

Machine Learning-Based Polycystic Ovary Syndrome Generative Modelling via Ensemble Learning and Neural Networks for Infertility Prediction

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Abstract

Higher health issues, such as diabetes and hypertension, are sacrosanct with Polycystic Ovary Syndrome (PCOS) and they greatly affect fertility in women. Therefore, irregular menstrual periods, acne, increased hair growth and several hormone-related disorders are prevalent in people with PCOS. The study employed variable distributions and correlations, and the experimental design made use of exploratory data analysis and heat map visualization. Principal Component Analysis (PCA) was used for feature selection to minimize dimensionality and pinpoint the most informative attributes. A thorough cross-validation evaluation that suggested models' generalizability, robustness, and performance was considered. To ensure a thorough evaluation of the PCOS diagnostic value, evaluation measures such as F1-score, precision, accuracy and recall were utilized on Random Forest (RF), Recurrent Neural Networks (RNN) and Support Vector Machines (SVM) algorithms to build the models. The performance results show that RF had the best accuracy result of 99.74% followed by SVM with 99.21% and RNN with the worst result of 65.09%. This means that RF had the highest accurate predictions of the total amount of input samples. SVM and RF had the same precision result of 1.00, which shows that the two models had no misclassification of the PCOS infertility outcomes. That is, both SVM and RF could correctly identify all the positive instances and all the negative instances. The higher the value of the F1-score, the more reliable the model's predictability. RF based on the highest F1-score of 0.9956 can be used for PCOS infertility modelling. The study concludes that RF is the golden model due to its superior performance for building a PCOS infertility prediction generative model. The study, therefore, suggests the implementation of federated learning and other deep learning algorithms for scalable performance using the big data paradigm.

Keywords: Deep learning, Infertility, Machine learning, Polycystic ovary syndrome, Random forest, Recurrent neural network, Reproductive health, Support vector machine, Women's health.

1.0 Introduction

Polycystic Ovary Syndrome (PCOS) is a hormonal condition often found in women of reproductive age. PCOS is a frequent hormone-related disorder. It causes insurgent menstrual cycles, excessive hair growth, acne, and infertility. The treatment for PCOS is determined by whether or not pregnancy is considered important. People with PCOS may be at a higher risk for certain health issues, including diabetes and hypertension [1]. Ten to fifteen percent of women of reproductive age are thought to be affected by PCOS, a complicated endocrine and metabolic condition. Hyperandrogenism, oligo-anovulation, and polycystic ovarian morphology are its defining characteristics, and they significantly increase the risk of infertility and chronic metabolic problems [2], [3]. Beyond reproductive dysfunction, PCOS is a serious global public health issue as a result of high correlations with obesity, insulin resistance, and elevated cardiovascular risks [4].

Clinical criteria like the Rotterdam consensus, hormone assays, and imaging techniques have historically been used to make diagnoses. However, subjectivity, demographic variability, and inconsistent feature selection are common problems with these traditional methods, which can result in delayed diagnosis and less-than-ideal care [5], [6]. Strong computational techniques that can capture the intricate, non-linear relationships between clinical, biochemical, and imaging data are desperately needed because PCOS manifests in a variety of phenotypes [7]. Recent developments in machine learning have demonstrated potential for enhancing early intervention tactics and increasing diagnostic precision. Notably, support vector machines (SVM) have shown good precision and recall metrics in their successful use in PCOS classification and optimization of pertinent feature subsets from high-dimensional datasets [5], [8]. To efficiently train deep learning models on big clinical datasets, gradient-based optimization techniques, specifically stochastic gradient descent (SGD), have further improved model convergence and generalization [9].

Recurrent neural networks (RNN) have become a powerful tool for modeling the sequential dependencies present in longitudinal clinical data, in addition to discriminative classifiers [10]. RNN architectures can improve prediction reliability by capturing the temporal evolution of metabolic and reproductive factors linked to PCOS by utilizing their capacity to process time-series inputs [2], [8]. Even with these encouraging advancements, there are still many obstacles to overcome. Reproducibility and interpretability are limited by the lack of standardized taxonomies of PCOS-relevant variables in many of the detection systems now in use [11]. Furthermore, the generative component of disease modelling, which is essential for creating representative patient profiles and simulating clinical scenarios, is frequently overlooked by traditional models [3], [12]. The scalability of machine learning techniques in this field is further limited by the lack of complete multimodal datasets and verified generating frameworks [13].

This study implements a unique machine learning-based generative modelling framework that integrates SVM, Decision Tree, and RNN architectures for Polycystic Ovary Syndrome (PCOS) infertility prediction to overcome these constraints. The method uses dense to optimize the training of RNN layers that can model temporal trends, while utilizing SVM's discriminative strength for initial feature selection and classification. To increase detection accuracy and facilitate longitudinal patient monitoring, this hybrid system attempts to integrate dynamic sequence modeling with static feature categorization. Significant percentage of women worldwide suffers from PCOS, a complex endocrine condition that continues to be major cause of infertility. Traditional diagnostic techniques frequently include a mix of biochemical indicators, clinical observation, and ultrasound imaging; however, these techniques are limited by subjectivity and population-specific variability [5]. Recent studies have shown that artificial intelligence (AI) [14] [15] and machine learning (ML) [16] are viable substitutes for enhancing diagnostic precision [17] and thus can help in simulating the diverse presentations of PCOS.

Support Vector Machine (SVM) classifier was used by [5] to forecast PCOS status using extensive clinical data. Linear SVM got the highest accuracy (90%) with balanced precision and recall scores, according to their study that examined linear, radial basis function, and polynomial SVM kernels. This result highlights SVM algorithms' ability to manage high-dimensional feature spaces and reliably categorize complicated medical diseases. The scientists also underlined that by eliminating unnecessary variables and keeping the most important predictors [18], incorporating feature selection techniques might increase classifier efficiency. Ensemble learning techniques for PCOS diagnosis have been investigated in complementary investigations. The effectiveness of ensemble classifiers incorporating Random Forest, Logistic Regression, and univariate feature selection techniques was shown by [2]. Their research showed that hybrid models, which take advantage of several viewpoints on data representation and decision boundaries, perform better than single classifiers [19]. By improving interpretability and prediction accuracy, these ensemble techniques help to overcome a significant drawback of conventional diagnostic frameworks.

[2] Conducted a thorough examination of ensemble learning frameworks for data-driven diagnosis of PCOS, offering additional evidence in favor of machine learning's significance in PCOS research. To lower dimensionality and improve model stability, the authors used principal component analysis with Random Forest and Logistic Regression classifiers. This method showed that ensemble learning may maintain good generalization capacities while accommodating the unpredictability present in clinical samples. Their results are consistent with more general trends in AI-driven healthcare, which favor hybrid and ensemble approaches more and more to strike a compromise between model transparency and predictive capability. Although ensemble learning models and discriminative classifiers like SVM have shown promise, generative modeling techniques are still relatively unexplored in PCOS prediction. To simulate representative patient profiles and comprehend the dynamic evolution of clinical conditions, generative frameworks are essential. RNN, one of the most current developments in deep learning, has showcased potential in identifying temporal connections in health data [2]. There is a significant research gap, nevertheless, as few studies have explicitly used RNN architectures to sequential PCOS datasets.

There is also growing recognition of the significance of explainability and model interpretability. Transparent machine learning frameworks are essential for fostering clinician trust and enabling meaningful integration into reproductive health workflows, as claimed by the authors [2]. To increase the acceptability and accountability of prediction models, the authors suggested methods for visualizing feature contributions and decision routes. Because reproductive health data is sensitive and clinical decision support systems must be transparent according to ethical standards, these factors are crucial. Apart from machine learning methods, exploratory data analysis (EDA) and data preprocessing have become essential elements of effective PCOS prediction pipelines. According to [5], thorough EDA, which includes correlation analysis and heat map visualization, is essential for finding hidden patterns and guaranteeing data quality. Principal Component Analysis (PCA) feature selection further refines the dataset, increasing computing efficiency and lowering the chance of overfitting. When working with complicated and diverse clinical information, these preprocessing techniques make it possible to create models that are more dependable and broadly applicable.

Even with these developments, there are still enduring difficulties. The generating ability necessary for continuous simulation of PCOS risk is not sufficiently addressed in many of the research studies that are currently available, which only concentrate on classification accuracy. Additionally, the clinical application of current techniques is hindered by the lack of defined evaluation methodologies [20] and the limited incorporation of temporal modelling frameworks, such as RNN. In order to close these gaps and enhance prediction accuracy, interpretability, and scalability, hybrid approaches combining generative models, gradient optimization methods, and discriminative classifiers must be developed. To address these issues, this study utilizes support vector machines (SVM) for initial classification. It combines RNN architectures for temporal modelling, and grows and uses multiple decision trees to create a “forest”. The suggested method seeks to improve the state of PCOS prediction and infertility risk assessment by utilizing ensemble learning principles, PCA-based feature selection, and rigorous cross-validation.

2.0 Methodology

A carefully selected PCOS dataset, comprising biochemical markers, anthropometric measurements, and ultrasound imaging data, was used for this study. To investigate variable distributions and correlations, the experimental design made use of exploratory data analysis and heat map visualization. Principal Component Analysis (PCA) was used for feature selection to minimize dimensionality and pinpoint the most informative characteristics. Thorough cross-validation evaluates the suggested models' generalizability, robustness, and performance. To ensure a thorough evaluation of the PCOS's diagnostic value, evaluation metrics such as F1-score, precision, accuracy, and recall were utilized.

2.1 Data Preparation

The Polycystic Ovary Syndrome dataset was prepared on the Jupyter Notebook IDE. Pandas was used to load the dataset. The dataset undergoes several preprocessing methods. The dataset was checked for missing values. Data scaling was performed on the dataset to fit within a specific range to ensure no data value is left out during model training. Standard Scalar was used to carry out the data scaling. Finally, data splitting was performed on the input data features labeled “independent variables”. The data cross-validation ratio employed a splitting of 70% training and 30% testing. Figure 1 shows the flowchart for the proposed model, which depicts the process flow for choosing the golden model.

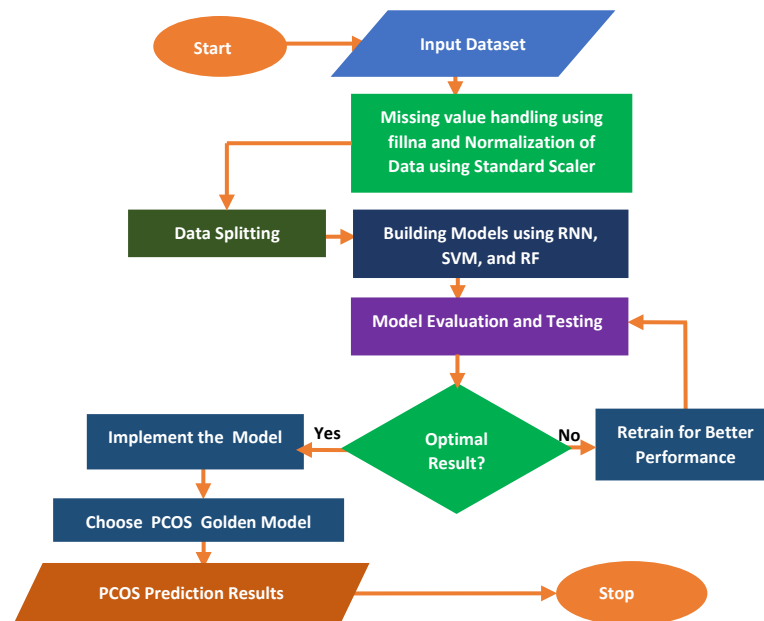


Figure 1: Flowchart for the PCOS Infertility Prediction Model

2.2 Mathematical Modelling for SVM, Random Forest and RNN

The mathematical models for the algorithms are elucidated accordingly.

2.2.1 Mathematical Modelling for Support Vector Machines

Consider a binary classification issue with two labels: +1 and -1. That is +1 is the presence of PCOS and -1 is the absence of PCOS. We have a training dataset made up of input feature vectors X and their matching class labels Y . The linear hyperplane equation can be defined thus:

$$w^T x + b = 0 \quad (1)$$

where:

w is the normal vector (w) is perpendicular to the hyperplane.

b is the offset or bias term that represents the hyperplane's distance from the origin along the normal vector (w).

Distance from a data point to the Hyperplane shows the hypothesis function for the classifier given thus:

$$\hat{y} = \begin{cases} 0 & : w^T x = b \leq 0 \\ 1 & : w^T x = b < 0 \end{cases} \quad (2)$$

where $\hat{y}$ is the predicted label of a data point.

2.2.2 Mathematical Modelling for Random Tree

This section explains the relationship between decision tree and random forest in model building. Ensembles of trees are used in making a random forest, after which a decision is made from a single decision path from the forest.

a) Decision Tree

For a randomly distributed dataset such as the Polycystic Ovary Syndrome dataset, it is critical to select a technique that reduces entropy while maximizing information gain. In that regard, the application of a Decision Tree for classification in this study is critical.

$$\text{Info}(D) = - \sum_{i=0}^m p_i \log_2 p_i \quad (3)$$

Where, P_i is the probability that an arbitrary tuple in D belongs to class C_i

$$\text{Info}_A(D) = \sum_{j=1}^v \frac{|D_j|}{|D|} \times \text{Info}(D_j) \quad (4)$$

$$\text{Gain}(A) = \text{Info}(D) - \text{Info}_A(D) \quad (5)$$

The gain ratio addresses the issue of bias by leveling the information obtained via Split Info. The gain ratio can be described as:

$$\text{GainRatio}(A) = \frac{\text{Gain}(A)}{\text{SplitInfo}_A(D)} \quad (6)$$

The Gini index favors greater divisions. It utilizes a squared percentage of classes. If everything was perfectly categorized, the Gini Index would be 0. Variable splits should have a low Gini index.

The algorithm operates as “ $1 - (P(\text{class1})^2 + P(\text{class2})^2 + \dots + P(\text{classN})^2)$ ”

$$\text{Gini} = 1 - \sum_{i=1}^C (P_i)^2 \quad (7)$$

The attribute with the biggest information gain becomes the splitting attribute at the decision tree's root node. The tuples are partitioned appropriately.

b) Random Forest

Random forests (RF) create several independent decision trees during training. The final prediction is made using the mode of the classes by pooling predictions from all trees when dealing with classification problems.

The relevance for each feature on a decision tree is then determined as shown in equation (8):

$$f_{i_i} = \frac{\sum_{j: \text{node } j \text{ splits on feature } i} n_{i_j}}{\sum_{k \in \text{all nodes}} n_{i_k}} \quad (8)$$

where:

$f_{i \text{ sub}(j)}$ = the importance of feature i and $n_{i \text{ sub}(j)}$ = the importance of node j

These are then normalized to a value between 0 and 1 by dividing by the total of all feature significance values.

$$\text{norm} f_{i_i} = \frac{f_{i_i}}{\sum_{j \in \text{all features}} f_{i_j}} \quad (9)$$

The ultimate feature significance at the Random Forest level is the average across all trees. The sum of the feature's significance value for each tree is computed and divided by the total number of trees as show in in equation (10).

$$RFfi_i = \frac{\sum_{j \in \text{all trees}} \text{normfi}_{ji}}{T} \quad (10)$$

where:

RFfi sub(i) = the importance of feature i calculated from all trees in the Random Forest model
 normfi sub(ij) = the normalized feature importance for i in tree j
 T = total number of trees

2.2.3 Mathematical Modelling for Recurrent Neural Networks

RNN relies on both current and historical inputs to determine its output. Let $\mathbf{I}_1$ be the initial input with a dimension of $\mathbf{n} \times \mathbf{1}$, where $\mathbf{n}$ is the length of the vocabulary. $\mathbf{S}_0$ represents the hidden state of the first RNN cell with $\mathbf{d}$ neurons. The input hidden state for each cell should be the preceding one. Because no past state is visible in the first cell, initialize $\mathbf{S}_0$ with zeros or a random value. $\mathbf{U}$ is another matrix of dimension $\mathbf{d} \times \mathbf{n}$, where $\mathbf{d}$ is the number of neurons in the first RNN cell and $\mathbf{n}$ is the size of the input vocabulary. $\mathbf{W}$ is another matrix of the size $\mathbf{d} \times \mathbf{d}$. $\mathbf{b}$ is bias, and its dimension is $\mathbf{d} \times \mathbf{1}$.

To determine the output from the first cell, another matrix $\mathbf{V}$ of dimension $\mathbf{k} \times \mathbf{d}$ is used, where $\mathbf{c}$ is the bias with dimension $\mathbf{k} \times \mathbf{1}$.

The first RNN cell produces the mathematical outputs shown in equations (11) and (12).

$$\mathbf{S}_1 = \mathbf{U}\mathbf{I}_1 + \mathbf{W}\mathbf{S}_0 + \mathbf{b} \quad (11)$$

$$\mathbf{O}_1 = \mathbf{V}\mathbf{S}_1 + \mathbf{c} \quad (12)$$

In general,

$$\mathbf{S}_n = \mathbf{U}\mathbf{I}_n + \mathbf{W}\mathbf{S}_{n-1} + \mathbf{b} \quad (13)$$

$$\mathbf{O}_n = \mathbf{V}\mathbf{S}_n + \mathbf{c} \quad (14)$$

In general, output $\mathbf{O}_n$ relies on $\mathbf{S}_n$, whereas $\mathbf{S}_n$ depends on $\mathbf{S}_{n-1}$. $\mathbf{S}_{n-1}$ depends on $\mathbf{S}_{n-2}$ as shown in equations (13) and (14). The process continues until $\mathbf{S}_0$ is obtained. This demonstrates that the output at the n th time step relies on all previous inputs.

2.3 Model Building for SVM, Random Forest and RNN

The Polycystic Ovary Syndrome dataset was imported into Python code in CSV format, utilizing tools and libraries such as Anaconda, Jupyter, pandas, NumPy, and matplotlib to create machine learning and deep learning models. During the model design phase, the dataset was split into training and testing sections, and some deep learning hidden layers, such as dense, activation, batch size, filament, input size, and epoch, were utilized to construct the recurrent neural network (RNN).

2.3.1 Support Vector Machines Model

The primary aim of SVM is to determine the best hyperplane that linearly divides the data points into two segments while maximizing the margin. Figure 2 shows the mathematical interpretation of the optimal hyperplane.

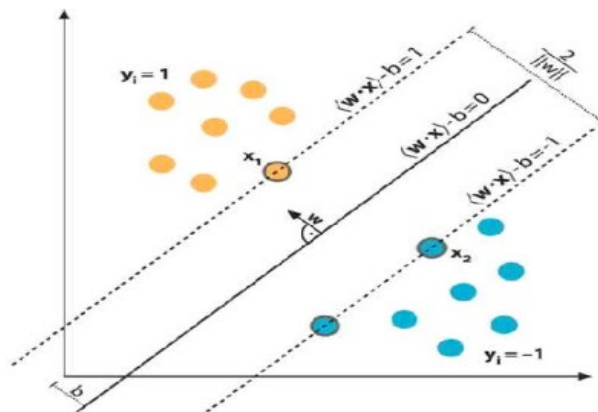


Figure 2: SVM optimal hyperplane

2.3.2 Random Forest Model

Random Forest (RF) is a machine learning system that employs a large number of decision trees to create better predictions. Each tree checks different random parts of the data, and the results are combined by voting for classification or averaging for regression. This increases accuracy and decreases mistakes. Random forest creates many more decision trees for accuracy improvement and reduction in errors.

Decision Trees (DTs) are supervised learning methods that are non-parametric (with a set number of parameters) and used for regression and classification. The idea is to train a model to predict the label of a target variable using simple decision rules generated from data characteristics. An algorithmic technique may be used to create decision trees that can partition the dataset in numerous ways depending on the criteria. Figure 3 shows the decision tree model implementation. Figure 4 shows the decision tree versus the random forest model implementation on how the decision path is made.

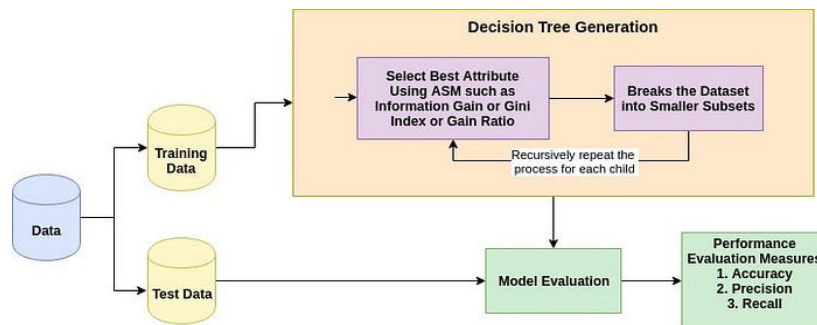


Figure 3: Decision tree model implementation

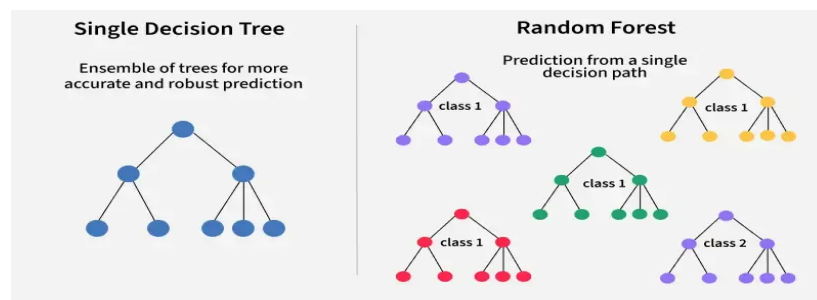


Figure 4: Decision tree versus random forest model implementation

2.3.3 Recurrent Neural Networks Model

RNN is a sort of neural network that takes variable-length input and generates variable-length output. It is used to create a variety of applications, including medical health analytics, time series stock forecasting, chatbots, language modelling, text-to-speech, machine translation, emotional analysis, and name entity recognition.

Figure 5 shows the RNN architecture, depicting the initial input, hidden state and dense layer.

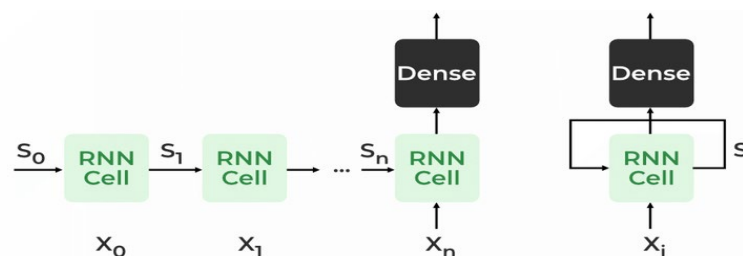


Figure 5: RNN model implementation

3.0 Results and Discussion

This section discusses the metric results obtained from the analysis using machine learning algorithms such as SVM, RF, and RNN deep learning algorithm to build the PCOS infertility generative models. After the model development, comparative analysis was carried out on the three models. Table 1 displays the performance evaluation results of the models, while Figure 6 gives the pictorial representation of the performance evaluation.

The performance results show that RF had the best accuracy result of 99.74% followed by SVM with 99.21% and RNN with the worst result of 65.09%. This means that RF had the highest accurate predictions of the total

amount of input samples. SVM and RF had the same precision result of 1.00, which shows that the two models had no misclassification of the PCOS infertility outcomes. That is, both SVM and RF could correctly identify all the positive instances and all the negative instances. Whereas for the RNN, the precision result was 0.35, which was very low. It means that RNN could not correctly identify all the positive instances. RF has the best recall result of 0.991, followed by SVM with 0.974 and RNN with 0.194. The higher the value of the F1-score, the more reliable the model becomes. It is evident that RF, based on the highest F1-score of 0.9956, can be used for PCOS infertility modelling.

Table 1: Performance Evaluation Results of the models

Models	Evaluation Metrics			
	Accuracy (%)	Precision	Recall	F1_score
SVM	99.21	1.00	0.974	0.9866
RF	99.74	1.00	0.991	0.9956
RNN	65.09	0.35	0.194	0.2486

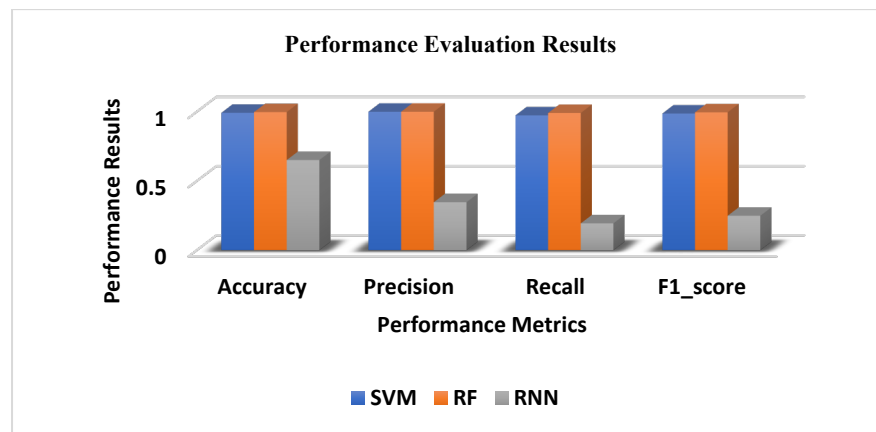


Figure 6: Performance evaluation results

4.0 Conclusion

The development of the PCOS generative model for infertility prediction represents a crucial stride towards enhancing women's reproductive health support and awareness. This study made use of SVM, RF, and RNN to build the models. According to the performance evaluation results, RF is the golden model because it outperformed other classifiers in all respects. This study concludes that Random Forest can be used as the best model to predict PCOS infertility in women to improve their reproductive health conditions. The study, therefore, suggests the implementation of federated learning and other deep learning algorithms for scalable performance using the big data paradigm for future work.

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