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Predicting Autism Spectrum Syndrome Employing Explainable Machine Learning and Deep Learning Approaches

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Abstract -- Autism Spectrum Disorder (ASD) is a neurodevelopmental condition characterized by difficulties in social communication and interaction, along with restricted interests and repetitive behaviors. Early screening can facilitate timely intervention and appropriate support. This study proposes an autism prediction framework using Machine Learning (ML) and Deep Learning (DL) techniques. A publicly available Kaggle dataset containing demographic information, screening questionnaire responses, and assessment scores is used for model evaluation. Decision Tree, Random Forest, CatBoost, LightGBM, LSTM, and BiLSTM models are investigated using accuracy, precision, and F1-score. Experimental results indicate that BiLSTM achieves the highest predictive accuracy among the evaluated models. Future research will focus on larger, diverse datasets and web-based screening applications to improve accessibility and generalizability. The proposed framework supports preliminary screening and does not replace professional clinical diagnosis.

Keywords: Autism Spectrum Disorder, Machine Learning, Deep Learning, LSTM, BiLSTM, Autism Screening.

I. INTRODUCTION

Autism Spectrum Disorder (ASD) is a neurodevelopmental condition characterized by challenges in social communication and interaction, along with restricted interests and repetitive behavioral patterns. Early identification and appropriate intervention are essential for providing timely support. With advancements in artificial intelligence, Machine Learning (ML) has emerged as a promising approach for analyzing behavioral and screening data to support preliminary autism prediction.

Previous studies have investigated ML-based autism screening using behavioral attributes and questionnaire responses. Research by Thabtah and colleagues explored ML techniques for autism-related classification, including rule-based approaches designed to improve model interpretability. Hasan et al. investigated automated approaches for early autism detection, particularly among children. Other studies have explored supervised learning techniques and the identification of behavioral patterns associated with autism, demonstrating the potential of data-driven screening methods.

Several algorithms, including Decision Tree, Random Forest, Support Vector Machine (SVM), and boosting techniques such as XGBoost and LightGBM, have been applied to autism prediction. Deep Learning (DL) architectures, including Long Short-Term Memory (LSTM) and Bidirectional LSTM (BiLSTM), have also been investigated for learning complex data patterns. In addition, emerging approaches incorporate neuroimaging, multimedia data, cloud computing, and Internet of Things (IoT) technologies to enhance screening capabilities.

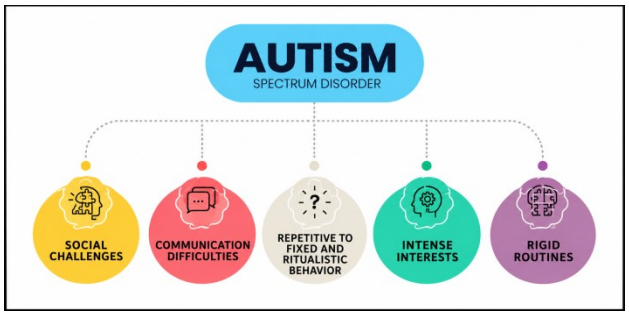


Figure 1: Autism Spectrum disorder.

This study develops an autism prediction framework using demographic attributes, screening questionnaire responses, and assessment scores from a publicly available Kaggle dataset. Decision Tree, Random Forest, CatBoost, LightGBM, LSTM, and BiLSTM models are implemented and evaluated. Python is used for development, with Pandas for data processing, Matplotlib and Seaborn for visualization, and Scikit-learn for model implementation and evaluation. Cross-validation and Randomized Search-based hyperparameter

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optimization are employed to assess model generalization and improve predictive performance.

The primary objective is to compare conventional ML and DL approaches and identify an effective model for preliminary autism screening. The proposed framework is intended to support early identification rather than replace professional clinical diagnosis.

II. Related Work

2.1 Machine Learning Algorithms in Autism

Early autism screening has gained considerable research attention due to the potential benefits of timely intervention and support. Various Machine Learning (ML) techniques have been investigated to improve the accuracy and reliability of autism prediction systems.

Thabtah et al. explored ML-based autism screening frameworks using questionnaire responses to support preliminary classification. Vyas and Gor evaluated algorithms such as Random Forest, Support Vector Machine (SVM), and Naïve Bayes, reporting comparatively better performance with Random Forest in their experiments. Ikotun and Olugbara investigated ensemble learning techniques for autism classification, highlighting the potential of combining multiple models to improve predictive performance. Sharma et al. examined a hybrid approach integrating Logistic Regression and SVM to address the limitations of individual classifiers. Alqahtani investigated CatBoost and LightGBM, which are suitable for classification tasks involving structured datasets.

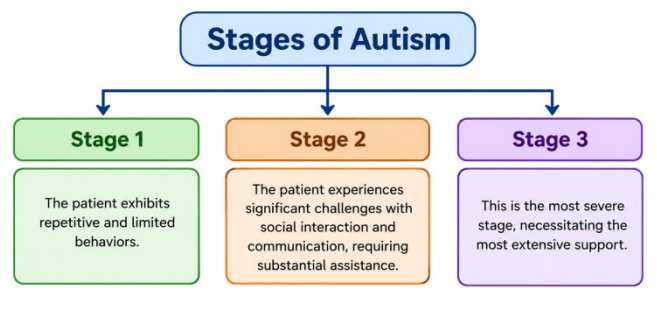


Figure 2: Stages of Autism

Although these studies demonstrate the potential of ML techniques for autism prediction, model performance and generalizability remain important considerations. Differences in dataset characteristics, feature selection, and evaluation procedures can influence predictive outcomes. Therefore, further investigation is required to compare conventional ML algorithms with Deep Learning (DL) architectures under consistent evaluation settings. This study addresses this need by evaluating Decision Tree, Random Forest, CatBoost, LightGBM, LSTM, and BiLSTM models for autism screening using a publicly available dataset.

Recent studies have highlighted the effectiveness of ensemble learning techniques, including Random Forest and boosting algorithms such as XGBoost, in Autism Spectrum Disorder (ASD) prediction. These methods can capture complex relationships in structured data and offer robustness across different classification tasks. Hasan et al. compared Support Vector Machine (SVM), Logistic Regression, and Random Forest, reporting superior accuracy for Random Forest in their evaluation. However, the interpretability of complex predictive models remains a concern, emphasizing the importance of explainable artificial intelligence (XAI). Deep learning architectures, such as Long Short-Term Memory (LSTM) and Bidirectional LSTM (BiLSTM), have also been explored for learning complex patterns from behavioral and sequential data. Nevertheless, their effectiveness on structured screening datasets requires systematic evaluation against tree-based ensemble methods.

To address this research gap, the present study compares conventional ML algorithms, including Decision Tree, Random Forest, CatBoost, and LightGBM, with LSTM and BiLSTM models for ASD prediction using a structured dataset. The comparative evaluation aims to identify an effective predictive model for screening applications involving demographic attributes and questionnaire-based features. Model performance is assessed using accuracy, precision, and F1-score, with cross-validation and hyperparameter optimization employed to support reliable evaluation and improve generalizability.

III. Proposed Methodology

3.1 Data collection and Visualization

The dataset used in this study was obtained from Kaggle and contains behavioral screening scores, demographic information, and classification labels for Autism Spectrum Disorder (ASD) prediction. The features include ten behavioral screening scores (A1–A10), age, gender, ethnicity, jaundice history, family history of autism, country of residence, previous screening status, total screening score, age category, and respondent relationship. An identification field is also provided to distinguish individual records.

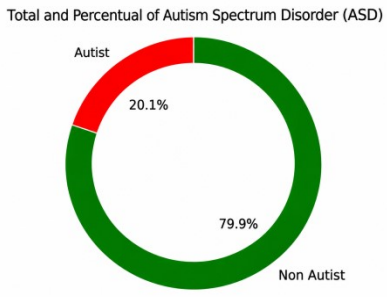


Figure 3: Dataset Visualization

The target variable, **Class/ASD**, represents the binary classification outcome, with 0 indicating a negative screening classification and 1 indicating a positive screening classification. The dataset is used to train and evaluate Decision Tree, Random Forest, CatBoost, LightGBM, LSTM, and BiLSTM models. Data preprocessing and feature selection are performed as required to support reliable model evaluation.

3.2 Data Preprocessing

Outlier detection is an important preprocessing step in machine learning, as extreme values may influence model performance. In this study, the Interquartile Range (IQR) method is used to identify potential outliers based on the first quartile (Q1) and third quartile (Q3). The IQR is calculated as (IQR = Q3 - Q1), and values below (Q1 - 1.5 \times IQR) or above (Q3 + 1.5 \times IQR) are identified as potential outliers.

Instead of removing these observations, the detected outliers are replaced with the median of the corresponding feature. The median is less sensitive to extreme values than the mean and provides a robust measure of central tendency. This approach retains the dataset's observations while limiting the influence of extreme numerical values during model training. However, outlier treatment is applied only to appropriate numerical features, ensuring that categorical attributes and valid screening scores are handled correctly.

3.3 Model Training

This study investigates four conventional Machine Learning (ML) algorithms—Decision Tree, Random Forest, CatBoost, and LightGBM—and two Deep Learning (DL) architectures, LSTM and BiLSTM, for Autism Spectrum Disorder (ASD) prediction.

Decision Tree classifies data by recursively splitting features according to decision rules. Although interpretable, it may overfit the training data. ***Random Forest*** combines predictions from multiple decision trees trained on randomly selected samples and features, improving robustness and reducing overfitting.

CatBoost is a gradient-boosting algorithm designed to handle categorical features effectively, while ***LightGBM*** uses a histogram-based learning strategy and leaf-wise tree growth to improve computational efficiency.

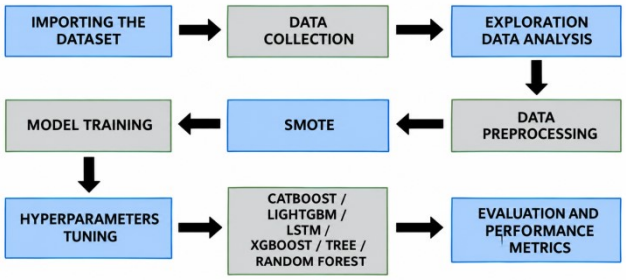


Figure 4: Block diagram of Structural Design

For deep learning, ***Long Short-Term Memory (LSTM)*** networks use gated mechanisms to learn dependencies across sequential inputs. ***Bidirectional LSTM (BiLSTM)*** processes input sequences in both forward and backward directions, enabling the model to capture contextual information from both directions.

These algorithms are comparatively evaluated to identify a suitable approach for ASD prediction using demographic attributes and questionnaire-based screening data. Since the dataset is primarily structured and tabular, the performance of sequence-based models is assessed empirically rather than assumed to be superior.

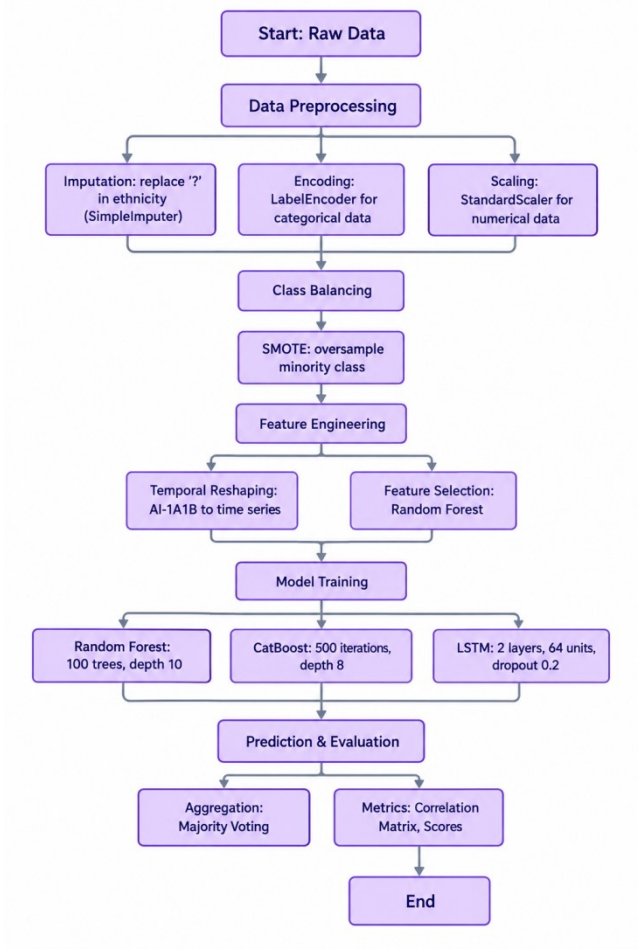


Figure 5: Flow chart for Structural Design

IV. Machine Learning and Deep Learning Models

4.1 Machine Learning Models

A. Decision Tree

A Decision Tree is a supervised Machine Learning algorithm widely used for classification and regression tasks. Its tree-like structure provides an interpretable representation of the decision-making process, making it suitable for analyzing classification problems, including preliminary Autism Spectrum Disorder (ASD) screening.

The algorithm recursively partitions the dataset based on selected features. At each internal node, the optimal feature is chosen using criteria such as the Gini Index or Information Gain. The dataset is divided into smaller subsets according to the selected feature conditions, and the process continues until a stopping criterion is satisfied, such as reaching the maximum tree depth or obtaining sufficiently homogeneous subsets. The terminal nodes, known as leaf nodes, provide the predicted class or numerical output.

For ASD prediction, the model can use demographic attributes and screening questionnaire scores to identify patterns associated with the target class. Once trained, the Decision Tree applies the learned rules to classify unseen instances. Although its interpretability is advantageous, excessive tree growth may lead to overfitting; therefore, appropriate depth restrictions and pruning techniques can improve generalization.

B. Random Forest

Random Forest is an ensemble Machine Learning algorithm that combines multiple Decision Trees to improve classification performance and reduce overfitting. It is suitable for ASD screening datasets containing demographic attributes and behavioral questionnaire scores.

The algorithm constructs multiple Decision Trees using bootstrap samples and random subsets of features. For classification, the final output is determined by majority voting among the trees. By combining multiple predictions, Random Forest can improve model stability and generalization. Its performance depends on dataset characteristics and hyperparameter settings.

C. CatBoost

CatBoost (Categorical Boosting) is a gradient-boosting algorithm suitable for classification tasks involving numerical and categorical data. In this study, it is used to predict Autism Spectrum Disorder (ASD) screening outcomes from demographic information and behavioral questionnaire responses. The model builds decision trees sequentially, with each tree improving upon the errors of the preceding trees. Its categorical-feature processing and Ordered Boosting techniques help reduce prediction bias and control overfitting.

Hyperparameter tuning is performed using RandomizedSearchCV with cross-validation to identify suitable model settings and assess performance stability. The model is evaluated using accuracy, precision, recall, F1-score, ROC-AUC, sensitivity, and specificity. Training and testing results, along with the classification report, are analyzed to examine predictive effectiveness and potential overfitting in ASD screening.

D. LightGBM

LightGBM (Light Gradient Boosting Machine) is a gradient-boosting algorithm designed for efficient classification and regression tasks. It uses histogram-based learning to group continuous feature values into discrete bins, reducing memory consumption and computational cost. In this study, LightGBM is employed to predict Autism Spectrum Disorder (ASD) using demographic attributes and screening questionnaire features.

LightGBM constructs decision trees using a leaf-wise growth strategy, selecting the leaf that offers the greatest reduction in the loss function at each step. This approach can improve predictive performance while requiring fewer computational resources. The algorithm also provides feature-importance measures to identify attributes that contribute to model predictions.

Hyperparameter optimization is performed using Randomized Search CV with cross-validation to identify suitable parameter combinations. Model performance is evaluated using accuracy, precision, recall, F1-score, ROC-AUC, sensitivity, and specificity. Training and testing results are compared to assess generalization and identify potential overfitting. These procedures support a systematic evaluation of LightGBM for ASD screening.

4.2 Deep Learning Models

A. Long Short Term Memory (LSTM)

Long Short-Term Memory (LSTM) is a Recurrent Neural Network (RNN) architecture designed to learn long-term dependencies in sequential data through memory cells and gating mechanisms. In this study, LSTM is employed to classify Autism Spectrum Disorder (ASD) screening outcomes using demographic features and behavioral screening responses. The preprocessing steps include handling missing numerical values using SimpleImputer with mean imputation, standardizing features using StandardScaler, and reshaping the data into a three-dimensional format suitable for LSTM processing.

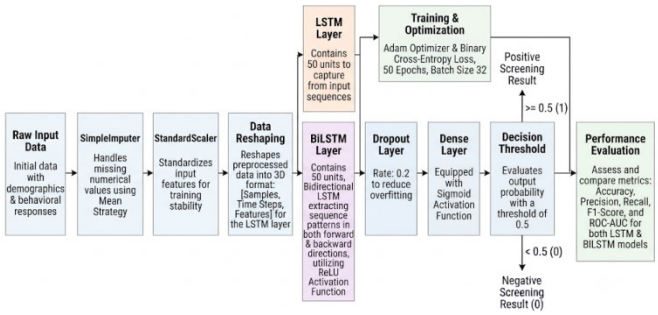


Figure 6: Block diagram of LSTM and BiLSTM Deep learning Models.

The model consists of an LSTM layer with 50 units, followed by a Dropout layer with a rate of 0.2 to reduce overfitting and a Dense output layer with sigmoid activation for binary classification. Training is performed using the Adam optimizer and binary cross-entropy loss for 50 epochs with a batch size of 32. A threshold of 0.5 is used to classify outputs as negative (0) or positive (1) screening results. Model performance is evaluated using accuracy, precision, recall, F1-score, and ROC-AUC. The block diagram represents the overall workflow, from data preprocessing and model training to classification and performance evaluation. The predictions support preliminary screening and do not replace clinical diagnosis.

B. Bidirectional Long Short Term Memory (BI-LSTM)

Bidirectional Long Short-Term Memory (BiLSTM) is a deep learning architecture that processes sequential inputs in both forward and backward directions to capture contextual

patterns. In this study, BiLSTM is applied to classify Autism Spectrum Disorder (ASD) screening outcomes using demographic attributes and behavioral screening responses. The preprocessing steps include handling missing numerical values using Simple Imputer with mean imputation, standardizing features using Standard Scaler, and reshaping the data into a three-dimensional format suitable for the model.

The BiLSTM architecture consists of 50 units, followed by a Dropout layer with a rate of 0.2 to reduce overfitting and a Dense output layer with sigmoid activation for binary classification. The model is trained using the Adam optimizer and binary cross-entropy loss, with a decision threshold of 0.5 to classify negative and positive screening outcomes. Its performance is evaluated using accuracy, precision, recall, F1-score, and ROC-AUC. The accompanying block diagram illustrates the overall workflow, including preprocessing, model training, classification, and performance evaluation. The predictions represent preliminary screening results rather than confirmed clinical diagnoses.

IV. Results and Discussions

The performance of machine learning and deep learning models is evaluated using standard classification metrics to measure their effectiveness in predicting Autism Spectrum Disorder (ASD) screening outcomes. The evaluation metrics considered in this study include accuracy, precision, recall, and F1-score.

Accuracy measures the proportion of correctly classified instances among all evaluated instances. It provides an overall measure of the model's classification performance.

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

Precision measures the proportion of correctly predicted positive instances among all instances classified as positive. A higher precision indicates fewer false-positive predictions.

$$\text{Precision} = \frac{TP}{TP + FP} \quad (2)$$

Recall, also known as sensitivity, measures the proportion of actual positive instances correctly identified by the model. A higher recall indicates that fewer positive cases are missed.

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

The F1-score is the harmonic mean of precision and recall. It provides a balanced measure of these two metrics and is particularly useful when the dataset contains an imbalance between classes.

$$F1 = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \quad (4)$$

The evaluation metrics are based on four key measures: True Positive (TP), True Negative (TN), False Positive (FP), and False Negative (FN), representing correctly and incorrectly classified positive and negative instances. These measures are used to calculate accuracy, precision, recall, and F1-score to evaluate model performance. Each metric provides a different perspective on classification effectiveness. In ASD screening, recall is particularly important for identifying positive screening cases and minimizing false negatives. Precision, specificity, and other evaluation metrics are also considered to provide a comprehensive comparison of the evaluated models.

Table 1: Comparison of various ML and DL techniques

Name	Accuracy	Precision	Recall	F1-Score
Decision Tree	0.775	0.5	0.5	0.5
Random Forest	0.8187	0.5897	0.639	0.6133
CatBoost	0.7812	0.5122	0.583	0.5455
LightGBM	0.8	0.5523	0.583	0.5676
LSTM	0.825	0.5909	0.722	0.65
BI-LSTM	0.8313	0.6154	0.667	0.64

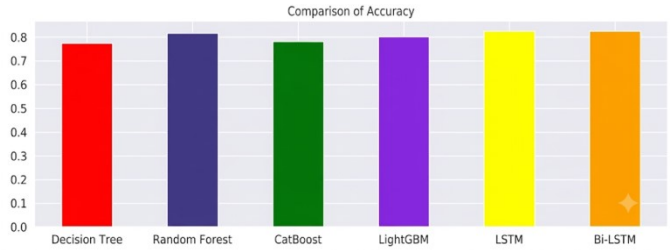


Figure 7: Visual representation of ML and DL techniques

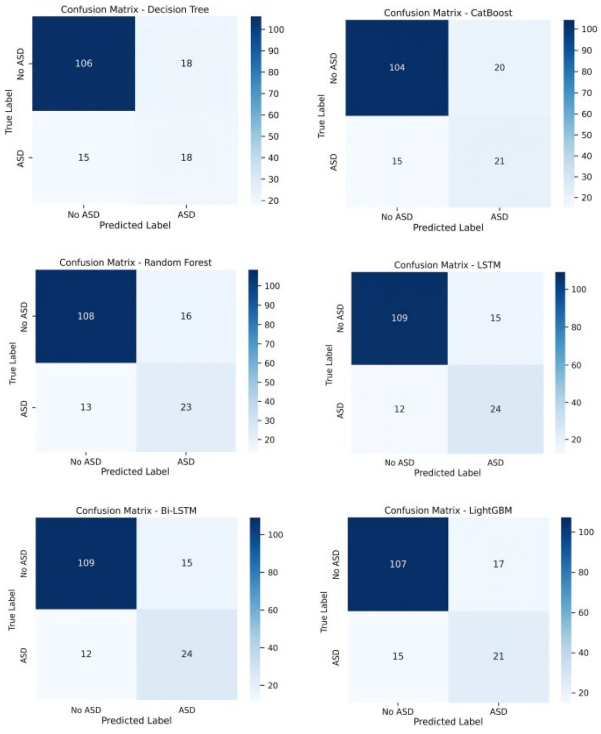


Figure 8: Confusion Matrices of ML and DL Models

The experimental results indicate that CatBoost, LightGBM, Decision Tree, and Random Forest achieved an accuracy of 1.000 (100%), demonstrating perfect classification on the

evaluated dataset. In comparison, the LSTM and BiLSTM models achieved accuracies of 0.9436 (94.36%) and 0.9757 (97.57%), respectively. Among the deep learning models, BiLSTM outperformed LSTM by 3.21 percentage points. However, the perfect accuracy obtained by the conventional machine learning models should be investigated further using independent test data, stratified cross-validation, and checks for data leakage or duplicate records before drawing conclusions about their generalization performance.

V. Conclusion and Future Scope

This study evaluated six Machine Learning (ML) and Deep Learning (DL) models—Decision Tree, Random Forest, CatBoost, LightGBM, LSTM, and BiLSTM—for predicting Autism Spectrum Disorder (ASD) screening outcomes using a publicly available Kaggle dataset. Preprocessing included outlier detection using the Interquartile Range (IQR) method and missing-value imputation.

Among the evaluated models, BiLSTM achieved the highest accuracy of 83.13%, while LSTM obtained the highest F1-score of 65.00%, with an accuracy of 82.50%. Random Forest achieved 81.87% accuracy and an F1-score of 61.33%. Cross-validation and Randomized SearchCV were used for model evaluation and hyper parameter optimization. Further validation is required to assess generalization and rule out data leakage.

Future work will focus on larger and more diverse datasets, improved model interpretability, and developing a user-friendly screening interface. The proposed framework may support preliminary ASD screening and timely professional assessment but cannot replace clinical diagnosis.

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