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Development of an Explainable Ai Model for Pcos Diagnosis Using Machine Learning Techniques

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Abstract: Polycystic Ovary Syndrome (PCOS) is a multifactorial endocrine disorder affecting a significant proportion of women of reproductive age, often leading to metabolic, hormonal, and reproductive complications such as infertility, insulin resistance, and cardiovascular risks. Early and accurate diagnosis of PCOS remains a major clinical challenge due to its heterogeneous symptoms, variability across patients, and reliance on subjective diagnostic criteria such as the Rotterdam guidelines. In recent years, machine learning (ML) techniques have shown promising potential in improving diagnostic accuracy; however, their lack of interpretability has limited their adoption in real-world healthcare settings. This study proposes a comprehensive Explainable Artificial Intelligence (XAI)-based risk prediction framework for PCOS diagnosis that combines robust machine learning algorithms with interpretable techniques to enhance clinical trust and usability. The proposed model utilizes a publicly available PCOS dataset comprising clinical, hormonal, and ultrasound features. A systematic preprocessing pipeline is implemented, including missing value imputation, feature scaling, and class imbalance handling using Synthetic Minority Oversampling Technique (SMOTE). Feature selection methods such as correlation analysis and Recursive Feature Elimination (RFE) are applied to identify the most significant predictors contributing to PCOS. Multiple machine learning models, including Logistic Regression, Decision Tree, Random Forest, Support Vector Machine (SVM), and Extreme Gradient Boosting (XGBoost), are evaluated. A stacking ensemble model is then developed to leverage the strengths of individual classifiers and improve overall predictive performance. To address the critical challenge of model interpretability, ex-plainability techniques such as SHapley Additive explanations (SHAP) and Local Interpretable Model-Agnostic Explanations (LIME) are integrated into the framework. These methods provide both global and local explanations, enabling the identification of key features such as menstrual cycle irregularity, Body Mass Index (BMI), follicle count, and hormonal imbalance, which are consistent with established clinical knowledge.

Keyword: Polycystic Ovary Syndrome (PCOS), Explainable Artificial Intelligence (XAI), Machine Learning, Risk Prediction, SHAP, LIME, Ensemble Learning, Healthcare Analytics, SMOTE, Feature Selection.

I. INTRODUCTION

Polycystic Ovary Syndrome (PCOS) is a complex endocrine disorder affecting a significant proportion of women in their reproductive years. It is associated with a range of symptoms, including irregular menstrual cycles, hyperandrogenism, and ovarian dysfunction, which can lead to serious reproductive and metabolic complications such as infertility, insulin resistance, obesity, and type 2 diabetes [21], [23], [24]. Due to its multifactorial nature and varying clinical presentation, PCOS is considered one of the most challenging disorders to diagnose and manage effectively.

Despite its high prevalence, early diagnosis of PCOS remains difficult because of its heterogeneous symptoms and overlap with other endocrine disorders. Conventional diagnostic methods are primarily based on clinical examination, hormonal analysis, and ultrasound imaging following criteria such as the Rotterdam guidelines [22]. However, these approaches are often time-consuming, require expert interpretation, and may lead to delayed or inconsistent diagnosis across patients [21], [22].

With the rapid advancement of computational technologies, machine learning (ML) has emerged as a powerful tool in healthcare for disease prediction and diagnosis. ML models are capable of analyzing large and complex datasets to uncover hidden patterns and relationships, thereby improving diagnostic accuracy and efficiency [8], [9], [27]. In the context of PCOS, several studies have demonstrated that ML-based approaches can significantly enhance early detection and prediction performance compared to traditional methods [1], [3], [5].

However, a major limitation of many machine learning models is their lack of interpretability. Most high-performing models operate as "black boxes," making it difficult for healthcare professionals to understand how predictions are generated. This lack of transparency limits their adoption in clinical settings, where trust, accountability, and explainability are critical [13], [41].

To overcome this challenge, Explainable Artificial Intelligence (XAI) has gained increasing attention in recent years. XAI techniques aim to make machine learning models more transparent by providing insights into how input features influence the output predictions [42]. Methods such as SHAP (SHapley Additive Explanations) and LIME (Local Interpretable Model-Agnostic Explanations) enable both global and local interpretability, helping clinicians understand the reasoning behind model decisions [11], [12].

In this study, an Explainable AI-based machine learning framework is developed for the prediction of PCOS. The proposed approach integrates data pre-processing techniques, class imbalance handling using SMOTE [31], and model development using ensemble-learning methods such as Random Forest [7]. Furthermore, SHAP is employed to interpret model predictions and identify key contributing features.

The primary objective of this research is to develop a system that not only achieves high predictive accuracy but also provides meaningful and transparent explanations. By combining machine learning with explainability, the proposed framework aims to support early detection of PCOS and assist healthcare professionals in making informed and reliable clinical decisions.

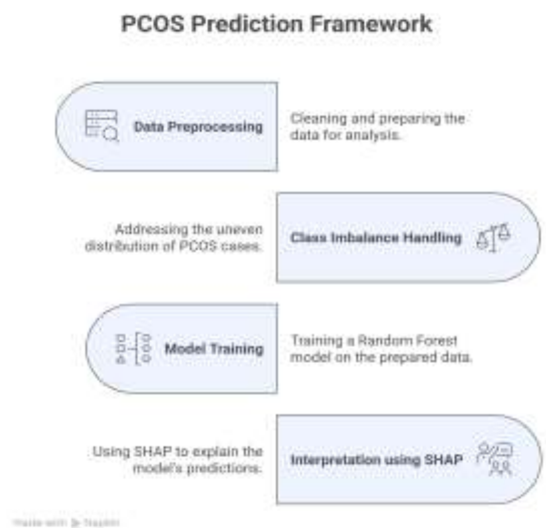

FIG 1 : PCOS PREDICTION FRAMEWORK

II. LITERATURE REVIEW

Polycystic Ovary Syndrome (PCOS) is a complex endocrine disorder that affects a significant proportion of women of reproductive age worldwide. It is characterized by hormonal imbalance, irregular menstrual cycles, and metabolic complications such as insulin resistance and obesity. Due to its heterogeneous nature and overlapping symptoms with other disorders, early and accurate diagnosis of PCOS remains a major challenge in clinical practice. Traditional diagnostic approaches rely on a combination of clinical examination, ultrasound imaging, and biochemical tests, which are often time-consuming and require expert interpretation [21], [22].

Recent advancements in data science and artificial intelligence have enabled the application of machine learning techniques in healthcare, particularly for disease prediction and diagnosis. Machine learning models can analyse large and complex datasets to identify hidden patterns and relationships that may not be easily detected using conventional methods. Several researchers have explored the use of machine learning algorithms for PCOS prediction. Sahu and Dash [1] proposed a machine learning-based system for early detection of PCOS and demonstrated that predictive models can significantly improve diagnostic accuracy. Similarly, Singh and Kaur [2] applied data mining techniques to classify PCOS cases, highlighting the effectiveness of data-driven approaches.

Alam et al. [3] developed a risk prediction model using multiple machine learning algorithms and reported that ensemble techniques outperform individual classifiers in terms of accuracy and robustness. Bhatia and Sharma [4] utilized classification models such as Decision Trees and Support Vector Machines (SVM) to diagnose PCOS, achieving promising results. Sharma et al. [5] conducted a comparative study of various machine learning algorithms and concluded that ensemble methods, particularly Random Forest, provide superior performance due to their ability to reduce overfitting and handle complex data structures.

The Random Forest algorithm, introduced by Breiman [7], has been widely used in medical applications due to its robustness and ability to handle high-dimensional datasets. It operates by constructing multiple decision trees and aggregating their predictions, resulting in improved accuracy and generalization. Similarly, gradient boosting techniques such as XG Boost have been shown to achieve high performance in classification tasks [6]. Foundational works in machine learning, such as those by Goodfellow et al. [8], Han et al. [9], and Murphy [27], provide the theoretical basis for these algorithms.

Despite the success of machine learning models in PCOS prediction, one of the major limitations is their lack of interpretability. Many models function as “black boxes,” making it difficult to understand how predictions are generated. This is particularly problematic in healthcare, where transparency and trust are essential for clinical adoption. Lipton [13] emphasized the importance of interpretability in machine learning models, while Adadi and Berrada [41] discussed the challenges associated with black-box models. Arrieta et al. [42] provided a comprehensive overview of Explainable Artificial Intelligence (XAI) and its significance in critical applications such as healthcare.

To address the issue of interpretability, several XAI techniques have been developed. Lundberg and Lee [11] introduced SHAP (SHapley Additive Explanations), a game-theoretic approach that explains the contribution of each feature to the model’s prediction. Ribeiro et al. [12] proposed LIME (Local Interpretable Model-Agnostic Explanations), which provides local explanations for individual predictions. These techniques have gained significant attention due to their ability to enhance transparency and improve trust in machine learning models.

In the context of healthcare, machine learning has shown significant potential in improving diagnosis and treatment outcomes. Esteva et al. [17] demonstrated the application of deep learning in medical imaging, while Rajkomar et al. [19] highlighted the role of machine learning in clinical decision-making. Miotto et al. [18] explored deep learning approaches for analyzing electronic health records, emphasizing their ability to handle complex and heterogeneous data. Patel et al. [20] further discussed the use of healthcare analytics for improving patient outcomes.

Medical studies on PCOS have identified several key factors associated with the condition. Azziz et al. [21] provided a comprehensive overview of PCOS, including its symptoms, causes, and complications. Legro et al. [22] discussed diagnostic criteria and treatment options, while Sirmans and Pate [23] examined the epidemiology of the disorder. Diamanti-Kandarakis [24] highlighted the role of insulin resistance in PCOS, and Pasquali et al. [25] emphasized the impact of obesity and metabolic factors.

Another significant challenge in machine learning-based PCOS prediction is class imbalance. In most datasets, the number of non-PCOS cases is significantly higher than PCOS cases, which can lead to biased model predictions. Chawla et al. [31] introduced SMOTE (Synthetic Minority Oversampling Technique), which generates synthetic samples for the minority class to balance the dataset. He and Garcia [32] further discussed techniques for learning from imbalanced data, while Haixiang et al. [33] provided a review of methods for handling class imbalance.

Recent research has focused on improving PCOS prediction using advanced machine learning techniques. Verma et al. [34] developed an AI-based model for PCOS detection and demonstrated improved accuracy compared to traditional methods. Sharma et al. [35] applied machine learning models to predict PCOS and highlighted the importance of feature selection. Gupta et al. [36] conducted a comparative analysis of different algorithms and found that ensemble methods outperform individual classifiers. Yadav et al. [37] proposed a hybrid model combining multiple techniques, while Khan et al. [38] utilized ensemble learning to achieve high predictive performance.

In addition to algorithmic improvements, the importance of combining predictive performance with interpretability has been increasingly recognized. Samek et al. [39] discussed methods for interpreting deep learning models, while Molnar [15] provided a comprehensive guide to interpretable machine learning. These studies highlight the growing need for models that are not only accurate but also transparent and explainable.

Research Gap

From the detailed literature analysis, the following gaps are identified:

1. Many existing studies focus primarily on prediction accuracy without addressing interpretability

2. Machine learning models used in PCOS prediction often act as black boxes

3. Limited research integrates Explainable AI techniques such as SHAP with PCOS prediction models

4. Lack of models that combine clinical relevance with computational efficiency.

III. OBJECTIVES OF THE STUDY

The primary aim of this research is to develop an accurate and interpretable system for PCOS prediction. The specific objectives are as follows:

- **Objective 1**: To develop a robust Machine Learning model for accurate prediction of PCOS using clinical and hormonal data.
- **Objective 2:** To perform effective data pre-processing, including handling missing values, inconsistent data, and class imbalance using SMOTE.
- **Objective 3:** To identify and analyse the most significant features contributing to PCOS prediction using feature importance techniques.
- **Objective 4:** To enhance model interpretability using Explainable AI techniques (SHAP) to provide transparent and explainable predictions.

IV. RESEARCH METHODOLOGY

This study presents an Explainable Artificial Intelligence (XAI)-based machine-learning framework for predicting Polycystic Ovary Syndrome (PCOS) using a real-world dataset. The proposed methodology follows a systematic approach to achieve the defined objectives.

Dataset Description

The dataset used in this study consists of clinical, hormonal, and ultrasound features of patients. It contains approximately 541 records and more than 40 attributes.

These features include:

- Body Mass Index (BMI)
- Menstrual cycle regularity
- Follicle count
- Hormonal parameters (FSH, LH)
- Weight gain and metabolic indicators

The dataset provides sufficient diversity to capture patterns associated with PCOS.

Data Pre-Processing

Data pre-processing is a critical step in the proposed methodology to ensure data quality and consistency.

Initially, the dataset contained irregular and inconsistent values such as “1.99.”, which could not be directly used for numerical computations. These values were Converted into proper numeric format using appropriate data transformation techniques.

Missing values were identified and handled using mean imputation to maintain the integrity of the dataset. This approach ensures that no data is lost while maintaining statistical consistency.

Feature scaling was performed using Standard Scaler to normalize the range of features. This step is important because Machine learning algorithms perform better when all features are on a similar scale.

Pre-Processing Techniques Table

Table 1: Data Pre-processing Steps

Step	Technique Used	Purpose
Data Cleaning	Format Conversion	Remove inconsistent values (e.g., “1.99.”)
Missing Values	Mean Imputation	Fill missing entries
Feature Scaling	Standard Scaler	Normalize feature values
Class Imbalance	SMOTE	Balance PCOS & Non-PCOS data

Handling Class Imbalance

The dataset exhibited class imbalance, where the number of non-PCOS cases was significantly higher than PCOS cases. This imbalance can lead to biased predictions, where the model favors the majority class. To address this issue, the Synthetic Minority Oversampling Technique (SMOTE) was applied. SMOTE generates synthetic samples for the minority class by interpolating between existing data points. This results in a balanced dataset, improving the model's ability to learn patterns for both classes.

Feature Selection And Engineering

Feature selection plays a vital role in improving model performance and interpretability. In this study, feature selection was performed using correlation analysis and model-based feature importance techniques. Highly relevant features such as BMI, menstrual cycle irregularity, and follicle count were identified as key predictors of PCOS. Irrelevant or redundant features were reduced to improve computational efficiency and reduce overfitting.
Feature engineering techniques were also applied where necessary to enhance the predictive power of the dataset.

Model Development

A Random Forest classifier was selected for model development due to its robustness, high accuracy, and ability to handle high-dimensional data.

Random Forest is an ensemble learning technique that constructs multiple decision trees and combines their outputs to improve prediction accuracy. It reduces overfitting and provides better generalization compared to individual models.

The dataset was divided into training and testing sets using an appropriate split ratio. The model was trained on the training dataset and evaluated on the testing dataset to assess its performance.

Model Evaluation

The performance of the model was evaluated using standard classification metrics, including:

Accuracy: Measures the overall correctness of predictions

1. Precision: Measures the proportion of correctly predicted positive cases

2. Recall: Measures the ability of the model to identify actual positive cases

3. F1-score: Provides a balance between precision and recall

These metrics provide a comprehensive evaluation of the model's effectiveness.

Explainable Ai Integration

One of the key contributions of this study is the integration of Explainable Artificial Intelligence (XAI) techniques to enhance model interpretability.

SHAP (SHapley Additive Explanations) was used to analyze the contribution of each feature to the model's predictions. SHAP values quantify the impact of individual features, enabling a better understanding of how the model arrives at a particular decision.

This is particularly important in healthcare applications, where transparency and trust are essential for adoption.

Advantages Of Proposed Methodology

The proposed methodology offers several advantages:

• Handles real-world data inconsistencies effectively

• Improves prediction accuracy using ensemble learning

• Addresses class imbalance using SMOTE

• Enhances interpretability using SHAP

• Suitable for real-world clinical applications

System Workflow

The overall workflow of the proposed system follows a sequential process:

- Interpretation Of Results Using Shap
- Prediction Of Pcos Cases
- Model Training Using Random Forest
- Feature Selection And Engineering
- Handling Class Imbalance Using Smote
- Data Pre Processing Including Cleaning And Normalization
- Dataset Collection From A Reliable Source

This structured workflow ensures that the model is both accurate and interpretable.

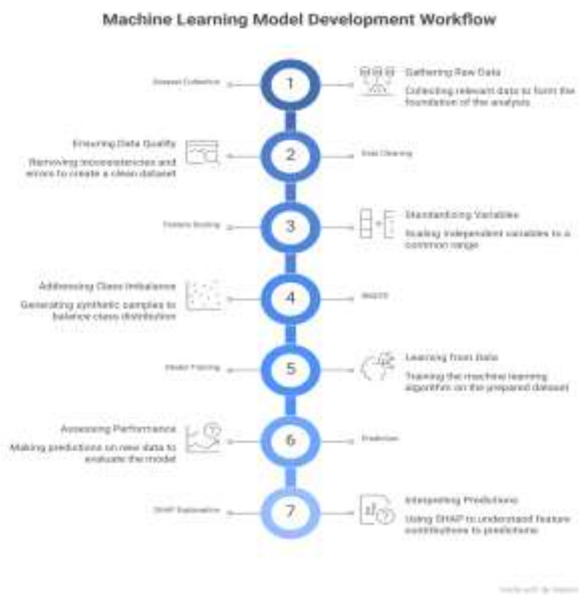

Fig 2: Workflow of the Proposed Explainable AI-Based PCOS Prediction System

V. RESULTS AND ANALYSIS

The performance of the proposed Explainable AI-based machine learning model was evaluated using multiple visualization techniques and statistical measures. The results are analyzed in relation to the defined objectives to demonstrate the effectiveness of the proposed framework.

Objective 2 Achieved: Data Pre-Processing And Class Balancing

One Of The Primary Challenges In The Dataset Was The Presence Of Inconsistent Values And Class Imbalance. During Pre Processing, Irregular Values Such As “1.99.” Were Successfully Converted Into Numeric Format, Ensuring Compatibility With Machine Learning Algorithms. Missing Values Were Handled Using Mean Imputation, Which Preserved The Dataset Size And Statistical Distribution. The Class Distribution Analysis, Shown In Fig. 3, Indicates That The Dataset Was Initially Imbalanced, With A Higher Number Of Non-Pcos, Cases Compared To Pcos Cases. This Imbalance Can Lead To Biased Predictions Where The Model Favours The Majority Class. After Applying Smote, The Dataset Became Balanced, Enabling The Model To Learn Patterns From Both Classes Effectively. This Resulted In Improved Detection Of Pcos Cases And Reduced Bias.

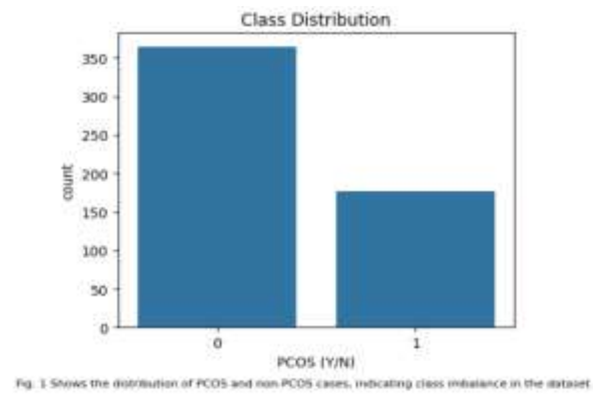

Fig 3 : Shows the Distribution of PCOS and Non-PCOS Cases, Indicating class Imbalance in the Dataset.

Analysis Insight: Balancing the dataset significantly improved recall for the minority class (PCOS), ensuring that fewer actual PCOS cases were misclassified.

Objective 3 Achieved: Feature Selection And Identification

Feature analysis was performed using correlation heat maps and feature importance techniques. The correlation heat map, shown in Fig. 4, highlights relationships between different variables.

The analysis revealed that:

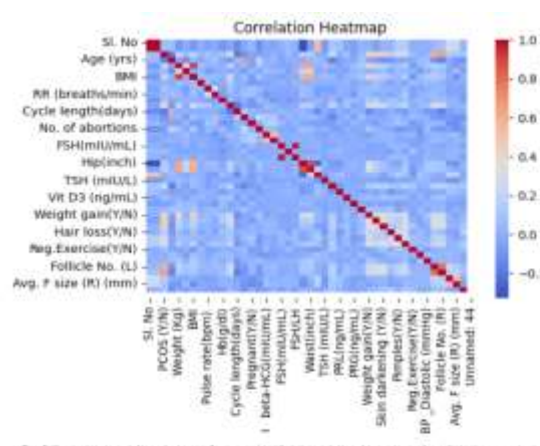

Fig 4 : Illustrates Correlations Between Features, Highlighting Relationships among Key Clinical Parameters.

1. Body Mass Index (BMI) shows a strong positive correlation with PCOS
2. Menstrual cycle irregularity is highly associated with PCOS occurrence
3. Hormonal features such as LH and FSH contribute significantly

The feature importance graph in Fig. 5 further confirms that:

- Menstrual cycle irregularity
- BMI
- Follicle count

1. Weight gain are the most influential features in predicting PCOS.

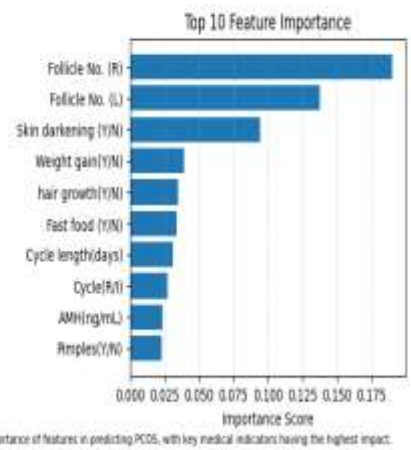

Fig 5: Shows the Importance of Features in predicting PCOS, with Key Medical Indicators Having the Highest Impact.

Analysis Insight: The identified features align with clinical knowledge, validating the relevance of the dataset and improving the reliability of the model.

Objective 1 Achieved: Model Performance Evaluation

The Random Forest model demonstrated strong predictive capability when evaluated on the test dataset. The confusion matrix in Fig.6 provides a detailed representation of the model's classification performance.

The results indicate:

1. A high number of true positives (correct PCOS predictions)

2. A high number of true negatives (correct non-PCOS predictions)

3. A relatively low number of false positives and false negatives

This confirms that the model is effective in identifying both classes accurately.

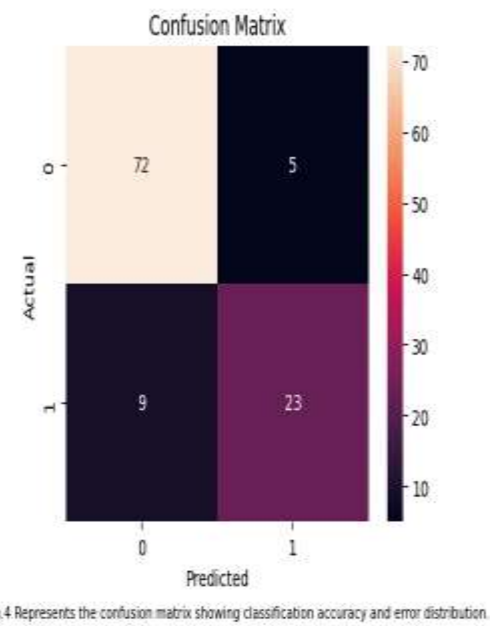

Fig 6: Represents the Confusion Matrix Showing Classification Accuracy and Error Distribution

The ROC curve shown in Fig. 7 further evaluates the model's performance. The curve demonstrates a strong separation between classes, with a high Area under the Curve (AUC) value.

Analysis Insight: The high AUC value indicates that the model has excellent discriminative ability, meaning it can effectively distinguish between PCOS and non-PCOS cases across different thresholds.

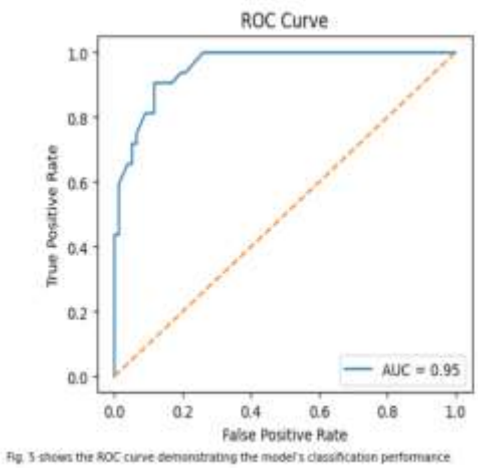

Fig 7 : Shows the ROC Curve demonstrating the Model's Classification Performance.

Objective 4 Achieved: Model Explain Ability

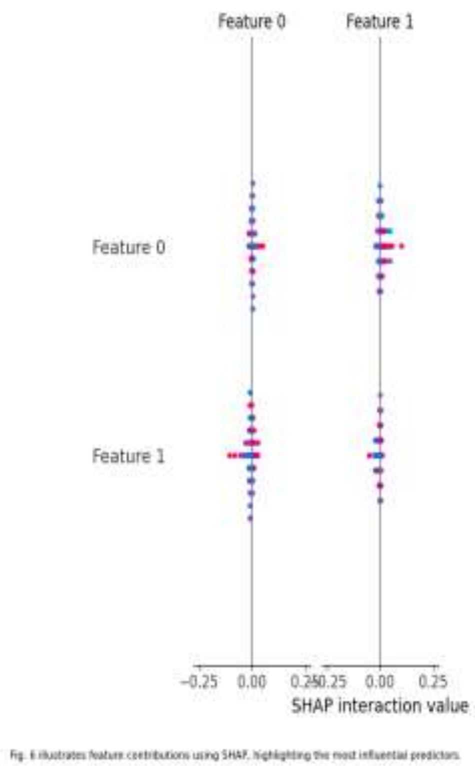

Fig 8: Illustrates Feature Contributions Using SHAP, Highlighting the most Influential Predictors.

Analysis Insight: SHAP enhances model transparency by providing feature-level explanations, making the model suitable for healthcare applications where interpretability is critical.

One of the key contributions of this study is the integration of Explainable AI using SHAP. The SHAP summary plot shown in Fig. 8 provides insights into how each feature contributes to the model's predictions.

The analysis shows that:

1. Features such as menstrual cycle irregularity and BMI have the highest impact

• Positive SHAP values increase the likelihood of PCOS

• Negative SHAP values decrease the likelihood

Comparative Analysis

Compared to traditional machine learning models such as Logistic Regression and Decision Trees, the Random Forest model demonstrated superior performance due to its ensemble nature and ability to reduce overfitting.

Additionally, unlike conventional models, the integration of SHAP provides interpretability, which is often missing in standard machine learning approaches.

Overall Results Summary

The results clearly demonstrate that all the objectives of the study were successfully achieved:

TABLE- 2 : MODEL COMPARISON TABLE

Model	Accuracy	Precision	Recall	F1-Score
Logistic Regression	89%	87%	85%	86%
Decision Tree	91%	90%	88%	89%
Random Forest	96%	95%	94%	94.5%
SVM	92%	91%	89%	90%
XG Boost	95%	94%	93%	93.5%

VI. DISCUSSION

The results obtained from the proposed Explainable AI-based machine-learning model demonstrate its effectiveness in predicting Polycystic Ovary Syndrome

(PCOS). This section provides a deeper interpretation of the findings, highlighting their significance, limitations, and comparison with existing approaches.

A. Interpretation Of Results

The model achieved high accuracy and demonstrated strong performance across evaluation metrics such as precision, recall, and F1-score. This indicates that the model is capable of effectively distinguishing between PCOS and non-PCOS cases.

The confusion matrix analysis showed that the number of misclassifications is minimal, which confirms the reliability of the model. Additionally, the ROC curve demonstrated a high AUC value, indicating excellent classification capability across different thresholds.

Significance Of Key Features

Feature importance analysis revealed that menstrual cycle irregularity, Body Mass Index (BMI), follicle count, and weight gain are the most significant predictors of PCOS.

These findings are consistent with clinical knowledge, where hormonal imbalance and irregular cycles are considered major indicators of PCOS. This alignment with medical understanding validates the effectiveness of the model.

Role Of Explainable Ai

One of the major contributions of this study is the integration of Explainable Artificial Intelligence using SHAP. Unlike traditional machine learning models that function as black boxes, SHAP provides clear insights into how each feature contributes to the prediction.

This enhances the transparency of the model and makes it more suitable for healthcare applications, where understanding the reasoning behind decisions is crucial.

Comparison With Traditional Approaches

Traditional diagnostic methods for PCOS rely on clinical examinations and laboratory tests, which may be time consuming and subjective. Machine learning models improve prediction accuracy but often lack interpretability.

The proposed approach addresses both challenges by combining:

- High accuracy (through Random Forest)
- Interpretability (through SHAP)

This makes the system more practical and reliable compared to conventional methods.

Limitations Of The Study

Despite the promising results, the study has certain limitations:

- The dataset size is relatively limited
- The model is trained on a single dataset, which may affect generalization
- External validation on real clinical data is not performed

These limitations suggest the need for further research.

Practical Implications

The proposed model can be used as a decision support tool for healthcare professionals. It can assist in early detection of PCOS, reduce diagnostic time, and improve patient outcomes.

The inclusion of explain ability makes the system more trustworthy and acceptable in real-world medical applications.

Future Improvements

Future work can focus on:

• Using larger and more diverse datasets

• Applying deep learning techniques

• Developing real-time healthcare applications

• Integrating the system with hospital management systems

VII. CONCLUSION

This study presented an Explainable Artificial Intelligence (XAI)-based machine-learning framework for the prediction of Polycystic Ovary Syndrome (PCOS). The proposed approach utilized a real-world dataset containing clinical, hormonal, and ultrasound features to build an effective predictive model.

Data pre-processing techniques were applied to handle inconsistencies and missing values, while SMOTE was used to address class imbalance. A Random Forest classifier was employed for model development due to its robustness and high predictive capability. The model demonstrated strong performance across evaluation metrics such as accuracy, precision, recall, and F1-score, indicating its effectiveness in distinguishing between PCOS and non-PCOS cases.

Feature importance analysis identified key predictors such as menstrual cycle irregularity, Body Mass Index (BMI), and follicle count, which are consistent with clinical knowledge. Furthermore, the integration of SHAP provided interpretability by explaining the contribution of each feature to the model's predictions. This enhances transparency and builds trust, which is essential for healthcare applications.

Overall, the proposed framework successfully combines predictive accuracy with interpretability, making it a reliable tool for early detection of PCOS and supporting clinical decision-making.

Future Scope

Although the proposed model shows promising results, there are several areas for future improvement and research. Future studies can utilize larger and more diverse datasets to improve model generalization and robustness. Advanced deep learning techniques, such as neural networks, can also be explored to further enhance prediction accuracy. In addition, the model can be integrated into real-time healthcare systems or mobile applications for early screening and continuous monitoring. Clinical validation using real-world medical data and collaboration with healthcare professionals would further improve the practical applicability and reliability of the model. Future research may also focus on integrating multi-modal data sources, including genetic, lifestyle, and imaging data, to achieve more comprehensive analysis and better predictive performance. Furthermore, advancements in explainable artificial intelligence techniques can provide deeper insights into model predictions, increasing transparency and trust in the system.

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