



An Interpretable PyCaret Approach for Alzheimer's Disease Prediction

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Abstract:

Alzheimer's Disease (AD) is a major global health concern. The research focuses on early and accurate diagnosis of AD for its effective treatment and management. This study presents a novel Machine Learning (ML) approach utilizing PyCaret and SHAP for early and interpretable AD prediction. PyCaret employs a span of classification algorithms and the study identifies the best model. SHAP value determines the contribution of individual features for the final prediction thereby enhancing the model's interpretability. The feature selection using SHAP improves the overall performance of the model. The proposed XAI framework improves clinical decision making and patient care by providing a reliable and transparent method for early AD detection.

1. Introduction

Alzheimer's Disease (AD) is a progressive neurological disorder which results in the decline of cognitive functions [1]. This condition frequently results in personality changes, impaired judgement and trouble in carrying out daily activities. Although there is no complete cure for the AD yet, early detection can help slow the progression of the disease. Brain MRI along with Machine Learning (ML) techniques can be used to analyze medical data and develop accurate models for AD prediction [2]. This has the potential to transform the diagnosis and treatment of AD thereby improving the lives of patients and their families. ML models are black-box in nature which fails to provide explanations for the predictions they make [3]. This makes the ML models untrustworthy for clinicians to accept and implement it. Explainable Artificial Intelligence (XAI) techniques have evolved to make these models understandable and transparent [4]. It is also validated that implementing feature selection techniques in ML models would improve the performance of the models [5-7].

Large sets of clinical as well as image data may be efficiently analyzed using ML algorithms. ML techniques have emerged as promising tools for

accurate as well as early detection and prediction of AD [8-15]. Although ML classifiers have demonstrated potential in the diagnosis of AD, clinical adoption is frequently hampered by their black-box nature. By offering insights into the model's decision-making process, XAI methodologies provide a solution that increases the model's credibility and interpretability [16-19]. While PyCaret has gained popularity as a low-code ML platform, its application in AD prediction is still in its infancy. Compared to the established frameworks like TensorFlow and PyTorch, there is a limited body of research specifically focused on AD prediction using PyCaret [20,21]. Table 1 summarizes the important researches carried out in the past 3 years using ML, XAI and PyCaret approaches for AD detection and classification. Traditional ML methods for AD prediction have high accuracy, but their lack of interpretability hinders clinical adoption. XAI techniques offer insights into model's reasoning, while it can be complex and time consuming. PyCaret streamlines the development process, allowing researchers to focus on interpretability. this approach improves AD prediction accuracy and patient outcomes. This paper proposes a novel XAI framework combining ML models and SHAP to predict AD in an intelligent way using only the relevant features.

Table 1. Summary of Researches using ML, PyCaret and XAI Techniques for AD Detection and Classification

| Research Study | Year | Problem Defined | Proposed Model | Accuracy (%) | Dataset Used | Explainability method |
|----------------|------|--|---|-----------------------------------|---|-------------------------|
| [8] | 2021 | AD prediction using ML and Principal Component Analysis | RELM | 77.62 (for binary classification) | ADNI | NIL |
| [9] | 2021 | Predicting progression of Mild Cognitive Impairment to AD using ML techniques | CNN | 78.5 | ADNI | NIL |
| | | | SVM | 75.4 | | |
| [10] | 2022 | Early-Stage AD Prediction Using ML Models | RF | 83 | OASIS | NIL |
| [11] | 2022 | Insights to AD using explainable ML approach | XGBoost | 84.2 | ADNI | SHAP |
| [12] | 2023 | ML Approach for Differential Diagnosis and Prognostic Prediction of AD | Ensemble Method | 91 | ADNI | SHAP |
| [13] | 2023 | Utilizing ML for the Early Diagnosis of AD | Voting Classifier | 96 | OASIS | NIL |
| [14] | 2023 | Early prediction of AD and related dementias using real-world electronic health records | Gradient Boosting Tree | 93.9 (AUC) | EHR data from OneFlorida + Clinical Research Consortium | SHAP |
| [15] | 2023 | Comparison of ML -based Approaches to Predict the Conversion to AD from MCI | Voting Classifier | 90 | ADNI | NIL |
| [16] | 2021 | Multilayer multimodal detection and prediction of AD using XAI | RF | 93.95 | ADNI | SHAP |
| [17] | 2022 | An explainable self-attention deep neural network for detecting mild cognitive impairment using multi-input digital drawing task | CNN+ multi-input+ self-attention mechanism + soft labelling | 81 | Live Patients from King Chulalongkorn Memorial Hospital | GradCAM |
| [18] | 2022 | Prediction of conversion to dementia using interpretable ML in patients with amnesic MCI | XGBoost | 80.7 | Live Patients at Samsung Medical Center | ICE+ SHAP |
| [19] | 2023 | AD stage prediction - CN, AD, EMCI, MCI, LMCI | EfficientNetB7 | 96 | - | Score-CAM or Grad-CAM++ |
| [20] | 2022 | Predicting conversion to AD in individuals with MCI using clinically transferable features | Ensemble | 74.9 | ADNI | NIL |
| [21] | 2022 | Classification and Interpretability of MCI Based on Resting-State Functional Magnetic Resonance and Ensemble Learning | XGBoost | 65.14 | From the Second Affiliated Hospital of Hangzhou Normal University | SHAP |

The framework is supposed to improve the classification performance by reducing the dimensionality of the dataset, demonstrating its feasibility in a Brain MRI dataset from the OASIS project. The paper contributes in the following manner: (i) this study uses PyCaret's user-friendly approach to streamline the machine learning workflow to predict AD, (ii) the model uses OASIS dataset to identify high-risk patients, (iii) SHAP values identify high-indicator features for the prediction thereby improving model's interpretability, (iv) SHAP explanations explore interactions and individual predictions, improving clinical understanding, (v) the feature selection technique reduces the number of attributes thereby increasing the computational efficiency and providing valuable insights beyond performance metrics.

The remainder of the paper is structured as follows: Section 2 frames the proposed methodology, Section 3 narrates the experiments, results and discussions, and Section 4 concludes the paper with a discussion of future improvements.

2. Methodology

2.1 Overview

The proposed system uses longitudinal brain MRI dataset from OASIS (Open Access Series of Imaging Studies) [22]. After pre-processing the dataset, PyCaret is applied to analyse the dataset using where various built-in ML classifiers are trained and evaluated to classify each instance as Demented or Non-Demented. The model performances are assessed using various metrics. Then SHAP algorithm is applied on the best model as a feature selection technique which could find out the individual features that have contributed most for the prediction. PyCaret is then applied on the new feature set which brought greater accuracy and improved performance in all the classifiers. Also, SHAP makes the results explainable both locally and globally. The proposed XAI framework architecture is shown in Figure 1.

2.2 Classification Using PyCaret

The proposed method aims to determine the reasons behind a person's elevated risk of developing AD. For that PyCaret, an open-source low-code ML toolkit in Python, is employed which expedites the workflow and automates the procedures [23]. The longitudinal brain MRI dataset from OASIS [22] is pre-processed by encoding categorical values and imputing missing values. PyCaret automates the pre-processing and preparation of data, making model training easier. A model for supervised binary classification is also included in the package.

Stratified cross-validation is used by the library to train and rank models for metric evaluation [23]. We can examine and contrast the model scores from the scoring grid for the performance evaluation of various classifiers.

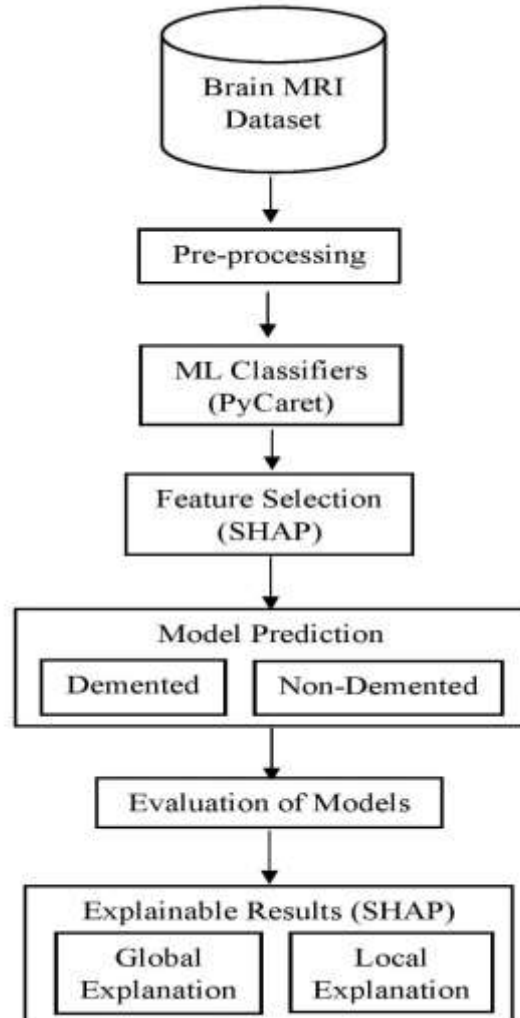


Figure 1. Architecture of the Proposed XAI Framework

2.3 Feature Selection

Data redundancy is a significant issue in high-dimensional datasets, and feature selection is a crucial step in ML pipelines. Feature selection involves choosing a subset of relevant features from the original dataset, improving model performance by reducing dimensions of the dataset [24]. There are three main techniques for feature selection: Filter, Wrapper, and Embedded. Filter techniques consider inherent properties of features, while wrapper methods train algorithms iteratively using specific features [25]. Embedded methods combine the advantages of filter and wrapper methods, such as L1 and L2 Regularization and Random Forest Importance [26]. But these methods fail to give adequate explanation for the selection or removal of particular features. In this study, SHAP serves as a

feature selection mechanism in addition to providing explanation to the results. SHAP helps to pick sufficient features to make the prediction and removes irrelevant features thereby reducing data dimensionality. When features cannot be simply removed in medical dataset, SHAP explain decisions during ML model construction and is grounded by strong mathematical formulae. The AD predictions made from the reduced dataset are more accurate with less computational cost and complexity.

2.4 Alzheimer's Disease Prediction

PyCaret trains and tests the new reduced feature dataset and the classifiers predict each new observation as either Demented or Non-Demented. It is also observed that all the PyCaret classifiers applied in the reduced feature set have improved their performance in terms of accuracy, precision, recall and F1-score when compared to the findings with all the features included in the dataset.

2.5 SHAP Explanations

Artificial Intelligence plays a crucial role in making decisions, but complex black box models often lack transparency, making them untrustworthy for clinicians to implement [27]. XAI aims to understand how a model works to make predictions, understand the relationship between input and output, and recognize the impact of each feature on prediction [28]. Interpretable ML algorithms can be of model-specific or model-agnostic in nature [29]. Model specific approaches such as LR and DT allow for easy interpretation of model parameters and internal structure. Model-agnostic approaches like LIME and SHAP, generate explanations in a human-understandable way, making them accessible to non-experts [30]. SHAP provides a strong foundation for analyzing ML models, allowing for understanding the role of every feature in a model's final prediction and identifying potential biases.

SHAP, based on game theory, helps explain individual predictions by computing the contribution of individual features to the prediction [31]. It computes Shapley values from coalitional game theory, calculating the marginal contribution of each feature in dataset. The marginal contribution is then averaged and used to determine the actual contributions of each feature [32]. The following equation can be used to determine the Shapley values of each feature.

$$\phi_i(f, x) = \sum_{Z' \subseteq x'} \frac{|Z'|!(F-|Z'|-1)!}{F!} [f_x(Z') - f_x(Z' \setminus i)](1)$$

Now, we shall understand what each variable in the eqn. (1) [8] represents.

$\phi_i(f, x)$ - shapley value for feature i of the given instance x in the black box model f

Z' - a subset of attributes

x' - the simplified input data

F- total number of features in the dataset

$f_x(Z')$ - Output of black box model- Prediction

$f_x(Z' \setminus i)$ - Output of black box model excluding feature i.

$[f_x(Z') - f_x(Z' \setminus i)]$ - contribution of feature i for the prediction

$\frac{|Z'|!(F-|Z'|-1)!}{F!}$ - weight. Contribution of each feature is multiplied by this weight.

If the weight increases by adding a new feature in the subset, then that attribute is considered to have significant contributions to the prediction. SHAP gives the model both global and local interpretability. Global interpretation involves averaging feature importance scores across instances, providing a positive or negative contribution to the output. SHAP Dependence Plot, Feature Importance Plot, Summary Plot, etc. gives global explanations [30]. Local explanation, achieved through individual SHAP values, explains the decision or individual prediction. Individual SHAP value plot, Force plot, Local bar Plot, Waterfall Plot, etc. provides local explanation to the model [30]. SHAP calculates the importance of features in the OASIS MRI dataset for predicting AD risk by calculating absolute Shapley values. It extracts relevant features from PyCaret classifiers and provides both global and local explanations. The global value is consistent with local values from each instance, and SHAP can explain individual predictions, providing local interpretation for each instance.

3. Experiments, Results and Discussions

3.1 Performance Evaluation

The XAI framework classifies AD into Demented or Non-Demented categories using PyCaret. SHAP is employed as a feature selection technique, which highlights feature relevance and eliminates irrelevant ones. SHAP also explains the reason behind the model predictions. The experiment is performed on brain MRI longitudinal dataset from OASIS project [22] and it is seen that the performance of the models has been enhanced after feature selection.

PyCaret module provides different ML Classifiers and plots for analyzing model performance in AD prediction. The models are trained using stratified cross-validation and ranked using metrics like average Accuracy, AUC, Recall, F1 Score, Kappa,

MCC and Training Time. In this experiment, Naïve Bayes (NB) achieves the best results. When all other parameters were considered, NB ranked highest, even though Ridge Classifier, Random Forest Classifier, Linear Discriminant analysis and ExtraTrees Classifier generated results with the same accuracy that of NB. Accuracy measures the proportion of correct predictions, while AUC is independent of class distribution. MCC considers True Positives, True Negatives, False Positives and False Negatives for comprehensive evaluation. A combination of metrics from the PyCaret library shown in Table 2 provides a more comprehensive view of each model's performance.

The PyCaret model successfully predicts AD, but understanding the rationale behind the predictions is crucial. SHAP provides a framework for interpreting the impact of individual features on the model's predictions. From table 2 it is evident that the performance scores of classifiers in training and classification of AD after applying SHAP feature selection technique is improved compared to the scores before applying feature selection. NB exhibited consistent performance in both phases,

achieving 91% accuracy in AD classification. By selecting the more relevant features, all the classifiers improved their performance in terms of all metrics such as AUC, recall, precision, F1-Score, Kappa, MCC and TT, with NB improving its accuracy score to 96%.

The PyCaret model's ability to forecast AD has been greatly enhanced by the use of SHAP for feature selection. SHAP values make the model more visible and intelligible by revealing how each feature contributes to the model's prediction. SHAP can be recommended as a good feature selection approach because all of the classifiers performed better in the SHAP reduced feature dataset than in the original dataset. When working with high-dimensional datasets, feature selection can help minimize overfitting and reduce dimensionality. A model with fewer features may be more efficient due to quicker training and inference periods.

3.2 Explanations from SHAP

SHAP provides model agnostic explanations for classification models, revealing important patterns

Table 2. Analysis of Classifiers Before and After Feature Selection using SHAP

| Classifier | Performance Evaluation of PyCaret Classifiers Before Feature Selection | | | | | | | | Performance Evaluation of PyCaret Classifiers After Feature Selection using SHAP | | | | | | | |
|--|--|---------|------------|-------------------|-----------------|---------------|-------------|-----------------|--|---------|------------|---------------|-----------------|---------------|-------------|-----------------|
| | Acc ura cy | AU C | Rec all | Pre cisi on | F1 Sco re | Ka pp a | M C C | TT (Se c) | Acc ura cy | AU C | Re call | Preci sion | F1 Sco re | Ka pp a | M C C | TT (Se c) |
| Naive Bayes (nb) | 91 | 94 | 82 | 100 | 89 | 82 | 84 | 0.01 40 | 96 | 99 | 95 | 100 | 97 | 90 | 90 | 0.0 040 |
| Ridge Classifier (ridge) | 91 | 92 | 82 | 100 | 89 | 82 | 84 | 0.02 20 | 95 | 94 | 94 | 100 | 97 | 88 | 88 | 0.0 050 |
| Random Forest Classifier (rf) | 91 | 94 | 84 | 98 | 89 | 82 | 83 | 0.10 80 | 94 | 99 | 93 | 100 | 96 | 91 | 92 | 0.0 870 |
| Linear Discriminant Analysis (lda) | 91 | 92 | 82 | 100 | 89 | 82 | 84 | 0.02 70 | 93 | 97 | 90 | 100 | 95 | 86 | 85 | 0.0 120 |
| Extra Trees Classifier (et) | 91 | 94 | 84 | 98 | 89 | 82 | 83 | 0.10 00 | 92 | 99 | 90 | 100 | 95 | 90 | 90 | 0.0 980 |
| Gradient Boosting Classifier (gbc) | 90 | 92 | 88 | 93 | 90 | 80 | 82 | 0.09 0 | 92 | 98 | 88 | 97 | 92 | 84 | 85 | 0.0 210 |
| Logistic Regression (lr) | 89 | 87 | 82 | 96 | 87 | 78 | 79 | 1.41 20 | 91 | 97 | 88 | 96 | 92 | 82 | 83 | 1.0 00 |
| Light Gradient Boosting Machine (lightgbm) | 88 | 91 | 84 | 93 | 87 | 76 | 77 | 0.18 10 | 90 | 91 | 84 | 95 | 89 | 81 | 81 | 0.0 820 |

| Classifier | Performance Evaluation of PyCaret Classifiers Before Feature Selection | | | | | | | | Performance Evaluation of PyCaret Classifiers After Feature Selection using SHAP | | | | | | | |
|---------------------------------------|--|-----|--------|-----------|----------|-------|-----|----------|--|-----|--------|-----------|----------|-------|-----|----------|
| | Accuracy | AUC | Recall | Precision | F1 Score | Kappa | MCC | TT (Sec) | Accuracy | AUC | Recall | Precision | F1 Score | Kappa | MCC | TT (Sec) |
| Extreme Gradient Boosting (xgboost) | 87 | 91 | 84 | 91 | 86 | 74 | 75 | 0.0550 | 88 | 95 | 85 | 92 | 88 | 79 | 79 | 0.0050 |
| Ada Boost Classifier (ada) | 86 | 92 | 84 | 89 | 85 | 72 | 73 | 0.0650 | 89 | 89 | 83 | 94 | 88 | 76 | 75 | 0.0150 |
| Decision Tree Classifier (dt) | 84 | 84 | 86 | 83 | 84 | 67 | 69 | 0.0140 | 85 | 97 | 81 | 87 | 84 | 80 | 81 | 0.0040 |
| Quadratic Discriminant Analysis (qda) | 76 | 78 | 88 | 77 | 79 | 52 | 55 | 0.0220 | 81 | 88 | 85 | 86 | 86 | 61 | 63 | 0.0010 |
| K Neighbors Classifier (knn) | 63 | 70 | 65 | 67 | 64 | 27 | 27 | 0.0250 | 72 | 71 | 77 | 82 | 80 | 43 | 45 | 0.0050 |
| SVM - Linear Kernel (svm) | 51 | 50 | 10 | 05 | 07 | 00 | 00 | 0.0170 | 52 | 52 | 58 | 71 | 64 | 04 | 04 | 0.0070 |
| Dummy Classifier (dummy) | 51 | 50 | 00 | 00 | 00 | 00 | 00 | 0.0180 | 51 | 50 | 10 | 51 | 17 | 00 | 00 | 0.0080 |

in behavior. SHAP values are used to explain classification results and gives benefits of interpreting AD predictions globally and locally by evaluating the contribution of each variable. Graphs are plotted for NB classifier since it performed consistently well before and after feature selection.

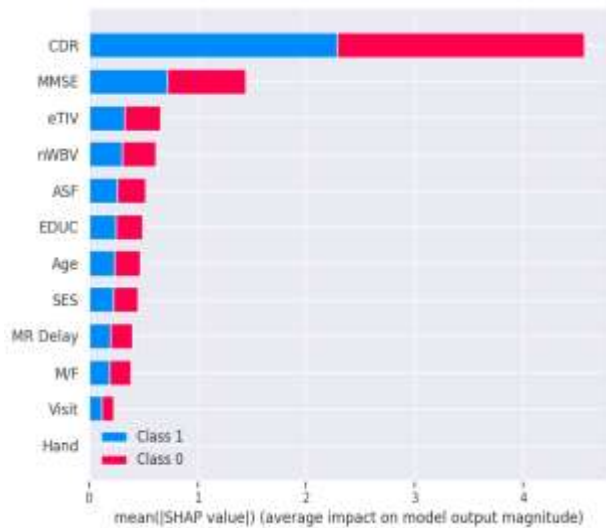


Figure 2. Feature Importance plot for AD prediction

Global Explanation

The SHAP Feature Importance plot represented in the Figure 2 shows the impact of each feature on the model output, ranking them in descending order of importance. Top features have higher Shapley

values, contributing more to the prediction and having higher predictive power. In the plot the feature CDR shows the most impact for the prediction, while Hand and Visit shows least importance. The classification results by NB is explained by SHAP values and it provides both global and local interpretation. Features with higher leads to a higher or lower prediction is determined by the position of the feature in horizontal location. absolute SHAP values have a stronger influence on the model’s overall predictions. Whether the value

The SHAP summary plot in Figure 3 shows the positive and negative relationships of input features with the target variable, displaying the average impact of each feature on the model's prediction. The plot rank features in descending order of importance, with Red indicating a positive influence and blue indicating a negative influence. The SHAP value discovers patterns in data and explains model decisions, benefiting from explainability and mathematical formulae. It also improves performance accuracy by classifying classifying the brain MRI dataset after feature selection by SHAP. Identifying important features from SHAP values reduces computational time and comes up with faster results. We can infer from the plot in figure 3 that a high CDR value has a positive and significant impact on AD prediction.

Local Explanation

Individual SHAP value plots are used to provide detailed explanations for individual observations in a model, making predictions for a single patient in a

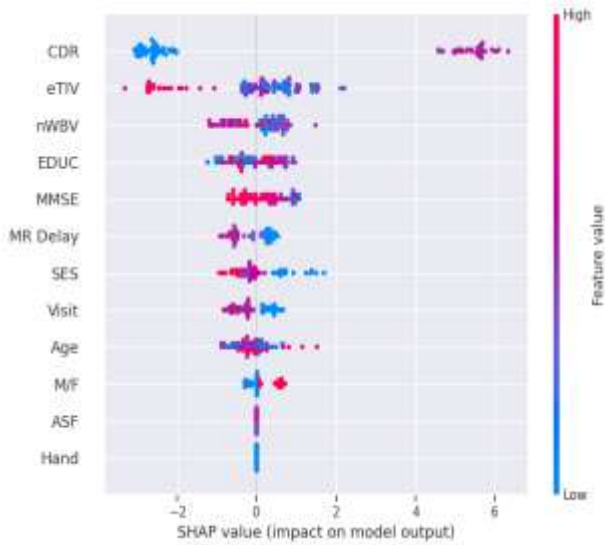


Figure 3. SHAP Summary Plot for AD Prediction

more sensible and adoptable manner. These plots explore the relationship between a specific feature and the model’s prediction for a single patient, revealing ho changes in that feature value affect the

predicted probability of AD. They are particularly useful for analyzing specific predictions and providing a deeper dive into their reasoning. Features with a positive correlation with the label contribute to the prediction. SHAP value plots visualize feature contributions to a model’s prediction using arrows, indicating their strength and direction. Figure 4 and Figure 5 shows two observations from the AD training dataset, one from the Demented category and the other from Non-Demented category represented using individual SHAP value plots.

Figure 4 shows the SHAP value plot for Obseravtion 1 in the training dataset shows that the predicted value 0 indicates Non-Demented, while the base value represents the mean model output. The attributes that drive the prediction higher are shown in Red and those drive the prediction lower are shown in Blue. The features CDR, MMSE, nBW and EDUC contribute to classifying the observation as Non-Demented. These features along with Age, ASF, SES and eTIV are positively related to the prediction, while the rest are negatively related. The absolutevSHAP values of these featuresare compared against their mean values showing that CDR, MMSE, nBW, Age and EDUC are all less than their mean values, indicating Non-Demented predictions.

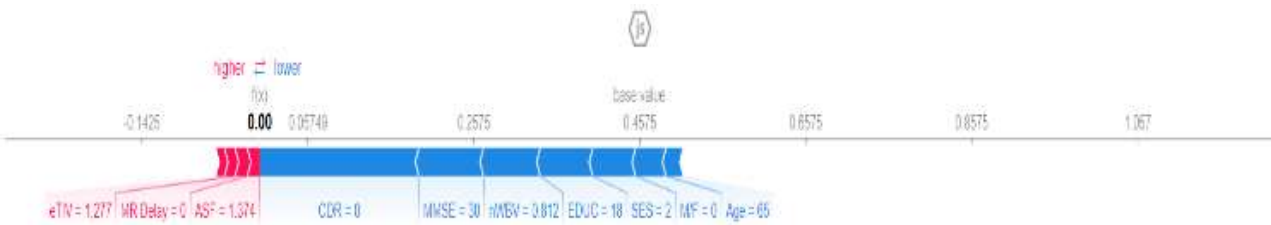


Figure 4. SHAP Value Plot for AD Prediction- Non-Demented Class

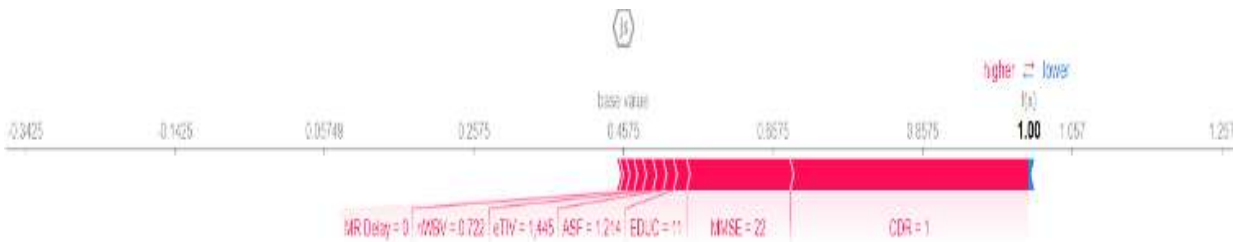


Figure 5. SHAP Value Plot for AD Prediction- Demented Class

Figure 5 shows the individual SHAP value plot for another observation - Observation 2. It classifies the patient as Demented where variable CDR has a positive impact pushing the prediction to the right. Conversely, the variable MMSE, EDUC and nWBV have low values, indicating a negative correlation with dementia. These low values push the prediction to the right.

SHAP transforms black-box models into glass-box models, improving prognosis of AD by incorporating feature selection methods. SHAP helps explain why a model predicts AD for a specific patient by revealing which features contributed most significantly. It is beneficial for displaying feature effects, exploring cumulative effects, identifying outliers and identifying typical prediction paths. This approach can be used to predict diseases and explain results, and can be extended to other domains where model transparency is vital, such as loan approval and spam detection. This paper presents a novel XAI framework for AD prediction and the key contributions include:

- Demonstrates high classification accuracy of 96% by Naive Bayes classifier in the OASIS dataset for AD prediction.
- Leveraging PyCaret enables rapid experimentation and provides a variety of performance metrics for evaluation.
- Utilizing SHAP enhances the model interpretability which leverages in understanding model's decision-making process.
- Employing SHAP to identify most influential features for AD prediction, leading to improved performance of the model and reduced complexity.
- Provides a transparent and explainable framework for early AD diagnosis, enabling clinicians to implement it confidently.
- With a broader focus on overall disease prediction, the proposed framework prioritizes different features compared to the State-of-the-Art (SOTA) methods discussed in the Literature Review and fills this gap by proposing a novel and insightful methodology.

4. Conclusions

Early detection of AD can improve patient's quality of life. ML models are increasingly used in AD prediction, but their interpretability is a challenge. Advancements in XAI techniques help overcome this issue. The proposed XAI framework uses PyCaret to analyze different ML models for AD prediction and SHAP, a popular interpretability technique for model explanation. The models are evaluated using Brain MRI OASIS dataset with metrics such as Accuracy, Precision, Recall, AUC, F1-Score etc. SHAP is also

used as a feature selection method, prioritizing features based on their contribution to model output. These findings imply that the suggested XIA framework may provide a dependable and explainable method for AD prediction by fusing the efficient exploration of PyCaret and interpretability of SHAP. It is a step towards a time when AI will enable medical professionals to combat AD.

Future work should focus on improving AD prediction performance by utilizing PyCaret library for conducting experiments in image datasets with multiclass classification, exploring more XAI techniques and incorporating casual knowledge. Advanced feature selection techniques, domain knowledge and evaluating feature selection's impact on different models can be explored. Additionally, developing interpretable DL models using attention mechanisms and layer-wise relevance propagation can enhance the accuracy, interpretability and clinical utility of ML which was used for different application in the literature [33-48].

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