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Enhancing sepsis detection using feed-forward neural networks with hyperparameter tuning techniques

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ABSTRACT

This paper investigates the use of feed-forward neural networks for sepsis detection, emphasizing class imbalance mitigation and hyperparameter optimization. Leveraging random oversampling, synthetic minority over-sampling technique (SMOTE), and random sampling techniques, we address class imbalance, significantly improving feed-forward neural network performance. The resulting model achieves an impressive 83% accuracy on the test set, with notable enhancements in precision, recall, and F1-score for the positive class. Hyperparameter tuning using RandomizedSearchCV identifies optimal parameters, including an alpha value of 0.01 and the logistic activation function, leading to a remarkable 57.5% test accuracy. GridSearchCV also contributes to model refinement, albeit with a slightly lower test accuracy of 51.5%. These findings underscore the importance of robust hyperparameter tuning methods in optimizing feed-forward neural network models for imbalanced datasets, particularly in sepsis detection. The insights gained hold promise for the development of more accurate diagnostic tools, ultimately improving patient outcomes in clinical practice.

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1. INTRODUCTION

Sepsis is a medical condition that requires immediate attention to avoid a life-threatening situation. This is a condition arises due to body's response to an infection. If this is not treated at the initial stage can lead to inflammation and dysfunction of organ and finally death. Sepsis can be triggered by various infectious agents such as bacteria, viruses, fungi, or parasites, and it can affect individuals of any age or health status. The immune system, designed to defend against infections, can go into overdrive during sepsis, releasing an excessive amount of inflammatory chemicals. Early identification and intervention is very much required to avoid sepsis to mitigate to severe stages like severe sepsis and septic shock [1]. If it's not treated in the early stage can lead to organ failure and even death their by increasing the mortality rate. Timely intervention includes antibiotics treatment to stabilize the initial symptoms. Sepsis remains a significant global health challenges. Machine learning plays a crucial role in detecting sepsis by leveraging computational algorithms and statistical models to analyze large datasets and identify patterns associated with the condition [2].

Predictive analytics can assist clinicians in identifying high-risk patients and implementing preventive measures. Machine learning algorithms can be integrated into clinical decision support systems to assist healthcare professionals in diagnosing sepsis. These systems analyze real-time patient data and provide recommendations or alerts based on established sepsis detection criteria. The current state of the art in sepsis detection and management emphasizes the importance of early identification and prompt intervention to prevent the progression of sepsis to severe stages, including septic shock. In this work feed-forward neural network model is developed and performance is checked using different metric like accuracy, precision, F1-score, and recall. To address class imbalance in datasets, techniques like random oversampling, synthetic minority over-sampling technique (SMOTE), and random sampling are employed, significantly improving the performance of feed-forward neural networks in detecting sepsis. Hyperparameter optimization methods, such as RandomizedSearchCV and GridSearchCV, are used to fine-tune these models, leading to improved accuracy and performance metrics. This work underscoring the importance of robust hyperparameter tuning methods in optimizing models for imbalanced datasets for detecting sepsis.

2. LITERATURE SURVEY

According to Lydia *et al.* [3], after evaluating multiple machine learning models, XGBoost stood out with a remarkable accuracy of 0.98, surpassing other models. Opting for efficiency, the study suggests using the lazy predict library and applies random search for hyper-parameter tuning of the XGBoost classifier. Introducing a lazy classifier to address classification challenges, the research achieves an impressive score of 0.99 using random search for optimal parameters, emphasizing the effectiveness of this approach with the XGBoost algorithm [3].

Kijpaisalratana *et al.* [4] have done hyper-parameter tuning using grid search on logistic regression model. Using a 5-fold cross-validation technique, the model's biases are minimized. Authors have compared the proposed model performance with the existing traditional scoring systems. They have used shapley additive explanation (SHAP) approach to explain the role of each feature in the prediction of sepsis. But this work has a limitation, as it's based on international classification of diseases (ICD) code which could be wrongly classified due to different types of error [4].

Ghias *et al.* [5] have used machine learning algorithms to effectively predict sepsis in the patients who are admitted to the intensive care unit (ICU). The features used here are the vital signs of the patients who are 18 and above aged. Here, the authors have used missforest algorithm for imputation of data. No hyperparameter tuning used, as they have used random forest, which can handle all the missing values. The XGBoost model outperformed with 0.98 accuracy [5].

Shashikumar *et al.* [6] have developed an recurrent neural network (RNN) model called deep artificial intelligence sepsis expert (DeepAISE) for early sepsis prediction. This model has achieved area under the curve (AUC) ranging from 0.87 to 0.90. Schamoni *et al.* [7] have developed an ensembling neural network (NN) to analyse medical data there by reducing error. This approach is exemplified in the early prediction of sepsis using real intensive care unit data, showcasing its efficacy in healthcare analytics. Here, authors have created a pool of individual learners. But they have not evaluated attribute inference attack. Through preventing membership inference, they were able to prevent attribute inference as well [7].

A novel hybrid meta heuristic algorithm, human mental search (HMS)-particle swarm optimization (PSO), used to optimize the deep neural network weights in early sepsis diagnosis. Here, local minima are reduced using PSO and HMS. System outperforms with mean square error (MSE) value of 0.22 [8]. This proposed system addresses the need to optimize the feed-forward neural network using hyper-parameter tuning, their by showcasing the effect of imbalance dataset on the model performance and addresses the need to hyper-parameter tuning to improve the overall performance of the model in sepsis detection [9].

3. METHOD

A feed-forward neural network is a type of artificial neural network in which information flows in one direction: forward, from the input layer to the output layer. It consists of multiple layers of interconnected nodes or neurons, organized into three main types of layers:

– Input layer: Input layer takes input data, and it has corresponding neurons as shown (1) and (2).

$$Y^{(1)} = X^{(1)}a + Z^{(1)} \tag{1}$$

$$a^{(1)} = \text{activation}(Y^{(1)}) \tag{2}$$

- Hidden layers: These are middle layers in the network. Each hidden layer has neurons and are connected to every other neurons in the previous layer.
- Output layer: The output layer consists of number of neurons, which is completely depending on the nature of the problem which we are solving.

A feed-forward neural network, at its core, is akin to a single-layer perceptron. It processes a sequence of inputs by multiplying them with weights. These weighted inputs are then summed to produce a total. If this sum surpasses a predetermined threshold (often set at zero), the output is typically 1; otherwise, it is -1. The single-layer perceptron is widely used for classification and can also integrate machine learning features [10].

3.1. Hyperparameter tuning

Hyperparameter tuning is a pivotal aspect in refining the efficacy of feed-forward neural networks, and GridSearchCV, RandomizedSearchCV, and random sampling techniques are commonly employed for this purpose [11]. By oversampling the minority class randomly, it helps alleviate class imbalance issues during the hyperparameter tuning process [12]. GridSearchCV systematically explores a predetermined hyperparameter grid, RandomizedSearchCV samples hyperparameter combinations from specified distributions, and random sampling involves selecting hyperparameter values at random. The incorporation of RandomOverSampler enhances the performance, especially when class imbalances [13], [14].

3.1.1. GridSearchCV

GridSearchCV is a hyperparameter tuning technique provided by scikit-learn that exhaustively searches through a predefined set of hyperparameter values for a given machine learning model. It performs a cross-validated grid search over a parameter grid, evaluating the model's performance for each combination of hyperparameters. Hyperparameter tuning finds the best possible settings to optimize the model's predictive performance. In hyperparameter tuning, you define a grid of hyperparameter values that you want to explore. This grid is essentially a set of points in the hyperparameter space [15], [6]. The grid search algorithm aims to find the optimal hyperparameters (h^*) by evaluating the model's performance across all combinations of hyperparameter values in the grid (H) .

GridSearchCV systematically explores this grid by training and evaluating the model at each point. It covers all possible combinations of hyperparameters specified in the grid. Cross-validation is an essential part of the process. The model is trained on some folds and tested on others, iteratively. GridSearchCV can be computationally expensive, especially when the hyperparameter space is large [16].

3.1.2. RandomizedSearchCV

Like GridSearchCV, the purpose of RandomizedSearchCV is hyperparameter tuning. Instead of exhaustively searching through all possible combinations of hyperparameters, RandomizedSearchCV randomly samples a specified number of combinations from the hyperparameter space. Similar to GridSearchCV, you define hyperparameter space to explore. However, instead of specifying exact values, you provide distributions from which values are randomly drawn [17].

The mathematical representation can be simplified as follows: Let H be the set of hyperparameters, M be the machine learning model, and P be the performance metric. The randomized search algorithm aims to find the optimal hyperparameters (h^*) by randomly sampling hyperparameter values from the distributions defined in the search space, as shown in (3).

$$h^* = \arg\max_{h \in H} P(M(h)) \tag{3}$$

Where $M(h)$ represents the machine learning model with hyperparameters h, $P(\cdot)$ is the performance metric used for evaluation, and $\arg\max_{h \in H}$ denotes the hyperparameter values that maximize the model's performance.

Hyperparameter tuning with RandomizedSearchCV is often more suitable when computational resources are limited or when you want to quickly get a sense of the hyperparameter space [18]. In summary, RandomizedSearchCV efficiently explores the hyperparameter space through random sampling, making it particularly useful when the search space is extensive and an exhaustive search is not feasible. It offers a good compromise between exploration and computational cost, providing an effective alternative to Grid-SearchCV. Figure 1 shows the proposed system architecture where feed-forward neural network is optimized using SMOTE, random sampling, GridCV, and RandomizedCV.

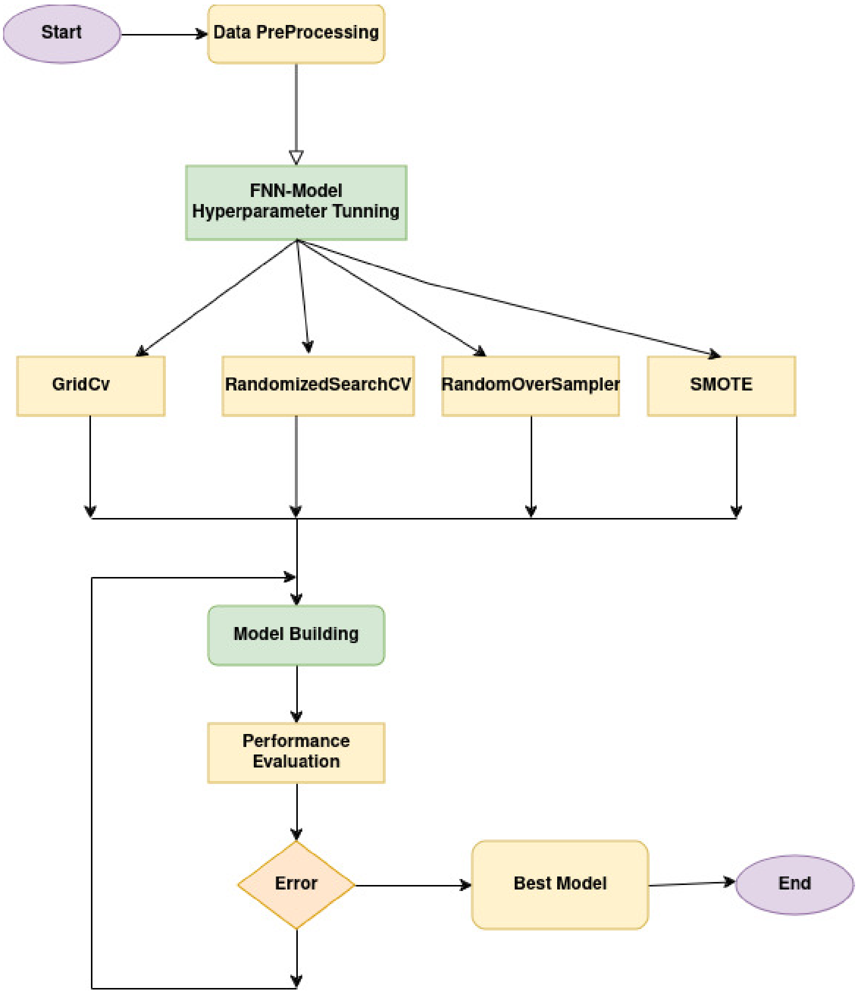

Figure 1. Proposed architecture

3.1.3. Random sampling

The main objective of oversampling techniques, such as RandomOverSampler, is to address class imbalance by generating synthetic instances for the minority class. The idea is to provide the model with more examples of the minority class, allowing it to learn a more robust decision boundary and reduce bias towards the majority class. RandomOverSampler takes a random selection approach to create additional samples for the minority class. Instead of relying on specific patterns within the minority class, it introduces randomness by duplicating instances at random. The random oversampling approach helps prevent overfitting to specific patterns in the minority class. If the oversampling were deterministic and always duplicated the same instances, the model might memorize these patterns, leading to poor generalization to new data [19].

3.1.4. Synthetic minority over-sampling technique

SMOTE is a technique used to address class imbalance. It works by generating synthetic instances for the minority class, and there by balancing the class. SMOTE helps balance the class there by improving the overall performance of the model [20].

4. RESULTS AND DISCUSSION

In this section, it is explained the results of research and at the same time is given the comprehensive discussion [21]. Dataset is taken from Physionet 2019 Challenge which has MIMIC III data [22]. Before tuning, the model showed low precision (0.0869) and recall (0.5417) for the minority class, resulting in an F1-score of 0.1497. However, after GridCV, precision significantly increased to 0.4875, achieving perfect recall (1.0000), and an improved F1-score of 0.6555. The classification report reflected this enhancement, with substantial gains in precision, recall, and F1-score for the minority class (1) while maintaining a reasonable accuracy of 0.49. Subsequently, the model was also evaluated using the SMOTE technique. Before GridCV, SMOTE demonstrated a balanced performance with precision, recall, and F1-score values around 0.57 for both classes. After GridCV, the model's hyperparameters were optimized, resulting in the best parameters being 'alpha': 0.1, 'hiddenlayersizes': (128,), and 'maxiter': 1500.

However, despite the parameter tuning, the performance improvements were moderate, with an accuracy of 0.51 and only slight enhancements in precision, recall, and F1-score for both classes. The SMOTE-enhanced model reflects the challenges in further improving the classification performance beyond a certain threshold, emphasizing the need for a comprehensive understanding of the dataset characteristics and potential limitations in model enhancement strategies [23], [24]. The classification report obtained from the evaluation of the feed-forward neural network with random oversampling for sepsis detection, where precision for detecting sepsis (class 1) is 8.86%. In this case, out of all instances predicted as sepsis, only 8.86% were true positive cases. Recall for detecting sepsis is 72.29%. A higher recall indicates better sensitivity. The F1-score is 15.79%. A higher F1-score is generally desirable. The overall accuracy of the model on this dataset is 83%. This metric represents the proportion of correctly classified instances among all instances. In the context of sepsis detection, while the model demonstrates high accuracy, the low precision suggests a high rate of false positives, and the F1-score indicates room for improvement in balancing precision and recall [25], [26].

Here's an explanation for the results obtained from the RandomizedSearchCV for hyperparameter tuning of a feed-forward neural network for sepsis detection as shown in Table 1.

- Best parameters: mlpclassifier__alpha: The optimal value found by the randomized search is 0.01. mlpclassifier__activation: The logistic activation function was found to be optimal.
- Best accuracy (training set): The best accuracy achieved on the training dataset is 56.12%. This indicates how well the neural network learned from the training data while adjusting its weights and biases based on the provided features.
- Test accuracy of best model is obtained when evaluated on an unseen dataset (not used during training), is 57.5%. This represents the ability of the tuned neural network to generalize and make accurate predictions on new data, specifically for sepsis detection.

Table 1. Best parameters and accuracy for feed-forward neural network with hyperparameter tuning

Best parameters	{'mlpclassifier__alpha': 0.01, 'mlpclassifier__activation': 'logistic'}
Best accuracy	0.561
Test accuracy of best model	0.575

The performance evaluation of feed-forward neural network model, employing hyperparameter tuning techniques, namely RandomizedSearchCV and GridSearchCV, is summarized herein. The test losses for the feed-forward neural network, obtained through RandomizedSearchCV, range from 0.0911 to 0.0931, showcasing consistent performance across multiple iterations as shown in Figures 2 and 3. Notably, RandomizedSearchCV yielded a test accuracy of 57.5%, with the optimal parameters being an alpha value of 0.01 and the logistic activation function as shown in Figure 4. In contrast, the GridSearchCV approach produced test losses within the range of 0.0915 to 0.0929, resulting in a slightly lower test accuracy of 51.5%. The optimal parameters identified through GridSearchCV include an alpha value of 0.01 and a hidden layer size of 64.

In the context of sepsis detection, these results suggest that the feed-forward neural network, with the specified hyperparameters, can achieve an accuracy of approximately 57.5% on unseen data. The results obtained from the GridSearchCV for hyperparameter tuning of a feed-forward neural network for sepsis detection as shown in Table 2 can be explained as follows: Best Parameters:`alpha` the optimal value found by the grid search is 0.01. The architecture of the neural network, specifying one hidden layer with 64 neurons. Best accuracy (training set): The best accuracy achieved on the training dataset is 52.63%. This indicates how well the neural network learned from the training data while adjusting its weights and biases based on the provided features. Test accuracy of best model is 51.5%. This represents the ability of the tuned neural network to generalize and make accurate predictions on new data, specifically for sepsis detection. In the context of sepsis detection, these results suggest that the feed-forward neural network, with the specified hyperparameters, can achieve an accuracy of approximately 51.5% on unseen data.

Figure 2. Feed-forward neural network test and validation loss

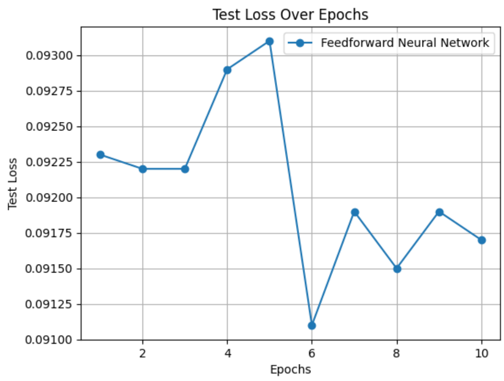

Figure 3. Feed-forward neural network test loss

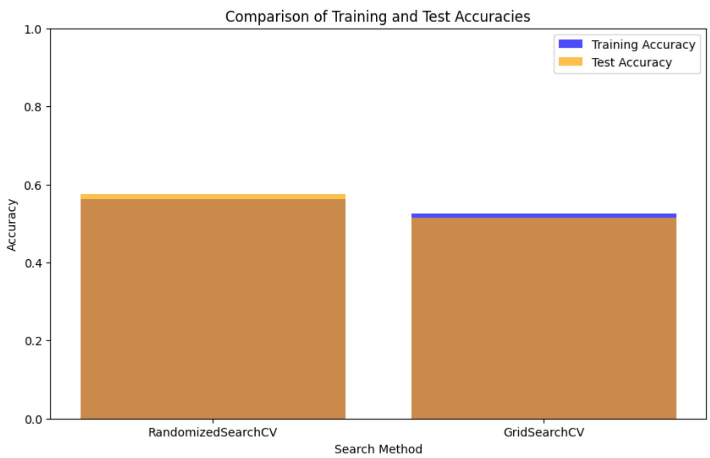

Figure 4. Feed-forward neural network training and test accuracy

Table 2. GridSearchCV results - feed-forward neural network

Best parameters	{'alpha': 0.01, 'hidden_layer_sizes': (64,)}
Best accuracy	0.526
Test accuracy of best model	0.515

5. CONCLUSION

Feed-forward neural network model achieved 83% accuracy on the test set with random oversampling, there is a substantial improvement in the precision, recall, and F1 score of the positive class compare to original imbalanced dataset. Optimal hyperparameter tuning like RandomizedSearchCV identified parameters like alpha value 0.01, logistic activation function with 57.5% accuracy. Whereas with GridSearchCV there was a down flow accuracy which is 51.5%. These findings underscore the role of robust hyper-parameter tuning methods in optimizing the feed-forward neural network for imbalanced datasets in detecting sepsis.

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