19]. The explanation is defined as:

$$\xi(x) = \underset{g \in G}{\text{argmin}} L(f, g, \pi_x) + \Omega(g) \tag{13}$$

This function minimizes the loss function $L(f, g, \pi_x)$ and the complexity $\Omega(g)$. The loss function is formulated as follows:

$$L(f, g, \pi_x) = \sum_{z, z' \in Z} \pi_x(z)(f(z) - g(z'))^2 \tag{14}$$

Here, $f(z)$ is the original model, approximated by a surrogate model, which is measured as:

$$g(z') = w_g . z' \tag{15}$$

And the proximity measure $\pi_x(z)$, is defined as:

$$\pi_x(z) = \exp(-D(x, z)^2 / \sigma^2 \tag{16}$$

b) SHAP: SHAP provides a global interpretability on the model predictions through feature contributions and local explanations to help understand why the model made a certain decision [20]. Explanation of a prediction can be stated as:

$$g(z') = \phi_0 + \sum_{i=1}^{M} \phi_i z_i' \tag{17}$$

Here, ϕ denotes the shapely value of a feature:

$$\phi_i(f, x) = \sum_{z' \subseteq x'} \frac{|z'|!\,(M - |z'| - 1)!}{M!} [f(z') - f(z_i')] \tag{18}$$

Here, x' is the simplified input of x using $x = h_x(x')$. z' is the subset of x'. M is thenum ber of features and $|z'|$ is the number of features in the subset. $f(z')$ and $f(z_i')$ are the outcome of a subset with and without the feature i respectively.

IV. Result and Discussion

This section demonstrates an overview of the dataset with preprocessing, selected features, assigned fuzzy memberships, and description of the experimental results with observations.

A. Overview of Dataset and Preprocessing

The thyroid dataset contains a significant class imbalance ('P': 92.1%, 'N': 7.9%), reflecting thyroid negative as the minority class. 7 features have been dropped including an empty feature (TBG). TSHmeasured, T4measured, etc features are removed as they indicate whether the test was taken, which can be inferred from test results (e.g., TSH=0 means TSH_measured='f'). The missing values in the sex attribute have been replaced with mode as it is a categorical feature. Categorical features have been converted through label encoding ('t':1, 'f':0) along with class label ('P':1, 'N':0). Table I displays the data characteristics before and after preprocessing.

TABLE I: Overview of the Original and Preprocessed Dataset

Dataset	Datatype	Data	Features	Result
Original	Numerical: 7 Categorical: 23	3770	30	Pos: 3479 Neg: 291
Preprocessed	Numerical: 6 Categorical: 17	3706	23	Pos: 3415 Neg: 291

B. Feature Threshold Selection:

TSH ranks as the most important attribute according to the absolute of the coefficient values shown in Fig. 2, while FTI ratings place it as the second most significant feature. Closest data of the opposite classes cluster around the intersection of the mean lines (TSH and FTI), as illustrated in Fig. 3.

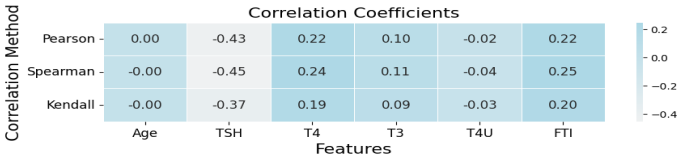


Fig. 2: Correlation coefficients of features.

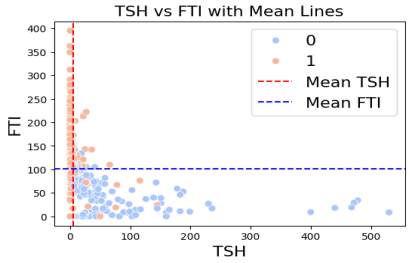


Fig. 3: Mean values as thresholds.

TABLE II: Fuzzy Membership of Training Data

Data	Index	Distance (TSH)	Distance (FTI)	Class	Linear	Exponential
1	38	1.742	9.663	1	0.126	0.026
2	45	4.342	70.338	1	0.117	0.002
3	52	4.142	35.338	1	0.122	0.003
4	115	4.259	30.338	0	1.44	0.028
5	121	4.859	26.667	0	1.446	0.016

C. Fuzzy Membership

Table II displays the assigned fuzzy memberships in five train samples. The 1st of three positive class data has obtained the highest memberships because of its lower distances. Although the distances from TSH threshold are nearly equal in the next two data points, lower memberships are assigned to the 2nd one (0.117 and 0.002) due to its high FTI threshold distance (70.338). The same event can be observed from the last two data points belonging to the negative class. There is a notable gap (1.32 and almost 0.02) between the memberships of the two classes, which indicates the efficacy of assigning higher membership to the minority class.

D. Experimental Results

The experiment result follows the steps stated below:

1) Exp. A: Evaluation of the Fuzzy SVM model.
2) Exp. B: Analysis of LIME Interpretation.
3) Exp. C: Key Findings of SHAP Investigation.

1) ***Result of Exp. A*** *:* Table III compares the SVM and Fuzzy SVM (Linear and Exponential) models, assessed with 5-fold cross-validation. The high sensitivity of the SVM indicates its ability to classify thyroid-positive patients accurately due to adequate data (3415). On the other hand, specificity results are in the range of 0.57 to 0.74, resulting in high FPRs (from 0.26 to 0.43). The model is unable to identify the negative class correctly due to insufficient data (291). The Gmean values show the imbalances (ranging from 0.75 to 0.86) between specificity and sensitivity. Although the model has low specificity, accuracy (95.55% to 96.90%) in each fold indicates the biasness of SVM towards the positive class. A significant growth can be observed in specificity in the FSVM models. Linear FSVM shows specificity values of 0.90 to 0.97, resulting in low FPR (0.034 to 0.1). Similarly in the exponential FSVM, high values of specificity (from 0.93 to 1.00) are noted. Especially the fold 2 has a perfect specificity score of 1.00. FPR values range from 0.0 to 0.069 in this case. The Gmean scores shown by the exponential FSVM are in the interval of 0.95 to 0.98. Linear FSVM demonstrates the geometric mean (Gmean) values from 0.93 to 0.97, indicating a balance in detecting both classes. The linear FSVM and exponential FSVM have an accuracy range of 95.56% to 97.57% and 96.22% to 97.57%, respectively. Assigning high membership values to the minority class data has contributed to the improved performance. As a result, the SVM has been outperformed by both linear and exponential FSVM, with average accuracy of 96.30%, 96.65%, and 97.22%, respectively.

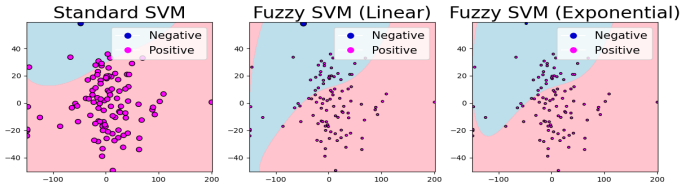
TABLE III: Result Comparison of Fuzzy SVM with SVM

Classifier	Fold	Sensitivity	Specificity	FPR	Gmean	Accuracy
SVM	1	0.99	0.61	0.39	0.78	96.23%
	2	0.99	0.57	0.43	0.75	95.55%
	3	0.99	0.74	0.26	0.86	96.76%
	4	0.99	0.59	0.41	0.76	96.09%
	5	0.99	0.72	0.28	0.85	96.90%
FSVM(Lin)	1	0.98	0.93	0.068	0.96	97.57%
	2	0.98	0.97	0.034	0.97	97.44%
	3	0.96	0.97	0.034	0.96	96.22%
	4	0.96	0.97	0.034	0.96	96.36%
	5	0.96	0.90	0.10	0.93	95.68%
FSVM(Exp)	1	0.98	0.98	0.017	0.98	97.71%
	2	0.97	1.00	0.00	0.99	97.57%
	3	0.97	0.98	0.017	0.98	97.44%
	4	0.98	0.93	0.069	0.95	97.17%
	5	0.96	0.95	0.052	0.96	96.22%

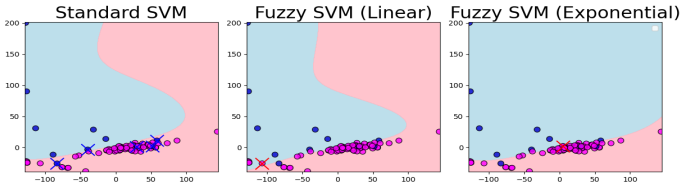
TABLE IV: Comparison of FSVM with Existing Approcahes

Research	Method	Accuracy	Sensitivity	Specificity
Alyas et al. [12]	RF	N/A	0.948	0.91
Mutasem [21]	HECFNN	96.10%	0.967	0.965
Proposed	FSVM(Exp)	**97.22%**	**0.97**	**0.97**

The exponential FSVM is compared with the existing thyroid classification approaches in Table IV since it has performed better than the linear FSVM. The exponential FSVM has surpassed the other models in terms of accuracy, sensitivity and specificity, which reflects its ability to be a benchmark for evaluating advanced models in thyroid diagnosis.



(a) Weighted train data



(b) Test data predictions

Fig. 4: Effect of fuzzy membership in decision boundary.

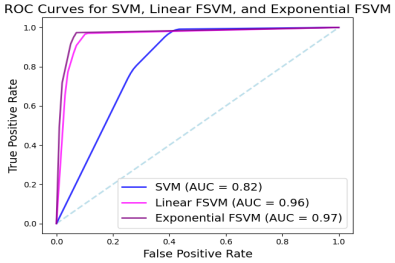
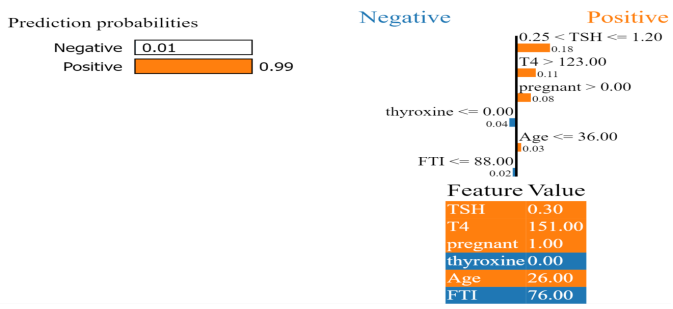


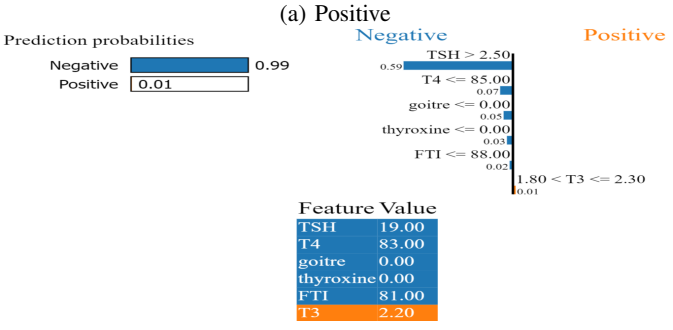
Fig. 5: ROC curve of SVM and Fuzzy SVM model.

- **Visualization of Fuzzy SVM Impact:** Fig. 4 (a) shows how fuzzy membership impacts the hyperplane. In the SVM plot, the negative train data get a smaller margin due to the lack of data. On the contrary, higher fuzzy memberships are assigned to these data in the FSVM model, contributing to the margin being far from negative class data. As a result, the hyperplane is more stretched in both of the FSVM models, indicating a larger margin for negative class data to obtain better prediction. In Fig. 4 (b), classification results of 100 test data can be observed in a 2D space. The SVM model has misclassified 5 negative samples. In contrast, only one wrong prediction is noticed in each of the Fuzzy SVMs, and there is no false positive. The decision boundaries of the Fuzzy SVMs are less tolerant of negative data being on the wrong side of the hyperplane. Due to the higher fuzzy membership, the FSVM ensures correct identification of the minority (negative) class data through a larger margin.

- **ROC Curve:** The ROC curve in Fig. 5 shows the tradeoff between TPR and FPR. The model performance is reflected by the area under curve (AUC). The effect of class imbalance is evident from the SVM curve being closer to the diagonal line (random performance). Increasing false positives reduces the overall performance of the SVM, resulting in an AUC of 0.82. Larger areas of 0.96 (linear) and 0.97 (exponential) are seen in the ROC curve of the FSVM models due to low FPR. Henceforth, the Fuzzy SVM is effectively minimizing false positives and enhancing class imbalance learning.



(a) Positive



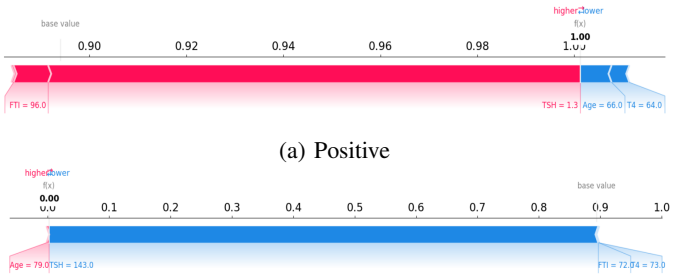
(b) Negative

Fig. 6: LIME explanation of prediction by linear FSVM.

*2) **Result of Exp. B**:* LIME interpretation for two predictions (positive and negative) is shown in Fig. 6 for the linear FSVM. TSH is the most significant factor in thyroid diagnosis, accounting for 40% (positive) and 77% (negative) of the contributions. A pregnant woman with low TSH and high T4 is diagnosed with thyroid disease in Fig. 6 (a). Conversely, in Fig. 6 (b), a patient with high TSH, low T4 and FTI, and without goitre is correctly detected as healthy.

*3) **Result of Exp. C**:*

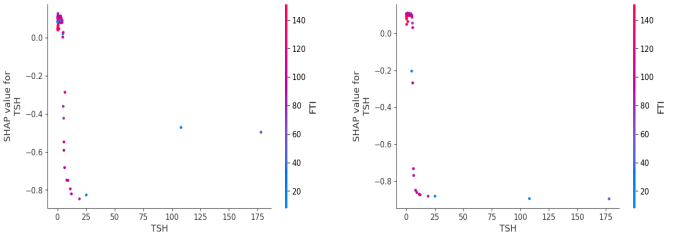
- **SHAP Force Plot:** The force plots of the exponential FSVM in Fig. 7 explain a positive and a negative prediction. The sum of SHAP values converts the base value (outcome without any feature) of 0.89 into the final outcome of 1 and 0. Low TSH and high FTI levels have contributed to the accurate thyroid prediction in Fig. 7 (a). Nevertheless, in Fig. 7 (b), the opposite test results indicate a negative outcome.
- **SHAP Dependence Plot:** In the dependence plots of both of the FSVMs in Fig. 8, the red dense areas imply that for people having TSH levels of 0–2, the likelihood of diagnosing thyroid disease rises for high FTI levels (120-140). Furthermore, data with negative SHAP values (up to 0.8) indicate the growing probability of thyroid negative diagnosis when TSH levels are greater than 5.
- **SHAP Summary Plot:** The summary plot of Fig. 9 illustrates global feature importance in thyroid forecasting, with TSH being the most contributed feature. TSH, FTI, T4, and T3 tests can be critical for diagnosing the early stages of thyroid. Besides, most of the thyroid patients seem to intake thyroxine medicine as a treatment.



(a) Positive

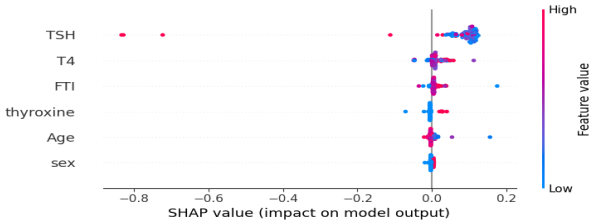
(b) Negative

Fig. 7: SHAP force plot of prediction by exponential FSVM.

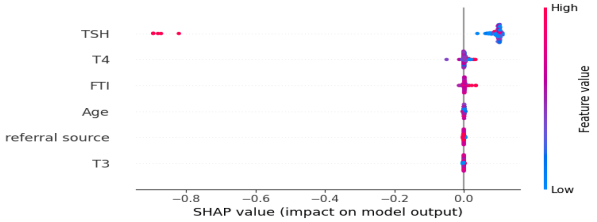


(a) Linear (b) Exponential

Fig. 8: SHAP dependence plot of TSH by Fuzzy SVM.



(a) Linear



(b) Exponential

Fig. 9: SHAP summary plot of Fuzzy SVM.

E. Findings and Implications for the Thyroid Diagnosis

- TSH, FTI, and T4 hormone tests are crucial for early thyroid detection.
- Pregnant women are at a higher risk of diagnosing thyroid dysfunction.
- Thyroxine dosage can be recommended as a treatment for thyroid illness.
- LIME and SHAP can benefit physicians in investigating model transparency and making decisions about the diagnosis of thyroid conditions.

V. Conclusion

The study proposes a Fuzzy SVM model to address the class imbalance problem in thyroid forecasting. The feature-based fuzzy membership function concentrates on the minority class data to minimize the impact of class imbalance, yielding an improved outcome. Both methods (Linear and Exponential) of the FSVM outperform the traditional SVM, and the exponential FSVM shows better results when compared to existing models. Furthermore, LIME and SHAP techniques provide insights into the model's decision, hence promoting transparency of the model as a black box and acknowledging vital features of thyroid dysfunction. Future studies will concentrate on reducing computational resource requirements and refining important model elements to improve performance with faster execution in large datasets.

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