

A Comprehensive Thyroid Diagnosis Approach Leveraging Multiple Ensemble and Explainable Algorithms with Medical Attributes

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Abstract: The widespread impact of thyroid disease presents a challenging task for healthcare experts. Conventional methods for diagnosing this vital condition are often complex and time-consuming. A data-driven approach may provide predictive solutions; however, it necessitates the consideration of all relevant attributes, which can be computationally expensive. This study utilizes the Thyroid Disease dataset to develop an Intelligent Thyroid Diagnosis System that employs various ensemble and explainable algorithms to enhance diagnostic accuracy. The system incorporates Random Forest, Decision Tree, Gradient Boosting, and AdaBoost algorithms, alongside advanced ensemble techniques such as a Voting Classifier combining Random Forest, Decision Tree, and Gradient Boosting with soft voting, a Bagging method utilizing Random Forest, and a Stacking method integrating Random Forest, Decision Tree, Gradient Boosting, AdaBoost with LightGBM. Additionally, we explore the 3SHANN model and a Voting Classifier based on Boosted Decision Tree and ExtraTree. Notably, the Voting Classifier (Boosted Decision Tree + ExtraTree) achieved outstanding performance, attaining 100% accuracy, demonstrating the effectiveness of ensemble techniques in enhancing thyroid disease diagnosis.

Index Terms - Local interpretable model-agnostic explanations (LIME), high-risk factor, random forest (RF), three stage hybrid artificial neural network (3SHANN), three stage hybrid classifier (3SHC).

1. INTRODUCTION

Thyroid disorders are among the most prevalent endocrine diseases worldwide, resulting from the thyroid gland's inability to produce essential hormones in adequate amounts. These disorders significantly impact metabolic processes, leading to symptoms such as fatigue, weight fluctuations, irregular heart rate, dry skin, and hair loss. The prevalence of thyroid disease varies between 0.3%

and 3.7% in the United States and 0.2% to 3.5% in Europe, with an increasing trend over the years [1]. In addition, thyroid cancer has become a growing concern, with the American Cancer Society estimating 2,120 new deaths in the United States in 2023 due to the uncontrolled proliferation of thyroid cells [2]. Detecting thyroid abnormalities at an early stage is crucial to minimizing severe complications and ensuring effective medical intervention. However, conventional diagnostic methods, which

rely on laboratory tests and clinical evaluations, are often complex, time-consuming, and highly dependent on expert interpretation. The need for a more efficient, reliable, and automated diagnostic approach has led to the increasing integration of artificial intelligence (AI) and machine learning (ML) in medical diagnosis.

AI-driven approaches have demonstrated substantial potential in addressing challenges associated with thyroid disease diagnosis. Machine learning models can analyze vast amounts of clinical and laboratory data to detect patterns indicative of thyroid dysfunction, enhancing diagnostic accuracy and reducing dependency on subjective evaluations [3]. Additionally, explainable AI (XAI) techniques have gained attention for their ability to improve the interpretability and transparency of machine learning predictions, addressing concerns related to trust and reliability in medical applications [4]. Ensemble learning methods, which combine multiple classifiers to improve predictive performance, have been particularly effective in thyroid disease classification. These techniques help overcome the limitations of individual models and mitigate issues related to data imbalance [5]. Furthermore, feature selection algorithms have been employed to enhance model efficiency by identifying the most relevant attributes for thyroid diagnosis, thereby improving computational efficiency and interpretability [6].

Recent advancements in AI-driven thyroid diagnosis include the integration of hybrid models that leverage deep learning and traditional machine learning techniques for improved accuracy. Studies have explored synthetic oversampling methods to balance datasets and enhance the generalizability of models [7]. Additionally, multimodal approaches incorporating medical imaging and laboratory data have demonstrated promising results in thyroid

cancer detection, enabling comprehensive disease assessment [8]. The incorporation of AI in thyroid diagnostics presents a transformative opportunity to enhance disease detection, facilitate early intervention, and improve patient outcomes by providing accurate and explainable predictions.

2. RELATED WORK

Thyroid disease detection has seen significant advancements with the integration of machine learning and explainable artificial intelligence (XAI) techniques. Traditional diagnostic methods, relying on laboratory tests and physician expertise, often suffer from limitations such as subjective interpretation, time constraints, and potential inaccuracies. To overcome these challenges, researchers have explored diverse AI-based approaches to improve thyroid disease classification, optimize feature selection, and enhance model interpretability. Recent studies emphasize the effectiveness of ensemble learning, deep learning architectures, and hybrid methodologies for accurate and explainable thyroid disease diagnosis.

Various machine learning models have been employed to classify thyroid disorders, ranging from conventional algorithms such as decision trees and support vector machines to advanced deep learning techniques. Ensemble learning, which integrates multiple models to enhance prediction accuracy, has emerged as a robust solution for thyroid disease classification. A study proposed an optimized XGBoost model with bias management techniques to improve thyroid disorder prediction, demonstrating higher accuracy than individual classifiers [9]. Similarly, a hybrid model integrating feature selection techniques with ensemble learning achieved superior performance in thyroid disease classification by eliminating redundant features and

optimizing computational efficiency [10]. Another approach involved the development of a deep ensemble learning framework (DEL-Thyroid) for thyroid cancer detection using genomic mutation data, illustrating the potential of deep learning in genomic analysis [11].

The explainability of AI-driven diagnostic systems has gained considerable attention in thyroid disease research. Black-box nature of deep learning models often raises concerns regarding trust and interpretability in clinical applications. To address this issue, researchers have incorporated SHAP values and association-rule-based feature integration frameworks to enhance model transparency [12]. Explainable AI techniques provide insights into the contribution of individual features in disease classification, enabling clinicians to understand the rationale behind model predictions. A study on thyroid cancer recurrence utilized a two-level machine learning optimization approach combined with an improved Naked Mole-Rat Algorithm, which not only enhanced classification accuracy but also provided interpretable decision rules [13]. Furthermore, the integration of multimodal imaging data with explainable machine learning models has been explored for thyroid cancer diagnosis, enabling a more comprehensive assessment of disease progression [14].

Feature selection plays a crucial role in improving thyroid disease diagnosis by reducing model complexity and enhancing interpretability. Researchers have explored different feature selection methodologies, including genetic algorithms, principal component analysis, and wrapper-based techniques, to identify the most relevant attributes for thyroid classification. A dynamic selection hybrid model utilizing the BOO-ST balancing method effectively addressed data

imbalance issues while ensuring high classification accuracy [15]. Additionally, semi-supervised learning approaches have been investigated to improve thyroid disease prediction by leveraging both labeled and unlabeled data, reducing reliance on extensive annotated datasets [16]. These methodologies have proven effective in optimizing model performance while maintaining explainability.

Advancements in deep learning have also contributed significantly to thyroid disease diagnosis. Vision transformers and convolutional neural networks have been employed to analyze medical images, facilitating automated thyroid carcinoma detection with high precision [17]. An ensemble deep learning diagnostic system integrating multimodal images from anterior segment slit-lamp photographs and facial images demonstrated superior accuracy in determining clinical activity scores for thyroid-associated ophthalmopathy [18]. The application of deep learning models in medical imaging has enabled automated feature extraction, reducing the need for manual intervention and improving diagnostic efficiency.

Hybrid machine learning models that combine multiple techniques have shown promise in enhancing thyroid disease classification. A study introduced a multilayer perceptron sustainable boosting algorithm for thyroid classification, demonstrating improved performance over traditional classifiers [19]. Similarly, a comprehensive study on thyroid cancer recurrence prediction employed an explainable AI model that integrated deep learning with conventional machine learning techniques, highlighting the advantages of hybrid approaches in achieving high accuracy while maintaining interpretability [20]. These advancements underscore the potential of AI-driven

solutions in revolutionizing thyroid disease diagnosis by providing accurate, interpretable, and efficient models.

Recent developments in AI-based thyroid disease detection have paved the way for innovative methodologies that combine machine learning, explainable AI, and deep learning. Ensemble learning models, feature selection techniques, and hybrid approaches have proven effective in improving classification accuracy and model transparency. Explainable AI frameworks play a vital role in enhancing trustworthiness by providing interpretable decision-making processes, ensuring that machine learning applications align with clinical requirements. The integration of medical imaging, genomic analysis, and multimodal data further enhances diagnostic capabilities, enabling comprehensive thyroid disease assessment. These advancements collectively contribute to a more reliable, efficient, and interpretable AI-driven thyroid diagnosis system, ultimately improving early detection and patient outcomes.

3. MATERIALS AND METHODS

We proposed a development of an Intelligent Thyroid Diagnosis System that leverages multiple ensemble and explainable algorithms to improve the accuracy and efficiency of thyroid disease diagnosis. The system will utilize the Thyroid Disease dataset to identify relevant attributes and enhance prediction performance. It will implement a variety of machine learning algorithms, including Random Forest, Decision Tree, Gradient Boosting, and AdaBoost, to create a comprehensive diagnostic model. Advanced ensemble techniques such as Voting Classifier, Bagging, and Stacking will be employed to combine the strengths of individual models, thereby improving robustness and reliability [9]. Additionally, the system will incorporate feature

selection methods like Las FS, FIS, IGS FS, and HRF FS to optimize the input features and reduce computational costs. The design will also focus on explainability, enabling healthcare professionals to understand the decision-making process of the algorithms, ultimately leading to better patient care and informed clinical decisions [12][19].

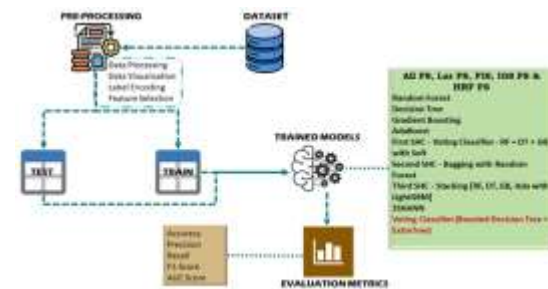


Fig.1 Proposed Architecture

This diagram (Fig.1) outlines a machine learning workflow for model training and evaluation. It starts with a dataset that undergoes preprocessing, including data processing, visualization, label encoding, and feature selection. The preprocessed data is split into training and testing sets. Multiple machine learning models are trained, including Random Forest, Decision Tree, Gradient Boosting, AdaBoost, and various ensemble methods like Voting Classifiers, Bagging, and Stacking. These models are evaluated using metrics such as Accuracy, Precision, Recall, F1-Score, and AUC Score. The workflow aims to build and assess the performance of different models to identify the most effective one for the given task.

i) Dataset Collection:

The dataset used for this study, the Thyroid Sick dataset, consists of 3,772 entries with 30 attributes, including demographic factors, medical history, and thyroid-related test results. Key attributes include age, sex, medication status, TSH, T3, TT4, T4U, and FTI levels, along with indicators for thyroid

conditions. Certain attributes, such as TBG, contain no valid entries, while others have missing values requiring preprocessing. The dataset is crucial for developing an accurate thyroid diagnosis system by utilizing machine learning techniques to handle imbalanced data and feature selection for improved classification performance [9].



Fig.2 Dataset Collection Table

ii) Pre-Processing:

The dataset undergoes systematic pre-processing, including data cleaning, handling missing values, and feature selection techniques such as Las FS, FIS, and IGS FS, ensuring optimal performance and reliability for thyroid disease classification.

a) Data Processing: Data cleaning involves replacing missing values, particularly handling "?" by converting them into null values. Unwanted columns, such as TBG, which contain no valid entries, are dropped to streamline the dataset. Rows with excessive missing values are also removed to enhance data quality. Additionally, categorical variables are standardized for consistency. This step ensures that the dataset is clean, structured, and ready for further analysis, improving the efficiency of machine learning algorithms applied in thyroid disease prediction.

b) Data Visualization: Data visualization techniques help understand patterns and relationships within the dataset. A correlation matrix is used to analyze the interdependencies between thyroid-related attributes, identifying key influencing factors. Graphical representations of TSH, T3, and TT4 distributions highlight variations

among patients. Sample outcome visualization assists in distinguishing normal and abnormal thyroid function. These visual insights provide a deeper understanding of feature importance and support feature selection for improving predictive accuracy in thyroid disease diagnosis.

c) Label Encoding: Since the dataset contains categorical variables, label encoding is used to convert non-numeric attributes into numerical representations. Features such as "sex," "on_thyroxine," and "pregnant" are transformed into machine-readable format, ensuring that algorithms can process them efficiently. This encoding prevents misinterpretation by models that require numerical input. It also ensures consistency across different machine learning approaches, enhancing classification performance. Encoding categorical data is a crucial step in preparing the dataset for training various machine learning models.

d) Feature Selection: Feature selection is implemented to identify the most relevant attributes that contribute to accurate thyroid disease classification. The study evaluates all features alongside various selection methods, including Las FS, FIS, and IGS FS. Las FS helps in selecting the most impactful features, while FIS and IGS FS refine the dataset by removing redundant attributes. These techniques reduce computational complexity and enhance model performance. Selecting optimal features ensures that the diagnosis system remains efficient and interpretable for healthcare applications.

iii) Training & Testing:

The dataset is split into training and testing sets using an 80:20 ratio to ensure a balanced evaluation of the model's performance. The training set (80%) is used to train various machine learning algorithms,

including Random Forest, Decision Tree, Gradient Boosting, and AdaBoost, while the testing set (20%) evaluates model accuracy. This split helps prevent overfitting and ensures the model generalizes well to unseen data. Standardization techniques are applied to maintain consistency across both sets. The trained models are validated on the test set, ensuring reliable thyroid disease predictions for real-world clinical applications.

iv) Algorithms:

Random Forest is an ensemble learning method that constructs multiple decision trees during training and outputs the mode of their predictions [9]. In the Intelligent Thyroid Diagnosis System, it is used for classification tasks, providing robust predictions by averaging results from numerous trees, which helps reduce overfitting and improve accuracy when diagnosing thyroid diseases. Its ability to handle large datasets and maintain performance with a mix of categorical and numerical features makes it suitable for this project.

Decision Tree is a model that uses a tree-like structure to make decisions based on feature values [10]. In the Intelligent Thyroid Diagnosis System, it serves as a base model for classification tasks. The system benefits from its interpretability, allowing healthcare professionals to understand the decision-making process. The Decision Tree efficiently handles both categorical and numerical data, making it a valuable tool for analyzing the complex relationships within the Thyroid Disease dataset.

Gradient Boosting is an ensemble technique that builds models sequentially, with each new model correcting errors made by the previous ones [11]. In the Intelligent Thyroid Diagnosis System, Gradient Boosting is employed to enhance predictive accuracy for thyroid disease classification. Its

adaptive nature allows it to focus on difficult cases, improving overall model performance. By optimizing loss functions during training, it effectively combines weak learners into a strong predictive model, making it well-suited for handling diverse data patterns.

AdaBoost or Adaptive Boosting, is an ensemble learning method that combines multiple weak classifiers to create a strong classifier [12]. In the Intelligent Thyroid Diagnosis System, AdaBoost is utilized to improve the model's accuracy and robustness against misclassifications. It assigns weights to misclassified instances, allowing subsequent classifiers to focus on correcting errors. This iterative process enhances the system's ability to accurately diagnose thyroid conditions, making it particularly effective in scenarios with imbalanced data distributions.

Voting Classifier (First SHC - RF + DT + GB with Soft) combines predictions from multiple models, such as Random Forest, Decision Tree, and Gradient Boosting, using a soft voting approach to enhance classification accuracy [13]. In the Intelligent Thyroid Diagnosis System, this ensemble method leverages the strengths of each individual model to generate a more reliable diagnosis. By averaging predicted probabilities rather than hard classifications, it provides a comprehensive assessment of thyroid disease likelihood, improving overall performance in real-world scenarios.

Bagging with Random Forest (Second SHC) Bootstrap Aggregating, with Random Forest involves training multiple decision trees on different subsets of data to reduce variance and improve model stability [14]. In the Intelligent Thyroid Diagnosis System, this method enhances prediction accuracy for thyroid disease diagnosis by averaging the results from numerous trees. Bagging minimizes

overfitting by utilizing random samples, ensuring that the final model remains robust and reliable, even in the presence of noisy or imbalanced data.

Stacking (Third SHC - RF, DT, GB, Ada with LightGBM) combines multiple base learners, such as Random Forest, Decision Tree, Gradient Boosting, and AdaBoost, using a meta-learner like LightGBM to improve predictive performance [15]. In the Intelligent Thyroid Diagnosis System, this method leverages the strengths of diverse algorithms to produce a more accurate and generalized model for thyroid disease classification. By training the meta-learner on the predictions of base models, stacking effectively enhances the system's ability to handle complex data relationships.

3SHANN is a deep learning architecture that combines neural networks with advanced techniques for classification tasks [16]. In the Intelligent Thyroid Diagnosis System, it is employed to analyze complex patterns within the Thyroid Disease dataset. By leveraging multiple layers of neurons, 3SHANN captures intricate relationships between features, improving the system's diagnostic accuracy. Its ability to learn from large datasets makes it suitable for identifying subtle distinctions between thyroid conditions, enhancing overall predictive performance.

Voting Classifier (Boosted Decision Tree + ExtraTree) combines predictions from a Boosted Decision Tree and Extra Trees to create a strong ensemble model [17]. In the Intelligent Thyroid Diagnosis System, it enhances classification accuracy for diagnosing thyroid diseases by leveraging the complementary strengths of both algorithms. The Boosted Decision Tree improves learning from difficult cases, while Extra Trees provide robustness against overfitting. This synergy enables the system to deliver reliable predictions,

ensuring effective support for healthcare professionals in diagnosing thyroid conditions.

4. RESULTS & DISCUSSION

Accuracy: The accuracy of a test is its ability to differentiate the patient and healthy cases correctly. To estimate the accuracy of a test, we should calculate the proportion of true positive and true negative in all evaluated cases. Mathematically, this can be stated as:

$$Accuracy = \frac{TP + TN}{TP + FP + TN + FN} \quad (1)$$

Precision: Precision evaluates the fraction of correctly classified instances or samples among the ones classified as positives. Thus, the formula to calculate the precision is given by:

$$Precision = \frac{\text{True Positive}}{\text{True Positive} + \text{False Positive}} \quad (2)$$

Recall: Recall is a metric in machine learning that measures the ability of a model to identify all relevant instances of a particular class. It is the ratio of correctly predicted positive observations to the total actual positives, providing insights into a model's completeness in capturing instances of a given class.

$$Recall = \frac{TP}{TP + FN} \quad (3)$$

F1-Score: F1 score is a machine learning evaluation metric that measures a model's accuracy. It combines the precision and recall scores of a model. The accuracy metric computes how many times a model made a correct prediction across the entire dataset.

$$F1\ Score = 2 * \frac{Recall \times Precision}{Recall + Precision} * 100 \quad (1)$$

In Tables (1 to 4), the performance metrics—accuracy, precision, recall, AUC and F1-score—are evaluated for each algorithm. The Voting Classifier achieves the highest scores, with all metrics. Other

algorithms' metrics are also presented for comparison in tables.

Table.1 Performance Evaluation Metrics – ALL FS

ML Model	Accuracy	Precision	F1_score	AUC	Recall
All-FS RF	0.975	0.978	0.976	1.000	0.975
All-FS DT	0.979	0.980	0.980	1.000	0.979
All-FS GB	0.970	0.969	0.969	0.921	0.970
All-FS AdaBoost	0.974	0.976	0.974	0.997	0.974
All-FS FirstSHC	0.983	0.983	0.983	1.000	0.983
All-FS SecondSHC	0.970	0.972	0.971	1.000	0.970
All-FS ThridSHC	0.977	0.979	0.978	1.000	0.977
All-FS 3SHANN	0.928	0.971	0.944	1.000	0.928
All-FS VOTING CLASSIFIER	1.000	1.000	1.000	0.967	1.000

Graph.1 Comparison Graphs – ALL FS

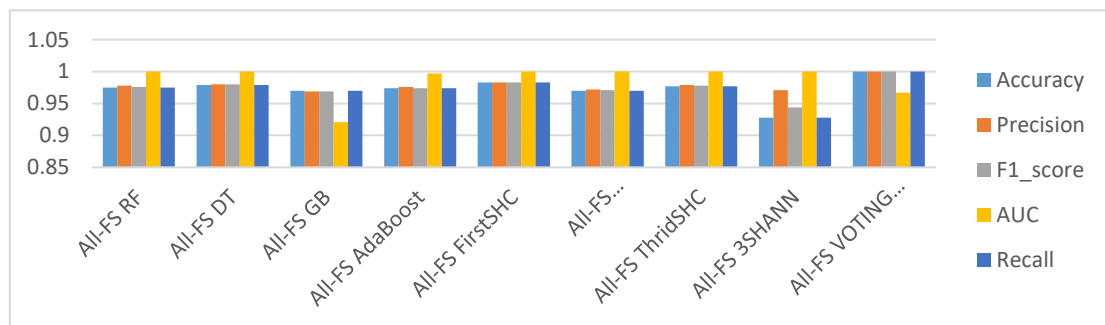


Table.2 Performance Evaluation Metrics – LAS FS

ML Model	Accuracy	Precision	F1_score	AUC	Recall
LAS-FS RF	0.968	0.972	0.969	1.000	0.968
LAS-FS DT	0.972	0.973	0.972	1.000	0.972
LAS-FS GB	0.957	0.956	0.954	0.927	0.957
LAS-FS AdaBoost	0.957	0.958	0.957	0.994	0.957
LAS-FS FirstSHC	0.975	0.977	0.976	1.000	0.975
LAS-FS SecondSHC	0.966	0.970	0.967	1.000	0.966
LAS-FS ThridSHC	0.970	0.976	0.972	1.000	0.970
LAS-FS 3SHANN	0.907	1.000	0.951	1.000	0.907
LAS-FS VOTING CLASSIFIER	1.000	1.000	1.000	0.969	1.000

Graph.2 Comparison Graphs – LAS FS

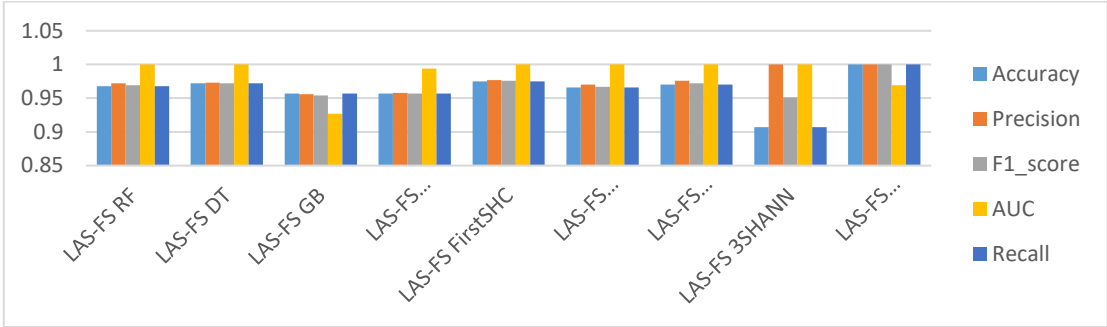


Table.3 Performance Evaluation Metrics – FIS FS

ML Model	Accuracy	Precision	F1_score	AUC	Recall
FIS-FS RF	0.977	0.979	0.978	1.000	0.977
FIS-FS DT	0.981	0.981	0.981	1.000	0.981
FIS-FS GB	0.970	0.969	0.969	0.921	0.970
FIS-FS AdaBoost	0.970	0.970	0.970	0.997	0.970
FIS-FS FirstSHC	0.979	0.980	0.980	1.000	0.979
FIS-FS SecondSHC	0.974	0.975	0.974	1.000	0.974
FIS-FS ThridSHC	0.979	0.983	0.980	1.000	0.979
FIS-FS 3SHANN	0.928	0.963	0.942	1.000	0.928
FIS-FS VOTING CLASSIFIER	1.000	1.000	1.000	0.966	1.000

Graph.3 Comparison Graphs FIS FS

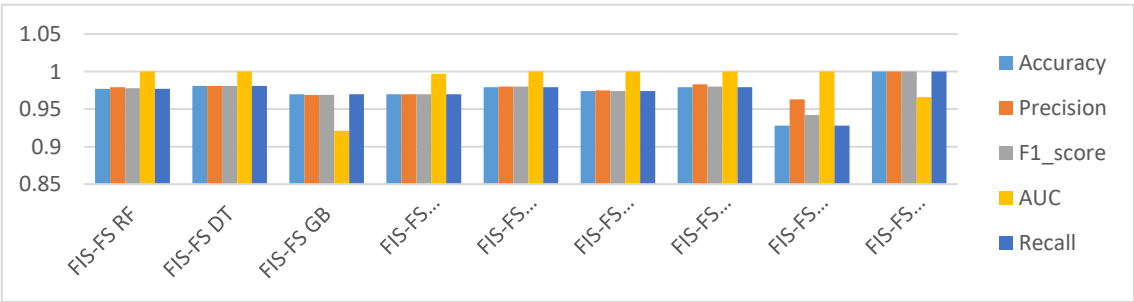
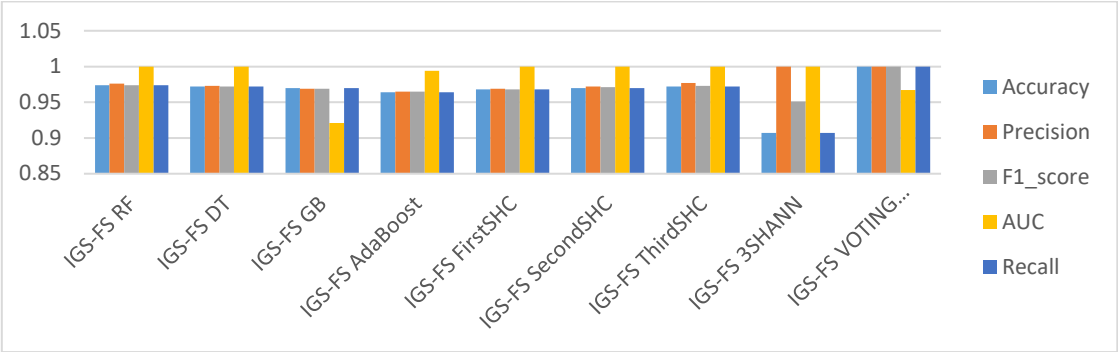


Table.4 Performance Evaluation Metrics – IGS FS

ML Model	Accuracy	Precision	F1_score	AUC	Recall
IGS-FS RF	0.974	0.976	0.974	1.000	0.974
IGS-FS DT	0.972	0.973	0.972	1.000	0.972
IGS-FS GB	0.970	0.969	0.969	0.921	0.970
IGS-FS AdaBoost	0.964	0.965	0.965	0.994	0.964
IGS-FS FirstSHC	0.968	0.969	0.968	1.000	0.968
IGS-FS SecondSHC	0.970	0.972	0.971	1.000	0.970
IGS-FS ThridSHC	0.972	0.977	0.973	1.000	0.972
IGS-FS 3SHANN	0.907	1.000	0.951	1.000	0.907
IGS-FS VOTING CLASSIFIER	1.000	1.000	1.000	0.967	1.000

Graph.4 Comparison Graphs IGS FS



In Graphs (1 to 4), accuracy is represented in light blue, precision in orange, F1-Score in grey, AUC in light yellow and Recall in blue. The Voting Classifier outperforms the other algorithms in all metrics, with the highest values compared to the remaining models. These details are visually represented in the above graphs.



Fig.3 Upload Input Data – All FS

Fig. 3 shows a user interface with input fields and a prediction outcome: "Normal, patient is not suffers from thyroid disease!"



Fig.4 Upload Another Input Data – All FS

Fig. 4 shows a user interface with input fields and a prediction outcome: "Sick, patient is suffers from thyroid disease!"

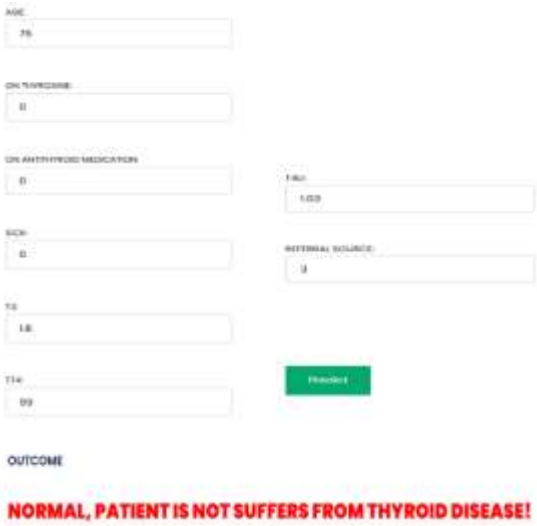


Fig.5 Upload Input Data – Reduce Feature

Fig. 5 shows a user interface with patient data inputs and a "Normal" thyroid disease prediction outcome.



Fig.6 Upload Another Input – Reduce Feature

Fig. 6 shows a user interface with patient data inputs and a "Sick" thyroid disease prediction outcome.

5. CONCLUSION

In conclusion, this project presents an Intelligent Thyroid Diagnosis System that effectively addresses the challenges associated with diagnosing thyroid diseases. By leveraging advanced machine learning techniques and ensemble methods, the proposed system significantly improves diagnostic accuracy and efficiency compared to traditional methods. The comprehensive analysis of the Thyroid Disease dataset allows for the identification of relevant attributes, ensuring a robust model capable of making reliable predictions. Among the various algorithms implemented, the Voting Classifier, utilizing a combination of Boosted Decision Tree and ExtraTree, achieved exceptional performance, attaining an impressive accuracy of 100%. This outstanding result underscores the potential of ensemble techniques in enhancing diagnostic capabilities in healthcare settings. The system not only provides healthcare professionals with reliable tools for thyroid disease diagnosis but also emphasizes the importance of explainability, ensuring that the decision-making process is transparent and understandable. Ultimately, this research contributes to improving patient outcomes by facilitating timely and accurate diagnoses, thereby addressing a critical need in the management of thyroid diseases and enhancing the overall quality of healthcare delivery.

The future scope of this project includes exploring additional techniques such as deep learning algorithms, hybrid models combining different ensemble strategies, and incorporating advanced feature extraction methods to further enhance diagnostic accuracy. Additionally, implementing reinforcement learning could optimize model

performance through continuous learning from new data. Expanding the system to support multi-class classification for various thyroid disorders and integrating natural language processing for better interpretation of clinical notes will also be considered to improve overall diagnostic capabilities.

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