Original Article

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Statistics Section

Development of a Preliminary Screening Tool for Predicting Polycystic Ovarian Syndrome using Machine Learning and Deep Learning Models with Non Invasive Qualitative Features: A Case-control Study

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ABSTRACT

Introduction: Polycystic Ovarian Syndrome (PCOS) is a prevalent endocrine disorder affecting women of reproductive age, characterised by irregular menstrual cycles, hyperandrogenism and polycystic ovaries. Despite its high prevalence, the diagnosis of PCOS remains challenging due to the variability in symptom presentation. Traditional diagnostic methods involve clinical evaluation, biochemical assays and ultrasound imaging. Machine Learning (ML) and Deep Learning (DL) models offer promising avenues for predicting probable cases of PCOS using non invasive qualitative features.

Aim: To develop and compare the performance of Random Forest (RF) and Feedforward Neural Network (FFNN) models in predicting PCOS using abundant non invasive qualitative features.

Materials and Methods: A retrospective case-control study was conducted with 100 cases and 100 controls, selected based on ultrasound-confirmed PCOS diagnosis in the Obstetrics and Gynaecology, Gayatri Vidya Parishad Institute of Healthcare and Medical Technology (GVP IHC MT), Medical College departments from February 2024 to October 2024. Data were collected using a structured questionnaire capturing demographic and clinical variables. Feature selection was performed using the Chi-square filter method, with 10 features identified as significant. The data were split into training (80%) and testing (20%) sets and stratified 5-fold cross-validation was applied. Model performance was evaluated using accuracy, precision, recall, F1 score and Area Under Curve (AUC).

Results: The RF model demonstrated high performance on the training set, with an average accuracy of 0.95, but exhibited variability on the testing set (accuracy of 0.80). The FFNN model showed consistent performance across both training (accuracy of 0.80) and testing datasets (accuracy of 0.82). The RF model identified irregular cycles and hirsutism as key predictors, while the FFNN model highlighted weight gain and abnormal Body Mass Index (BMI) as important features. The RF model required significantly less computational time compared to the FFNN model.

Conclusion: The RF model is preferable for tasks requiring computational efficiency, while the FFNN model offers better generalisation. The complementary feature importance rankings suggest that integrating insights from both models could enhance the understanding of PCOS predictors. In epidemiological investigations, these models can be used as preliminary screening tools for identifying probable cases of PCOS using non invasive qualitative features, especially in areas where diagnostic facilities are not available.

Keywords: Feedforward neural network, Hirsutism, Irregular cycles, Random forest

INTRODUCTION

The PCOS represents one of the most prevalent endocrine disorders affecting women of reproductive age globally, with estimates suggesting its incidence could be as high as one in ten women [1]. It is characterised a spectrum of symptoms, including irregular menstrual cycles, hyperandrogenism and polycystic ovaries [2]. PCOS poses significant challenges in both diagnosis and management. Traditionally, diagnosis has relied on clinical evaluation, biochemical assays and ultrasound imaging [3]. However, the multifaceted nature of PCOS, coupled with variations in symptom presentation among individuals, often leads to delayed or inaccurate diagnosis. This underscores the urgent need for innovative approaches to enhance diagnostic accuracy and facilitate timely intervention for affected individuals.

Now-a-days, ML and DL models play a vital role in predicting diseases. Early-stage disease prediction can significantly alleviate long-term health complications [4-11]. Present study aimed to apply ML and DL models to predict PCOS using non invasive features. These models have the potential to aid in early diagnoses and treatment.

MATERIALS AND METHODS

The chosen research framework for this epidemiological inquiry adopts a retrospective case-control study design, relying on ultrasound scans to discern the presence or absence of PCOS. Within this investigation, a case designation is attributed to females diagnosed with a positive PCOS outcome, while a control status pertains to those with a negative PCOS diagnosis. This study was conducted in the Department of Obstetrics and Gynaecology at GVP IHC and MT Medical College, Vizag, Andhra Pradesh, India, from February 2024 to October 2024.

Inclusion criteria: Subjects aged between 20 and 30 years were included in the study.

Exclusion criteria: Subjects who were not willing to participate were excluded from the study.

Sample size calculation: The following formula [12] was used to determine the minimum sample size in each group.

$$n_{case}=n_{control}\geq\frac{Z^2_{1-\frac{\alpha}{2}}\,V(AUC)}{d^2}$$

where, n_{case}=sample size for cases, $n_{control}$=sample size for controls, $n_{1-\alpha/2}$=1.96 (Z-score corresponding to the 95% level of confidence), d=desired margin of error

V(A ∪ C)= Variance of the AUC estimator $=(0.0099\times e^{-a^2/2})\times(6a^2+16)$

where $a=Z_{AUC}\times 1.414$, Z_{AUC}=Z-score corresponding to the AUC value Anticipating Area Under the Curve (AUC) is 0.8, Estimation error (d)=0.1. The minimum number of PCOS cases needed was 46 and a minimum number of controls needed was 46. In the present study, 100 cases and 100 controls are enrolled.

Data collection: A structured closed-ended questionnaire was used to collect demographic, clinical and diagnostic variables. PCOS is the dependent variable. Abnormal Waist-Hip Ratio (WHR), abnormal Body Mass Index (BMI), unexplained weight gain, physical inactivity, hirsutism, hair loss, irregular cycles, skin darkening, acne, stress and fast food consumption were considered as independent variables, all of which are binary variables.

STATISTICAL ANALYSIS

ML and DL models: For the FE model, default parameters were employed where the number of trees (estimators) was set to 100. Each tree was allowed to grow fully unless further constraints on splitting were naturally met within the data. No maximum depth was specified, allowing the trees to expand until they reached pure or nearly pure nodes. Decision nodes and leaf nodes were determined based on the natural splits of the data, guided by the Gini impurity measure. A random state of 42 ensured reproducibility in the results.

The FFNN model consisted of three layers, with two hidden layers and an output layer. The first hidden layer contained 32 neurons and used the ReLU activation function, while the second hidden layer included 16 neurons with the same activation function. The output layer had a single neuron with a sigmoid activation function to classify the binary target. The FFNN model for 10 epochs were trained, using a batch size of 32. The model was compiled with the Adam optimiser and binary cross-entropy loss, which is suitable for binary classification.

RF model in ML: RF is an ensemble learning method that consists of a collection of decision trees, where each tree is built on a random subset of the data and features [13]. It is primarily used for classification and regression tasks.

RF model for a binary dependent variable: Given a training dataset $\{(X_i, Y_i)\}_{i=1}^{n}$, where X_i represents the feature vector for the *i*th observation and Y_i represents the binary target variable (either 0 or 1), the RF model is a collection of M decision trees. Each decision tree m is built using a random subset of the training data (bootstrap sample) and a random subset of the features at each split.

The prediction of the RF model for a new observation X is the aggregated prediction of all individual decision trees:

$\hat{Y} = \frac{1}{M}\sum_{m=1}^{M} f_m(X)$ where $f_m(X)$ is the prediction of the mth decision tree for observation X.

The decision trees in the RF model are typically grown to full depth (unpruned) to reduce bias. The randomness introduced during training helps reduce variance and prevents overfitting, making the model more robust to noise and outliers.

FFNN models in DL: Neural networks can also be used for regression tasks, including those with binary dependent variables [14]. However, representing the mathematical notation of a neural network for binary regression can be quite complex due to the intricate nature of neural network architectures.

Mathematical notation of a neural network regression model for a binary dependent variable:

Given a training dataset $\{(X_i, Y_i)\}_{i=1}^{n}$, where X_i represents the feature vector for the ith observation and represents the binary target variable (either 0 or 1).

A basic FFNN consists of multiple layers:

Input layer: The input layer receives the feature vector X_i as input.

Hidden layers: One or more hidden layers process the input data through a series of weighted transformations using activation functions. Each layer consists of nodes (neurons) that apply linear transformations followed by non linear activation functions.

Output Layer: The output layer produces the final prediction for the binary dependent variable. For binary regression, a single output node with a sigmoid activation function is commonly used to generate a continuous output between 0 and 1, representing the predicted probability of the positive class.

The mathematical notation for a single neuron in a neural network layer can be represented as:

$$Z_j = \sum_{i=1}^{n} w_{ij}\, x_i + b_j$$

$$a_j = \sigma(z_j)$$

where: z_j is the weighted sum of inputs to the neuron j. w_{ij} is the weight connecting neuron i in the previous layer to neuron j. x_i is the input to neuron j. b_j is the bias term associated with neuron j. σ (.) is the activation function, typically a non-linear function like the sigmoid function for binary regression.

The output of the neural network is computed as the composition of multiple layers:

$\hat{y}_i = f(x_i)$ Where, $\hat{y}_i$ represents the predicted probability of the positive class for observation i and $f(x_i)$ represents the forward propagation through the neural network.

Training a neural network involves optimising the network's parameters (weights and biases) to minimise a loss function, typically the binary cross-entropy loss function, which measures the difference between the predicted probabilities and the true labels. The optimisation process, often performed using gradient descent or its variants, adjusts the weights and biases iteratively to improve the model's performance on the training data.

Model evaluation metrics: The comparative analysis employs a diverse set of performance metrics such as accuracy, precision, recall, F1 score and AUC in the Receiver Operating Characteristic curve (ROC).

Feature important scores: The RF model used average impurity reduction to assess each feature's contribution, with scores normalised for straightforward comparison. In contrast, the FFNN employed permutation importance, where the performance decline from shuffling each feature indicated its influence. This approach enabled us to identify and rank the most critical features for both models effectively.

Preprocessing and feature selection: The Chi-square filter method was adopted for features selection. Among the 11 features, 10 variables are associated with PCOS at a 5% level of significance, which include abnormal BMI, abnormal WHR, physical inactivity, weight gain, hair loss, hirsutism, irregular cycles, stress, skin darkening and fast food consumption, except for acne. The Variance Inflation Factor (VIF) method was used to identify multicollinearity. It was observed that there is no multicollinearity between the features, as all the features' VIF values were less than 5.

Training and testing: An 80% of the data was used to train the model and the remaining 20% was used for testing. The effectiveness of the models was assessed using a stratified 5-fold cross-validation method [15].

RESULTS

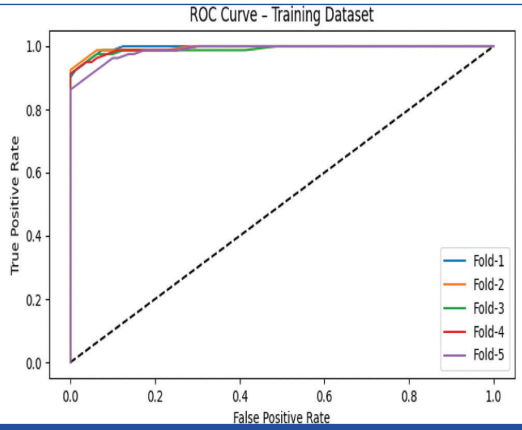
The age distribution between the PCOS-positive and PCOS-negative groups shows a similar median age of 27 years. The PCOS-negative group has less variability (IQR of 3) compared to the PCOS-positive group (IQR of 5). Both groups exhibited slight negative skewness and a relatively normal distribution. The Mann-

Whitney U test indicates no significant difference in age distribution between the groups (p-value=0.502).

[Table/Fig-1] depicts that the RF model exhibited strong performance on the training dataset, with high average metrics: an accuracy of 0.95, precision of 0.96, recall of 0.95, F1 score of 0.95 and AUC of 0.95 [Table/Fig-2]. These results suggest that the RF model was highly effective at fitting the training data, showing excellent precision and recall with minimal trade-offs between the two.

Cross-validation	Evaluation metrics				
	Accuracy	Precision	Recall	F1 score	AUC
Fold-1	0.96	0.95	0.96	0.96	0.96
Fold-2	0.96	0.96	0.96	0.96	0.96
Fold-3	0.96	0.99	0.93	0.95	0.96
Fold-4	0.96	0.96	0.95	0.96	0.96
Fold-5	0.93	0.94	0.93	0.93	0.93
Average	0.95	0.96	0.95	0.95	0.95

[Table/Fig-1]: Evaluation metrics by RF model of 5-fold cross validation on training dataset.



[Table/Fig-2]: ROC curve of RF on train dataset.

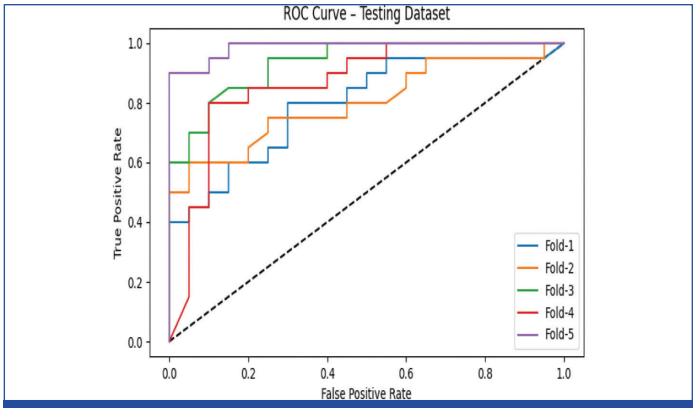
[Table/Fig-3] illustrates that in the testing dataset, the RF model displayed a more variable performance, with an average accuracy of 0.80, precision of 0.79, recall of 0.82, F1 score of 0.80 and AUC of 0.80 [Table/Fig-4]. These results indicate that while the RF model is strong in terms of generalisation, its performance is somewhat less stable on unseen data compared to its performance on the training dataset.

Cross-validation	Evaluation metrics				
	Accuracy	Precision	Recall	F1 score	AUC
Fold-1	0.70	0.67	0.80	0.73	0.70
Fold-2	0.73	0.76	0.65	0.70	0.73
Fold-3	0.80	0.77	0.85	0.81	0.80
Fold-4	0.85	0.89	0.80	0.84	0.85
Fold-5	0.93	0.87	1	0.93	0.92
Average	0.80	0.79	0.82	0.80	0.80

[Table/Fig-3]: Evaluation metrics by RF model of 5-fold cross validation on testing dataset.

[Table/Fig-5] shows that the FFNN model demonstrated consistent performance across the five folds of cross-validation on the training dataset, with an average accuracy of 0.80, precision of 0.81, recall of 0.79, F1 score of 0.80 and AUC of 0.80 [Table/Fig-6]. These metrics indicate a balanced model with good generalisation capabilities, showing that it can identify positive cases with reasonable precision and recall.

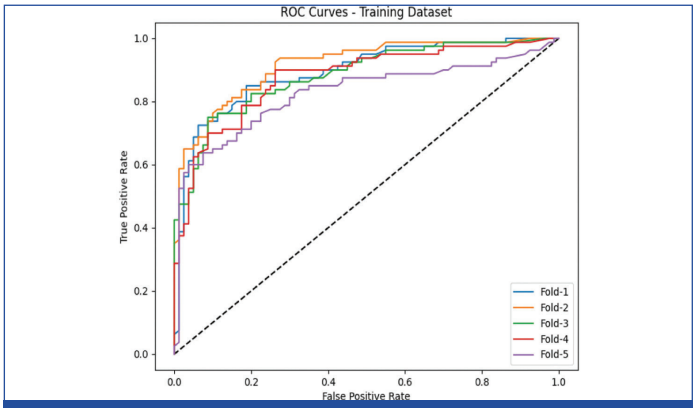
[Table/Fig-7] indicates that in the testing dataset, the FFNN model showed slightly better performance, with an average accuracy of 0.82, precision of 0.85, recall of 0.80, F1 score of 0.81 and AUC of 0.82 [Table/Fig-8]. The model maintained its balance but



[Table/Fig-4]: ROC curve of RF on test dataset.

Cross-validation	Evaluation metrics				
	Accuracy	Precision	Recall	F1 score	AUC
Fold-1	0.81	0.84	0.78	0.81	0.81
Fold-2	0.83	0.85	0.79	0.82	0.83
Fold-3	0.81	0.80	0.83	0.81	0.81
Fold-4	0.79	0.80	0.79	0.79	0.79
Fold-5	0.76	0.76	0.77	0.77	0.76
Average	0.80	0.81	0.79	0.80	0.80

[Table/Fig-5]: Evaluation metrics by FFNN model of 5-fold cross validation on training dataset.



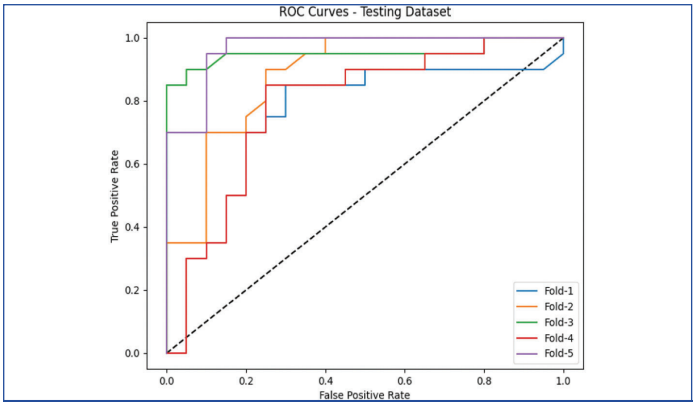
[Table/Fig-6]: ROC curve of FFNN on train dataset.

Cross-validation	Evaluation metrics				
	Accuracy	Precision	Recall	F1 score	AUC
Fold-1	0.83	0.93	0.70	0.80	0.83
Fold-2	0.76	0.87	0.65	0.74	0.77
Fold-3	0.85	0.79	0.95	0.86	0.85
Fold-4	0.75	0.78	0.70	0.74	0.75
Fold-5	0.93	0.87	1	0.93	0.92
Average	0.82	0.85	0.80	0.81	0.82

[Table/Fig-7]: Evaluation metrics by FFNN model of 5-fold cross validation on testing dataset.

demonstrated slight variability across the folds, indicating that it performs well on unseen data, although with some variations in recall and precision depending on the specific fold.

[Table/Fig-9] explores that the RF and FFNN models highlighted different features as the most important in predicting PCOS. The RF model emphasised irregular cycles and hirsutism as the top predictors, while the FFNN model prioritised weight gain, abnormal BMI and irregular cycles. This divergence in feature importance suggests that while both models agree on certain key features, their internal mechanisms differ in how they weigh the importance of various factors. The FFNN model appears to distribute importance more evenly across multiple features, whereas the RF model focuses more heavily on a few key predictors.



[Table/Fig-8]: ROC curve of FFNN on test dataset.

Feature	RF		FFNN	
	Average score of 5-fold CV	Rank	Average score of 5-fold CV	Rank
Abnormal WHR	0.10	4	0.19	5
Abnormal BMI	0.07	8	0.20	2
Physical inactivity	0.05	10	0.18	9
Weight gain	0.14	3	0.21	1
Hair loss	0.08	5	0.19	5
Hirsutism	0.17	2	0.20	4
Irregular cycles	0.17	1	0.20	3
Stress	0.08	6	0.17	10
Skin darkening	0.08	7	0.19	8
Fast food consumption	0.06	9	0.19	7

[Table/Fig-9]: Feature importance scores and their ranks of each model.

Computational time: The FFNN model required an average of 2.47 seconds per fold during 5-fold cross-validation, reflecting its computational complexity due to multiple layers and parameters. In contrast, the RF model was much more efficient, averaging just 0.25 seconds per fold. Its parallel processing of decision trees required significantly less computational time.

DISCUSSION

Thakre V conducted a study predicting PCOS using various invasive and non invasive variables, where the RF model outperformed four other models, achieving an impressive 89.0% AUC on test data and a 90.9% training accuracy [16]. Similarly, Subha R et al., used the RF algorithm with Chi-square feature selection to predict PCOS, resulting in an AUC of 0.889 in the ROC analysis [17]. Elmannai H et al., explored ML models for forecasting PCOS, finding that the Stacking ML approach with REF feature selection achieved perfect performance, surpassing other models [18]. Additionally, a meta-analysis by Bharali MD et al., highlighted the high incidence of PCOS among Indian women, with a prevalence of nearly 10% using Rotterdam's and Androgen Excess Society (AES) criteria, compared to 5.8% using National Institutes of Health (NIH) criteria, emphasising the need for standardised diagnostic criteria [19]. Moreover, Shan B et al., identified significant risk factors for PCOS, including a family history of infertility (OR=11.953), diabetes (OR=7.008), menstrual disorders (OR=5.824), maternal menstrual irregularities (OR=2.557), mood disturbances (OR=2.852) and low physical activity (OR=1.866) [20].

Performance metrics: Indicate that the RF model outperformed the FFNN model in terms of accuracy, precision, recall, F1 score and AUC on the training dataset, emphasising the robustness of ensemble methods like RF in handling complex, non linear interactions between features [21]. However, the RF model's performance on the testing dataset showed more variability, suggesting potential overfitting, a common challenge in ML models trained on high-dimensional data [22]. On the other hand, the FFNN model, despite having slightly lower training accuracy, demonstrated more consistent performance on the testing data, indicating better generalisation, which is often a strength of neural networks [23].

Several studies provide a basis for comparing model accuracy in PCOS prediction. Hosseini A et al., achieved an accuracy of 0.85 with a RF model using both invasive (e.g., blood hormone levels) and non invasive features, which was slightly higher than the present study's RF model accuracy of 0.80, which relied solely on non invasive features [24]. Kumar R and Choudhury T's FFNN model, using only non invasive markers, reached an accuracy of 0.78, lower than the present study's FFNN accuracy of 0.82, highlighting the potential of non invasive data for consistent PCOS prediction [25]. Li Z et al.'s, Support Vector Machine (SVM) model reached 0.88 accuracy with invasive measures like hormonal assays suggesting higher accuracy from additional tests, while the present study's non invasive approach still achieves competitive accuracy [26]. Zeng H et al., reported that their RF model attained an accuracy of 0.81 using a mix of invasive and non invasive data, similar to the present study's RF accuracy of 0.80, supporting the utility of non invasive methods alone [27]. Lastly, Jones H et al., used logistic regression with non invasive features alone, reporting a lower accuracy of 0.76, indicating that models like RF and FFNN can yield better results without invasive diagnostics [28].

Feature importance: The RF model identified irregular cycles and hirsutism as the most influential predictors of PCOS, consistent with clinical evidence that these symptoms are strongly associated with the syndrome [28]. Conversely, the FFNN model assigned higher importance to weight gain and abnormal BMI, reflecting the model's ability to capture complex, non linear relationships between these features and PCOS. This divergence in feature importance underscores the complementary nature of these models, suggesting that integrating insights from both could provide a more comprehensive understanding of PCOS risk factors [29].

Computational efficiency: The RF model's significantly shorter computational time (0.25 seconds per fold on average) compared to the FFNN model (2.47 seconds per fold) is noteworthy and consistent with literature that highlights the efficiency of ensemble methods. The longer computational time for the FFNN model reflects the complexity of neural networks, which involve multiple layers of computation and require extensive hyperparameter tuning, a trade-off often considered in deep learning applications [30,31].

The differing feature importance rankings also suggest that using both models in tandem could provide a more comprehensive understanding of the predictors of PCOS. In epidemiological investigations, these models serve as preliminary screening tools for identifying probabilistic cases of PCOS using non invasive qualitative features, especially where diagnostic facilities are not available.

Limitation(s)

The absence of data for key features, such as family history of PCOS, resulted in the exclusion of this variable from the analysis due to the majority of data being missing. This may limit the model's ability to account for hereditary influences on PCOS risk. Additionally, the case-control design used in this study could introduce selection bias, affecting the generalisability of the findings. A prospective cohort study may yield more comprehensive results by allowing for temporal data collection and a clearer understanding of how various risk factors contribute to the development of PCOS over time.

CONCLUSION(S)

The choice between RF and FFNN depends on the specific requirements of the task. If computational efficiency and quick deployment are priorities, the RF model is a clear winner. However, for applications where consistent performance and generalisation to new data are more important, the FFNN model offers a compelling advantage.

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PLAGIARISM CHECKING METHODS: [Jain H et al.]
- Plagiarism X-checker: Sep 10, 2024
- Manual Googling: Nov 04, 2024
- iThenticate Software: Nov 06, 2024 (9%)

ETYMOLOGY: Author Origin

EMENDATIONS: 6

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- Was Ethics Committee Approval obtained for this study? No
- Was informed consent obtained from the subjects involved in the study? Yes
- For any images presented appropriate consent has been obtained from the subjects. No

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