Makerere University

INTERPRETABLE MULTI-STRATEGY LEARNING FOR PREDICTIVE THERAPEUTIC ADHERENCE TO OSTEOPOROSIS TREATMENT AMONG CHRONIC PATIENTS

by

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Declaration

I ...Busingye Caroline............ hereby declare that this thesis is my own work and effort and that it has not been submitted anywhere for any award. Where other sources of information have been used, they have been acknowledged.

Signed: Busingye.

Date: 19. 12. 2025

Approval

This Dissertation titled **Interpretable Multi-strategy for predictive therapeutic Adherence to Osteoporosis treatment among Chronical patients**, has been approved by the following supervisors.

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Dedication

I dedicate this thesis to my supervisors, Dr. Daudi Jjingo and Mr. Ggaliwango Marvin, for their constant guidance and support. To Makerere University, thank you for providing a solid foundation, resources, and platform for this research. I am deeply grateful to my colleagues for their encouragement and to my dear husband and children for their love, patience, and prayers that carried me through. Above all, I thank God for the strength and wisdom to complete this journey.

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I would like to express my deepest appreciation to my supervisors, Dr. Jjingo Daudi and Ggaliwango Marvin, whose expertise, understanding, and patience, added considerably to my graduate experience. I also thank them for their encouragement and insightful critiques of my research work.

I would like to express my heartfelt gratitude to my family for their unwavering support and encouragement throughout my academic journey. Their love and motivation have been instrumental in helping me navigate the challenges of researching and writing this thesis. Special thanks to my husband, Twijukye Benon, for his patience, understanding, and unwavering support. This achievement would not have been possible without them, and I am forever grateful. Thank you Lastly, my thanks also go out to my colleagues and university staff who have been part of my journey. Their continual support will be forever valuable.

Abstract

This study presents an interpretable multi-strategy learning framework to predict therapeutic adherence to osteoporosis treatment among chronic patients, advancing the use of Artificial Intelligence (AI) in adherence prediction. Traditional, ensemble, deep learning, and hybrid models were developed and evaluated using Explainable AI (XAI) techniques LIME, SHAP, and Permutation Feature Importance to identify key adherence factors.

The Extreme Gradient Boosting (XGBoost) model achieved the best overall validation performance with 68.3% accuracy, 66.3% F1 score, and 73.4% AUC-ROC and was deployed as a web-based prediction tool on Render for real-time adherence prediction.

XAI results showed that lifestyle factors like smoking, low physical activity, and inadequate calcium intake negatively affected adherence, while regular exercise and sufficient vitamin D intake improved it. These findings highlight an interpretable, data-driven pathway for clinicians and researchers to support personalized interventions and enhance adherence outcomes in osteoporosis management. Deep Learning, Explainable Artificial Intelligence (XAI), Feature Importance, LIME, Machine Learning Interpretability, Osteoporosis, Postmenopausal, SHAP, Therapeutic Adherence, XGBoost

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List of Acronyms

AI	Artificial Intelligence
AUC	Area Under the Curve
BMD	Bone Mineral Density
GRU	Gated Recurrent Unit
IDSS	An Intelligent Decision Support system
LIME	Local Interpretable Model-agnostic Explanations
ML	Machine Learning
ROC	Receiver Operating Characteristic Curve
SHAP	SHapley Additive Explanations
SOLSSA	Self-Organizing Linear Search Simulated Annealing
SVM	Support Vector Machines
XAI	Explainable Artificial Intelligence

Chapter 1

Introduction

1.1 Background of the Study

Osteoporosis is a chronic skeletal disorder characterized by a reduction in bone mineral density and deterioration of bone tissue microarchitecture, leading to bone fragility and an increased risk of fractures [1]. In simpler terms, it causes the bones to become weak and brittle, making even minor falls or movements potentially harmful. According to the IOF, approximately 200 million people are affected globally, and 1 in 3 women over the age of 50 will experience an osteoporosis-related fracture [2, 3]. Men are also at risk, though at a lower rate, with 1 in 5 men over 50 expected to suffer from an osteoporosis-related fracture [4]. Osteoporosis is a great disability burden with an expected cost increase of almost 50% by 2025. Due to its long-term treatment, approximately 50- 70% of patients withdraw from their osteoporosis medications within the first year of initiation. This requires an urgent need for improved osteoporosis and pharmacologic management tools, especially for pregnant women, postmenopausal women and the elderly to ensure therapeutic adherence of patients during treatment [5].It is a skeletal disorder characterized by loss of bone mass(BM), microarchitectural deterioration of bone tissue, decline in bone quality, leading to increased bone fragility and the risk of fractures [6].Therapeutic adherence is the extent to which patients follow prescribed treatments [6, 7]. Osteoporosis treatment focuses on strengthening bones, reducing fracture risk, and managing pain. This involves a combination of lifestyle changes, medications, and supplements such as calcium and vitamin D supplements [5]. There is an increasing treatment gap for patients at high fracture risk [2] Therapeutic adherence is a notable challenge in the treatment of osteoporosis, long-term patient compliance is crucial to prevent fractures and worsen disease spread. Recently, advances in deep learning have provided powerful predictive models for therapeutic adherence. However, the complexity and lack of transparency of these models make them difficult to interpret by healthcare providers, potentially limiting their application. Therefore, interpretable multi-strategy learning models are being explored to predict adherence while offering clear insights for physicians. Multi-strategy learning is the use of multiple learning algorithms, techniques, or strategies to improve the performance of a machine learning model.To achieve better predictive accuracy compared to using a single strategy. Interpretable AI in Healthcare is the development of machine learning models whose decision-making processes can be easily understood and well explained by human experts and beneficiaries and helps stakeholders to trust AI systems [6].

1.2 Problem Statement and research gap

Numerous machine learning and deep learning models have been developed to predict osteoporosis-related outcomes such as fracture risk — for example, using Logistic Regression, Random Forest, SVM, and Deep Neural Networks [8]. However, relatively few models focus on predicting therapeutic adherence rather than fracture risk. Moreover, many existing predictive models lack interpretability, making their predictions difficult for clinicians to trust and act upon. Deep learning models, though powerful, often operate as black-boxes"and do not readily explain why a patient may or may not adhere to treatment [9]. Additionally, much prior research has relied on single-strategy approaches, which limit flexibility and generalizability. Few studies have explored multi-strategy learning frameworks, combining multiple algorithms to improve performance while also providing deeper, more clinically meaningful insights. This gap in explainability and adaptability poses a major barrier to the practical adoption of AI in clinical osteoporosis management [10].

1.2.1 Research Motivation

This study seeks to bridge these gaps by developing an interpretable multi-strategy learning framework that predicts therapeutic adherence while offering transparent explanations of influencing factors. By integrating Explainable AI (XAI) techniques such as LIME, SHAP, and Permutation Feature Importance, the study provides actionable insights for clinicians and supports personalized, data-driven intervention strategies. Ultimately, the research aims to enhance both the predictive accuracy and interpretability of adherence models, improving trust and usability in real-world healthcare settings.

1.2.2 Proposed Solution

This research proposes an Interpretable Multi-Strategy Approach for predicting therapeutic adherence to osteoporosis treatment among chronic patients with the primary goal of developing a robust, explainable, and deployable machine learning model that identifies key factors influencing patient adherence while enhancing interpretability using Explainable AI techniques. The implementation of ensemble of deep learning models, including Long Short-Term Memory (LSTM), Gated Recurrent Units (GRU), to analyze structured patient data as well as hybrid models. These models uses patient demographics, lifestyle habits, medical history, treatment adherence records. The core model selection bases on performance metrics such as accuracy, precision, recall, F1-score, and AUC-ROC.

1.2.3 Explainability and Interpretability

To ensure transparency in decision making, LIME (Local Interpretable Model-agnostic Explanations) and SHAP (SHapley Additive Explanations) are integrated to explain the predictions of the model. These methods help patients, clinicians and researchers understand which factors most significantly contribute to adherence predictions.

1.3 Research Objectives

1.3.1 Main Objective

To develop and evaluate an interpretable multi-strategy learning framework that combines the strengths of linear and non-linear models to improve the prediction of therapeutic adherence to osteoporosis treatment, thus supporting personalized treatment planning and patient outcomes.

1.3.1.1 The specific objectives

(i) To build and evaluate multiple predictive models like traditional, ensemble, deep learning, and hybrid for classifying patient adherence to osteoporosis treatment.

(ii) To derive and implement model explainers including LIME, SHAP, and Permutation Feature Importance to interpret the contribution of clinical and lifestyle factors influencing adherence and enhancing model transparency and clinician trust.

(iii) To design, deploy, and integrate a web-based monitoring tool that provides real-time adherence predictions and interpretable insights for clinical decision support.

1.3.2 Anticipated outcomes

(i) This study is important in the advancement of artificial intelligence through the implementation of robust machine learning models optimized for imbalanced datasets and to ensure accurate predictions and early interventions for non-adherence.

(i) The study Improves interpretability, fostering trust and usability among healthcare professionals.

(i) Designing a monitoring tool for seamless integration into clinical settings will enable personalized treatment planning, thus improving patient outcomes.

Chapter 2

Related work

2.1 Introduction

This section discusses various articles including key factors that influence the adherence of osteoporosis treatment, the role of machine learning and Artificial intelligence and the use of interpretable AI in identifying nonadherence risks and improving patient outcomes.

2.2 Factors Influencing Osteoporosis Treatment Adherence

Factors influencing osteoporosis medication adherence, such as patient demographics, beliefs, accessibility to healthcare care, and regimen complexity. Gears the need for tailored interventions to improve adherence rates, enhancement of treatment adherence strategies in management of osteoporosis. [11].Key issues like lack of knowledge, dissatisfaction with doctor visits, side effects, and forgetfulness, while providers highlighted knowledge gaps, structural barriers, side effects, and difficulties tracking adherence and the development of a randomized trial to test and evaluate targeted interventions is proposed [12].Positive and negative determinants of adherence to osteoporosis treatment in clinical practice Simplifying treatment and improving patient education are emphasized to enhance adherence to osteoporosis therapy [13,14]. Some factors such as fear of side effects, lack of understanding of osteoporosis, and low perceived need for medication are the major barriers to adherence, physician recommendations, education, and the belief in the benefits of treatment, improved patient education and communication to address these barriers are positive influencers [15]. In [16] the understanding these socio demographic influencers can guide personalized support strategies and improve disease management and quality of life, approximately 20–30% of patients taking daily or weekly treatments may suspend their treatment within 6 to 12 months of initiating therapy. In [3] Patients with poor adherence increase their risk of osteoporotic fractures and hospitalization.

2.3 Adherence in Healthcare and Predictive Modeling for osteoporosis

Machine learning Algorithms have been deployed in prediction of various aspects of Medical Adherence and osteoporosis risk prediction [17]. Machine learning and natural language processing were implemented to predict adherence to medications in patients with fibromyalgia based on social forum data [18].Various Machine Learning techniques to identify patterns and risks of osteoporosis seen in [19]. Therapeutic adherence to osteoporosis treatment, addressing the critical challenge of non-adherence among chronic patients is done in [20]. Osteoporotic hip fractures prediction in postmenopausal women done with models like support vector machines (SVM), random forests, and logistic regression trained using finite element derived biomechanical parameters and patient data, Assessments based on each patient's unique bone structure and biomechanical profile enabled descision making [21]. An intelligent decision support system (IDSS) for predicting osteoporosis risk with a hybrid of neural networks and decision trees enabled more accurate early diagnosis and personalized intervention strategies for patients [22]. There is a growing potential of machine learning for large-scale, data-driven osteoporosis prediction, enabling more targeted and preventative healthcare strategies [**?**]. AI-driven models show promise in identifying high-risk individuals more effectively than traditional methods [23].

2.4 Machine Learning Interpretability and Explainable Artificial Intelligence

Explainable artificial intelligence and machine learning interpretability are acquiring significant attention among practitioners and researchers [24]. Most of machine learning and AI methods are nontransparent with respect to their working mechanism, referred as black box models prohibiting straight forward explanation constituting severe problems for a number of fields including the health sciences [25]. Arguments have been brought forward in favor of XAI by policies like DPR (European Parliament and Council of the European Union 2016) [26]. Interpretable machine learning (IML) methods can be used to discover knowledge, to debug or justify the model and its predictions, and to control and improve the model and vital for trust, accountability, regulatory compliance, and effective deployment in sensitive domains [27,28]. Key tools that include feature attribution using approaches like LIME and SHAP , visualization using saliency maps, rule-based methods, and surrogate models and then highlights the need to balance accuracy with interpretability [29].Tools like SHAP and ELI5 were used in predicting diabetes to interpret model predictions, identifying key factors influencing diabetic and non-diabetic classifications emphasising both global and local interpretability [29]

2.5 Multi-Strategy Learning Approaches

Multi-strategy learning refers to use of various learning methods to improve predictive power [30]. A hybrid machine learning approach that identified secondary testosterone deficiency, ten base classifiers, optimized with stratified K-fold cross-validation, and integrated them into ensemble frameworks, including weighted averaging and stacking with a logistic regression meta-classifier, Using advanced sampling techniques like SMOTE(Synthetic Minority Over-sampling Technique) and repeated Edited Nearest Neighbors were employed to address data imbalance. The effectiveness of hybrid and ensemble strategies like improved prediction accuracy, creating robust, cost-effective diagnostic tools was seen for testosterone deficiency [31]. Machine learning based decision support system for predicting bone mineral density (BMD) response in osteoporosis patients after treatment, multiple machine learning models were trained, selecting Random Forest as the best-performing model [32]. The impact of feature selection on prediction accuracy is analysed, applying algorithms such as Support Vector Machines (SVM), Decision Trees, Naive Bayes, and the AdaBoost ensemble method used in early diabetes prediction with advanced sampling methods handling imbalanced data thus achieving significant improvements in precision [33]. Ensemble machine learning framework integrating multiple algorithms, such as decision trees and support vector machines, using bagging, boosting, and stacking techniques to analyze diverse medical datasets addressing challenges of data variability and limited accuracy in standalone models through improving prediction robustness and generalization. [34]. Various supervised machine learning algorithms, models, such as decision trees, support vector machines, and random forests classified individuals as diabetic or non-diabetic based on relevant features and achieved the better accuracy used performance metrics such as accuracy, precision, and recall being used for evaluation [28]. Cardiovascular disease risk assessment using the self-organizing linear search simulated annealing (SOLSSA)-CatBoost model by integrating the self-SOLSSA algorithm for feature selection and the CatBoost gradient boosting algorithm was used, offered an optimal and reliable tool for early identification of Cardio Vascular Disease risk and supporting preventive healthcare strategies [34]. Multi-strategy learning approaches improve performance but face challenges such as increased model complexity, high computational demands, data dependency, and the risk of over-fitting, mitigated through careful parameter tuning [35].

2.6 Current State of art

Machine learning approaches have widely been utilized in osteoporosis-related outcomes such as fracture risk and therapeutic adherence: Predictive models such as Logistic Regression, SVM, Random Forest, and Gradient Boosting have shown effectiveness in classification tasks within bone health research [36].

Deep learning has shown improved performance but remains clinically opaque and difficult to interpret([37]. Explainability in AI-driven clinical decision support systems is now a critical requirement [38].

2.7 Conclusion

Much as significant advances have been made in using machine learning to predict therapeutic adherence, many existing models lack the transparency and adaptability required for clinical integration. Current approaches often rely on single-model strategies that are unable to address the complex and individualized nature of patient adherence behavior [39]. This research bridged this gap by introducing an interpretable multistrategy learning framework to predict adherence to osteoporosis treatment. The combination of diverse machine learning models and integration of explainable AI techniques offered both accurate and transparent predictions hence enhancing clinical decision making and provide personalized insights for improved treatment outcomes.

Chapter 3

Methodology

3.1 Introduction of the methodology

This study adopted a multi-strategy learning approach by combining traditional, ensemble, deep learning, and hybrid models rather than relying on a single algorithmic strategy the rational is as explained below.

3.1.1 Limitations of Single-Model Approaches

Much as machine learning has shown promise in osteoporosis-related prediction tasks, many studies adopt single-model learning strategies, which exhibit several limitations that hinder clinical usefulness:

- Inability to Capture Complex and Heterogeneous Adherence Behavior. Therapeutic adherence is influenced by interactions among diverse demographic, clinical, and behavioral factors. Single-model methods struggle to model such non-linear and individualized relationships.Forexample a Random Forest-only model for adherence prediction performed well but failed to capture heterogeneous behavior across subgroups [40].

- Restricted Generalizability Across Patient Populations Single models often overfit to limited clinical cohorts, reducing performance when applied in broader healthcare settings.A Logistic Regression-only fracture prediction model showed significant performance drop on external validation cohorts [41].

- Black-box models such as deep neural networks achieve high accuracy but lack the interpretability required for clinical trust. XAI literature shows that relying solely on opaque models limits their applicability in healthcare, as demonstrated in fracture prediction studies where DNN-only systems lacked the explanations clinicians need. This supports the adoption of multi strategy approaches that integrate accuracy with transparent, clinically meaningful explanations [42].

- Bias Toward One Type of Relationship (Linear / Non-linear Only) Single-model approaches are limited because they capture only one type of relationship either linear or non-linear—but not both. Linear PRS models miss interaction effects between genetic variants, while non-linear models alone may overlook strong additive relationships. Evidence showed that incorporating non-linear learners like XGBoost alongside PRS significantly improved predictive performance across multiple traits.

Similar limitations are seen in clinical models, where single algorithms like SVM-only approaches fail to capture complex patient-specific interactions, later justifyied the use of multimodal or ensemble approaches [43].

3.1.2 Why a Multi-Strategy Learning Framework Was Proposed

Combining multiple model types is more effective than relying on a single model because each contributes unique strengths: tree-based models capture non-linear interactions, deep learning models learn high-level patterns, and XAI methods provide essential transparency. Recent AI reviews show that such multimodal, explainable approaches consistently improve accuracy, generalization, and trust. This supports the use of an interpretable multi-strategy learning framework for predicting osteoporosis treatment adherence [44].

A multi-strategy framework was chosen to ensure comprehensive, interpretable, and reliable prediction of therapeutic adherence, outperforming single-model strategies that are often limited by bias toward specific data patterns.

The methodology involves data acquisition, preprocessing a healthcare dataset, developing interpretable machine learning models, evaluating their performance using both accuracy metrics and explainability techniques. The aim is to provide actionable insights for improving adherence among chronic patients as illustrated in Figure 3.1.

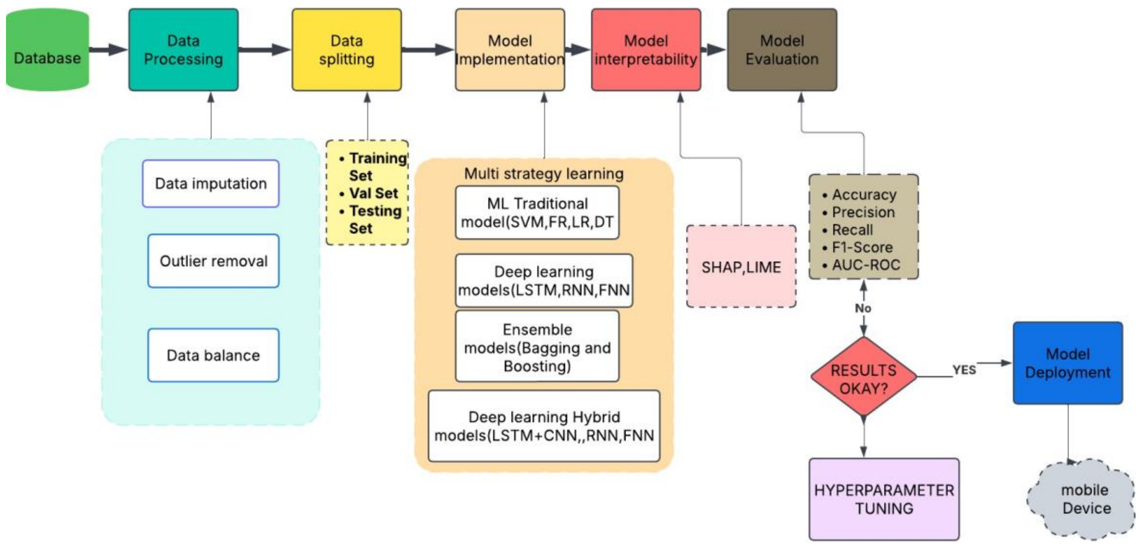


Figure 3.1: Visualization of the methodology

3.1.2.1 Data acquisition

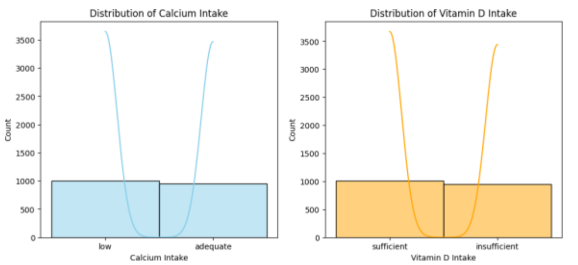
The dataset used in this research covers behaviors, treatment patterns, and factors influencing therapeutic adherence in osteoporosis publicly available on IEEE DataPort and can be accessed via DOI: https://dx.doi.org/10.21227/02nz-pa46 This is a valuable data set for building predictive machine learning models and deep learning models, as well as implementing interpretability analyzes. The description of the characteristics is shown in Table 3.1.

Table 3.1: The table showcasing Patient related features used in the study and Their Descriptions

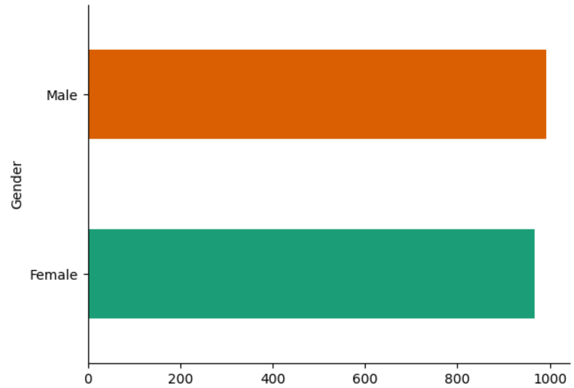
Feature	Description	Data type
ID	patient identifier	integer
Age	Patients Age	Integer
Gender	Male/Female	Categorical
Hormonal Changes	Hormonal status	Categorical
Family History	Family osteoporosis history	Categorical
Race	Patient's race/ethnicity	Categorical
Body Weight	Weight in kg	Float
Calcium Intake	Low/Adequate intake	Categorical
Vitamin D Intake	Sufficient/Insufficient	Categorical
Physical Activity	Activity frequency	Categorical
Smoking	Smoking habit	Categorical
Alcohol Consumption	Alcohol intake	Categorical
Medical Conditions	Health conditions	Categorical
Medications	Current medications	Categorical
Prior Fractures	Previous fractures	Categorical
Osteoporosis	Diagnosis presence	Categorical
Adherence	Treatment adherence	Categorical

3.1.3 Exploratory data Analysis

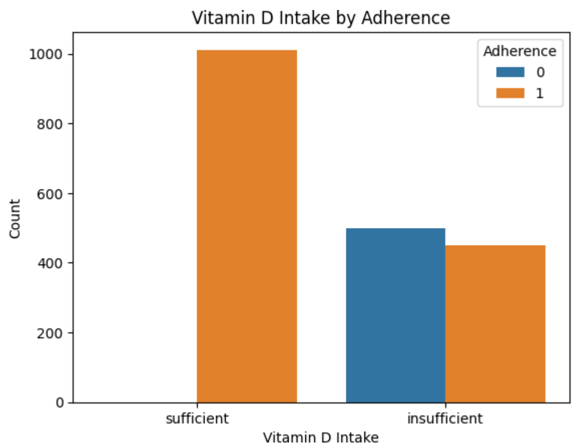
The exploratory data analysis phase was conducted to understand the structure, distribution and relationships within the data set and helped to detect data uncertainties such as missing values, detecting outliers by analyzing feature distributions through statistical summaries and visualizations as shown in Figures 3.2a, 3.2b, 3.2c, 3.2d, 3.3a, 3.3c, 3.3b.



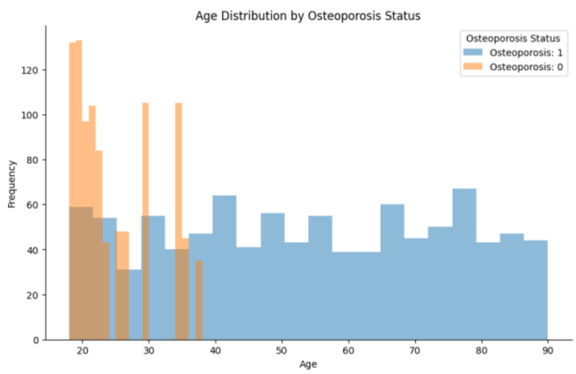
(a) Histogram with KDEs showing Calcium and Vitamin D Intake distribution among patients.



(b) Horizontal bar chart showing equal gender distribution in the dataset.

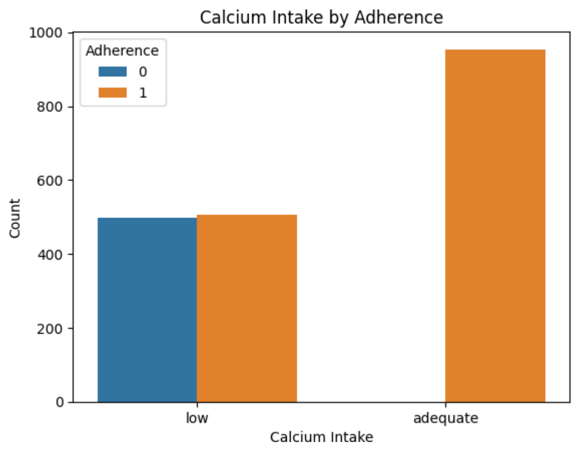


(c) Bar plot of Vitamin D intake levels by adherence status.

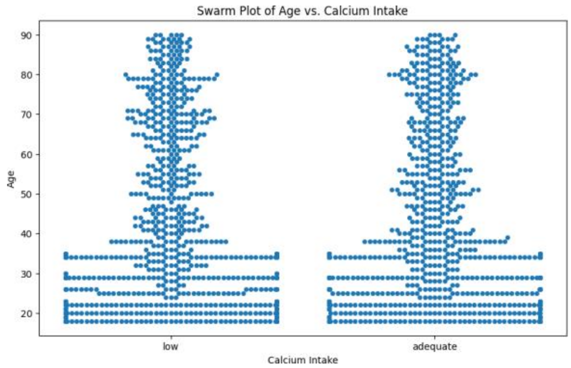


(d) Histogram showing more younger people in the dataset.

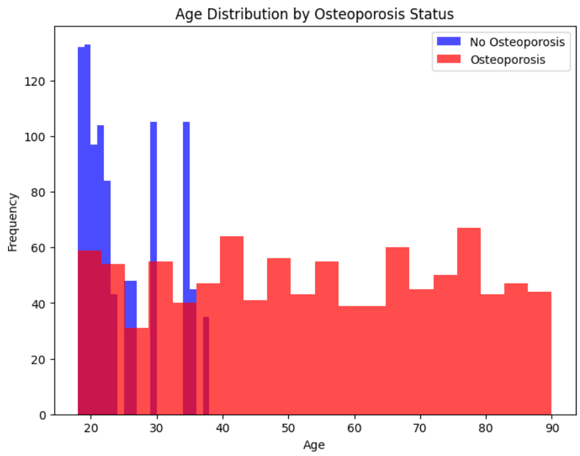
Figure 3.2: Exploratory Data Analysis Plots: Intake distributions, gender, and age insights.



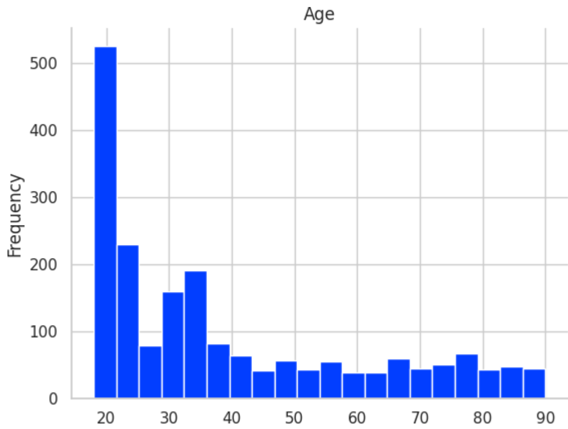
(a) Calcium intake levels grouped by adherence. Higher adherence with adequate intake.



(b) Swarm plot: Calcium intake decreases with increasing age.



(c) Overlapping histograms: Older individuals more likely to have osteoporosis.



(d) Histogram showing majority of participants are younger.

Figure 3.3: Additional EDA Plots: Calcium intake, age, and osteoporosis insights.

3.1.4 Data preparation and processing

Data preparation involved converting raw data into a suitable format for model training and evaluation. Missing values were handled by imputing categorical variables with the mode, while numerical data were normalized using Min-Max scaling to ensure consistency. Categorical variables were encoded using Label Encoding for ordinal variables and One-Hot Encoding for nominal vari- ables. Normalization was applied to scale numerical features, ensuring all values fell within a similar range for better model performance. To address class imbalance and prevent model bias, SMOTETomek was applied. This technique improved pre- dictive performance by preventing the model from skewing toward the majority class and poorly predicting the minor- ity class. By using SMOTE, the model learned meaningful patterns from both classes, enhancing its overall performance.Figure 3.4 shows before data imbalance whereas Figure 3.5 shows after data was balanced.

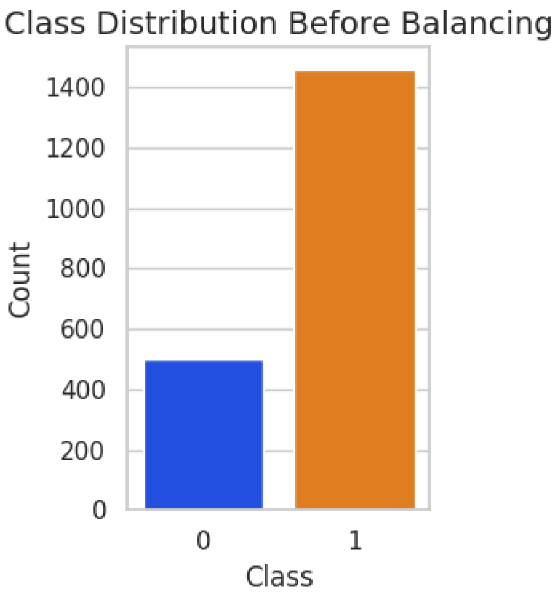


Figure 3.4: The count plot illustrates an imbalance between the two adherence classes, with a significantly higher number of samples in adherent class.

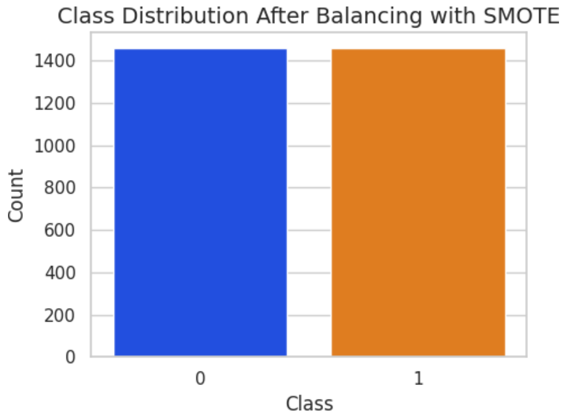


Figure 3.5: The count plot shows that the dataset was successfully balanced, with both adherence classes having an equal number of samples

3.1.4.1 Data splitting

The splitting was performed in two stages using stratified sampling to maintain class balance. First, 60% of the data were allocated to the training set, and the remaining 40% was split into validation sets (75%) and test sets (25%). This ensured a final 60:30:10 distribution, optimized model performance, and prevented overfitting.

3.2 Data Computational Modeling.

To effectively predict therapeutic adherence to osteoporosis treatment among chronic patients, a diverse set of machine learning and deep learning models grouped into three main categories were employed ranging from traditional, ensemble, to hybrid approaches. Traditional models included logistic regression, support vector machine (SVM), closest neighbor K (KNN), decision tree, and naive Bayes classifiers, serving as baselines for performance and interpretability. The ensemble methods comprised Random Forest, Bagging, Stacking, XGBoost, and Gradient Boosting, selected for their ability to improve prediction accuracy through model combination and boosting strategies. Advanced hybrid architectures such as XGBoost + LSTM, KNN + SVM, were integrated to leverage both sequential data handling and robust boost capabilities. This comprehensive modeling strategy ensured robust comparative evaluation and supported the objective of the study.

3.2.1 Logistic Regression

Due to its simplicity and interpretability of its coefficients, making it effective in identifying the influence of each characteristic on adherence as well classifying binary adherence,Logistic regression a traditional machine learning model was used. It helped to classify whether a patient is likely to adhere or not adhere to treatment as shown in Figure 3.6

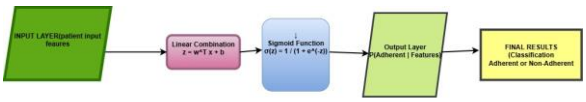


Figure 3.6: Logistic Regression Architecture for Osteoporosis Treatment Adherence Prediction: From Patient Data to Adherence Classification

The logistic regression model consisted of the following components: Input layer: The input layer included of various patient features, such as age, sex, medical history, medication, lifestyle factors. Weighted Sum Calculation: Each input feature is assigned a weight, and the weighted sum was computed as:

Mathematical representation

$$z = w_1x_1 + w_2x_2 + \cdot\cdot\cdot + w_nx_n + b \quad (1)$$

where:

- x_i represents the input features
- w_i represents the learned weights
- b is the bias term

The sigmoid activation function transformed the linear output into a probability between 0 and 1:

$$P(Y = 1) = \frac{1}{1 + e^{-z}} \quad (2)$$

where:

- If $P(Y = 1) > 0.5$, the prediction is **Adherent (1)**

- If $P(Y = 1) < 0.5$, the prediction is **Non-Adherent (0)**

Output Layer: The final probability score determined the classification of adherence. Regression made it easy to analyze the influence of factors on adherence.

3.2.2 The Decision Tree Classifier.

It modeled non-linear relationships and provided transparent decision rules, making it easy to understand the factors driving adherence. The tree was built by recursively splitting the characteristics based on the data set such as age, calcium intake, and physical activity, with the aim of minimizing impurity by splitting the data at each node based on the characteristic as shown in Figure3.7.

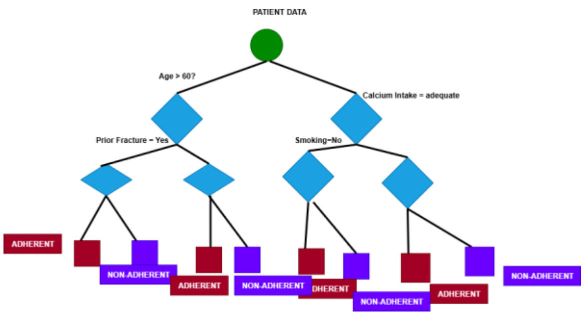


Figure 3.7: This diagram illustrates a simplified Decision Tree model for classifying osteoporosis patients as adherent or non-adherent to treatment based on key features such as age, prior fracture history, calcium intake, and smoking status. The root node (green) represents the first decision split, internal nodes (blue diamonds) represent intermediate decision conditions, and leaf nodes (colored squares) indicate the final predicted adherence class.

Impurity can be measured using *Gini Impurity* or *Entropy*.
The Gini impurity for a node is calculated as:

$$Gini = 1 - \sum_{i=1}^{c} p_i^2 \tag{3}$$

Where:

- p_i is the probability of class i in the node,
- c is the number of possible classes (for example, Adherence or Non-Adherence).

The entropy for a node is defined as:

$$Entropy = -\sum_{i=1}^{c} p_i \log_2(p_i) \tag{4}$$

Where:

- p_i is the probability of class i in the node.

Information Gain To select the best feature for splitting, the algorithm calculates the Information Gain, which measures the reduction in entropy after the split:

$$IG = Entropy(S) - \sum_{v \in V} \frac{|S_v|}{|S|} Entropy(S_v) \tag{5}$$

' Where:

- S is the set of data before the split,
- S_v are the subsets after splitting by feature v,
- $|S|$ and $|S_v|$ represent the number of instances in S and S_v, respectively.

The Decision Tree was constructed by selecting the feature with the highest Information Gain at each node and recursively splitting the data until a stopping criterion was met [45].

3.2.3 Naive Bayes

A probabilistic classifier, was used for its efficiency in handling small datasets and categorical data, providing a fast and interpretable approach to predict adherence and the model based on Bayes' theorem, assumed a conditional independence among features as shown in Figure3.8.

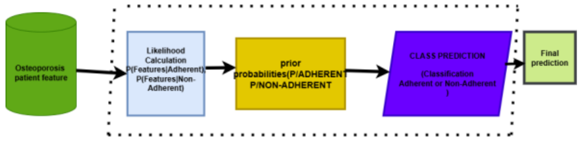


Figure 3.8: Naive Bayes architecture for Osteoporosis Treatment Adherence Prediction Based on Patient Features.

Bayes' Theorem The fundamental equation governing the Naive Bayes classifier follows as:

$$P(C_k|X) = \frac{P(X|C_k)P(C_k)}{P(X)} \tag{6}$$

where:

- $P(C_k|X)$ is the posterior probability of class C_k given the input features X.
- $P(X|C_k)$ is the likelihood of observing X given class C_k.
- $P(C_k)$ is the prior probability of class C_k.
- $P(X)$ is the marginal probability of the input data.

The independence assumption of Naive Bayes Naive Bayes assumed that features are conditionally independent given the class label, meaning:

$$P(X|C_k) = \prod_{i=1}^{n} P(x_i|C_k) \tag{7}$$

where x_i represents the individual feature values. This assumption simplifies the computation and allows efficient probability estimation.

Classification Decision The predicted class is determined by selecting the class C_k that maximizes the posterior probability:

$$C^* = \arg\max_{C_k} P(C_k) \prod_{i=1}^{n} P(x_i|C_k) \tag{8}$$

With this study, Naive Bayes calculated the probability of adherence and non-adherence, selecting the most probable category.

3.2.4 Support Vector Machine (SVM)

A support vector machine (SVM) is a supervised machine learning algorithm classified data by finding an optimal line or hyperplane that maximizes the distance between each class in an N-dimensional space. In this study, it found the optimal hyperplane that separates factors influencing treatment adherence from those that do not.

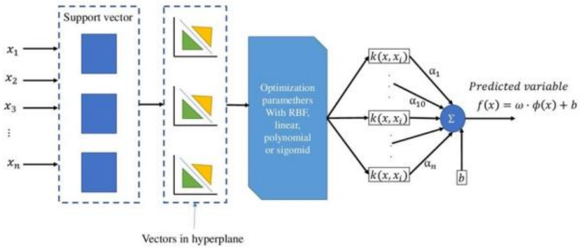


Figure 3.9: Support Vector Machine (SVM) architecture for predicting osteoporosis adherence, illustrating the optimal hyperplane for classification of adherent and non-adherent patterns.

Mathematical Formulation Given a training set (x_i, y_i), where $x_i \in \mathbb{R}^n$ and $y_i \in \{-1, 1\}$, the SVM optimization problem is:

$$\min_{w,b} \frac{1}{2}||w||^2 \tag{9}$$

subject to:

$$y_i(w^T x_i + b) \geq 1, \quad \forall i \tag{10}$$

For non-linearly separable data, the soft-margin SVM introduces slack variables ξ_i:

$$\min_{w,b,\xi} \frac{1}{2}||w||^2 + C \sum_{i=1}^{n} \xi_i \tag{11}$$

subject to:

$$y_i(w^T x_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad \forall i \tag{11}$$

Kernel Trick To handle non-linearly separable data, SVM employs a **kernel function $K(x_i, x_j)$ to project data into a higher-dimensional space:

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j) \tag{13}$$

Common kernels include: - Linear Kernel: $K(x, x') = x^T x'$ - Polynomial Kernel: $K(x, x') = (x^T x' + c)^d$ - Radial Basis Function (RBF) Kernel: $K(x, x') = \exp(-\gamma||x - x'||^2)$

3.2.4.1 K-Nearest Neighbors (KNN)

This was employed for its ability to model nonlinear decision boundaries and its effectiveness with various patient characteristics. AS a non-parametric, instance-based learning algorithm used for classification and regression tasks, It relied on measuring the similarity between data points using distance metrics and classifying a sample based on the majority class of its nearest neighbors.

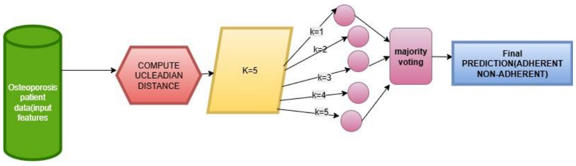


Figure 3.10: KNN model architecture, showcasing voting basing on the nearby points to give the prediction.

Distance Metric KNN determined the similarity between an input sample X and all training samples using a distance function. The metric was the Euclidean distance, defined as:

$$d(X, X_i) = \sqrt{\sum_{j=1}^{n} (x_j - x_{ij})^2} \tag{14}$$

where:

- $X = (x_1, x_2, ..., x_n)$ is the feature vector of the new instance.
- $X_i = (x_{i1}, x_{i2}, ..., x_{in})$ represents the feature vector of the i-th training instance.
- n is the number of features.

after computing the distances, the K nearest neighbors were selected, and the class label was assigned based on the majority vote:

$$C^* = \arg\max_{C_k} \sum_{i \in N_k} \delta(y_i, C_k) WS \tag{15}$$

where:

- N_k is the set of the k nearest neighbors.
- y_i is the class label of neighbor i.
- $\delta(y_i, C_k)$ is an indicator function that returns 1 if $y_i = C_k$, otherwise 0.

For this study, KNN classifies patients as adherent or non-adherent by evaluating similarities in patient attributes such as age, lifestyle habits, medication history, and medical conditions. The algorithm identifies patients with similar profiles and predicts adherence behavior based on the majority class of the closest neighbors.

3.2.5 Random Forest Classifier.

This is an ensemble learning method that builds multiple decision trees and combines their results to improve classification accuracy and reduce overfitting. Trains several decision trees on different random subsets of the data and aggregates their predictions through majority voting.

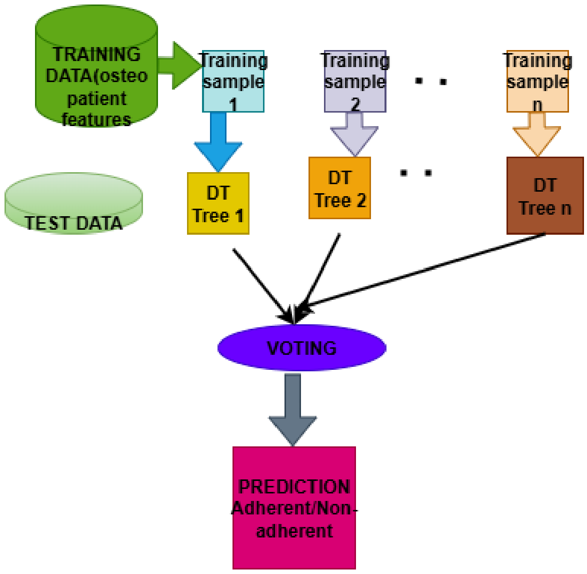


Figure 3.11: Random Forest Model Architecture for Predicting Therapeutic Adherence:An ensemble of multiple decision trees trained on different patient data samples, whose outputs are combined through a majority voting mechanism to classify osteoporosis patients as adherent or non-adherent

Mathematically, the final prediction $y\hat{}$ in classification is obtained by taking the majority vote across T decision trees:

$$y\hat{} = \text{mode}\{h_1(x), h_2(x), ..., h_T(x)\} \tag{16}$$

where $h_t(x)$ represents the prediction of the t-th decision tree for input x.

Each decision tree is trained on a **bootstrap sample** (random sampling with replacement), and at each node, a **random subset of features** is considered for splitting instead of using all features. This helps in reducing correlation between trees and improves generalization.

The impurity of each node is measured using metrics like **Gini impurity** or **Entropy**:

Gini Impurity:

$$Gini = 1 - \sum_{i=1}^{C} p_i^2 \tag{17}$$

where p_i is the probability of class i and C is the number of classes.

Entropy (Information Gain):

$$H(S) = -\sum_{i=1}^{C} p_i \log_2 p_i \tag{18}$$

where $H(S)$ represents entropy at a node.

It reduces overfitting by averaging multiple trees compared to individual decision trees

.

3.2.6 Extreme Gradient Boosting(XGBoost)

XGBoost is an optimized gradient-boosting algorithm designed to improve predictive accuracy while maintaining computational efficiency. It constructs a set of decision trees sequentially, where each new tree corrects errors made by previous trees using gradient descent optimization, as shown in Figure **??**. *Mathematical Representation* The objective

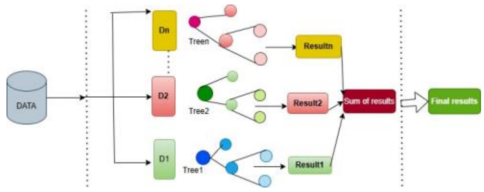


Figure 3.12: XGBoost model architecture: An ensemble of decision trees built sequentially, where each tree corrects the errors of the previous ones. Gradient descent optimizes tree weights and minimize the loss function.

function in XGBoost consists of two main parts: the loss function and the regularization term:

$$L(\vartheta) = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k) \tag{19}$$

where:

- $l(y_i, \hat{y}_i)$ is the loss function measuring the difference between actual and predicted values. XGBoost typically uses squared error loss for regression and logistic loss for classification.
- $\Omega(f_k) = \gamma T + \frac{1}{2}\lambda \sum w^2$ is the regularization term that controls model complexity, where T is the number of leaves in a tree, w is the leaf weights, γ is the complexity penalty, and λ controls L2 regularization.

Gradient Boosting Update Rule

New trees are added to minimize the loss function:

$$\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + \eta f_t(x_i) \tag{20}$$

where η is the learning rate, and $f_t(x_i)$ is the new tree predicting the residuals.

XGBoost helps analyze factors influencing osteoporosis treatment adherence by identifying patterns in patient data. Its efficiency and strong performance and the ability to allow construction of sequential decision trees to correct previous errors is why it was chosen.

3.2.7 Stacking

Combined the predictions of different classifiers using a meta-model, thus enhancing overall performance. Stacking ensemble architecture

*Stacking Model: Mathematical Representation

Let X be the input features and y be the target variable. The stacking ensemble consists of **base models** $f_1, f_2, ..., f_n$ and a **meta-model** g.

*1. Base Model Predictions (Level-0 Learners) Each base model f_i is trained on X to produce predictions:

$$\hat{y}_i = f_i(X), \qquad \text{for } i = 1, 2, ..., n \tag{21}$$

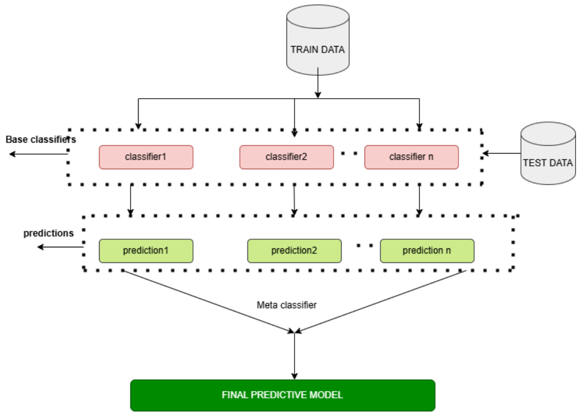


Figure 3.13: Illustration of a stacking ensemble model architecture showing Random Forest, XGBoost, and SVM base models trained in parallel, and their combined predictions by a Logistic Regression meta-classifier to improve adherence prediction

These predictions form a new feature set Z:

$$Z = [\hat{y}_1, \hat{y}_2, ..., \hat{y}_n] \tag{22}$$

2. Meta-Model Training (Level-1 Learner)

A meta-model g was trained on Z to learn how to best combine base model predictions:

$$\hat{y} = g(Z) = g(\hat{y}_1, \hat{y}_2, ..., \hat{y}_n) \tag{23}$$

Final Prediction

$$\hat{y} = g(f_1(X), f_2(X), ..., f_n(X)) \tag{24}$$

The key Advantage: Instead of taking a simple average, stacking learned the optimal combination of predictions thus improved performance and generalization.

3.2.8 Bagging

Bagging is an ensemble method that involved training multiple models independently on random subsets of the data and aggregating their predictions through voting or averaging as shown in Figure 3.14

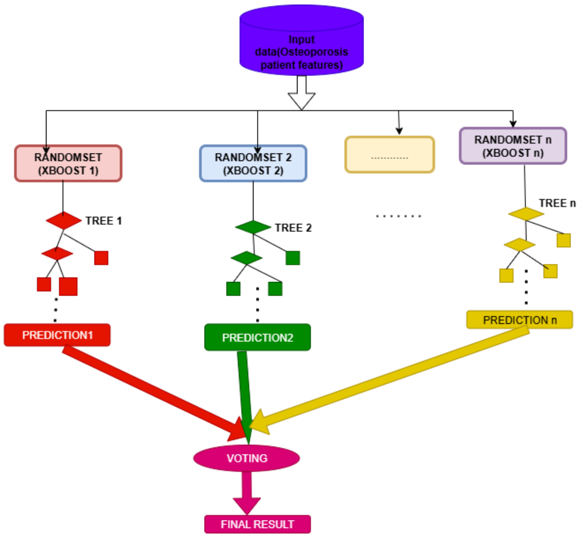


Figure 3.14: An illustration of a bagging ensemble showing each bootstrap sample trained an independent XGBoost base learner, each consisting of an ensemble of decision trees. The outputs of these learners were aggregated to produce the final adherence prediction.

3.2.9 Gradient Boosting

In this study, a gradient boost classifier (GBC) was used to predict therapeutic adherence to osteoporosis treatment by learning complex patterns within the data set. Gradient Boosting was chosen because it constructs an ensemble of weak learners, typically shallow decision trees, that are added sequentially. Each new tree was trained to correct the residual errors made by the combined ensemble up to that point as shown in Figure 3.15

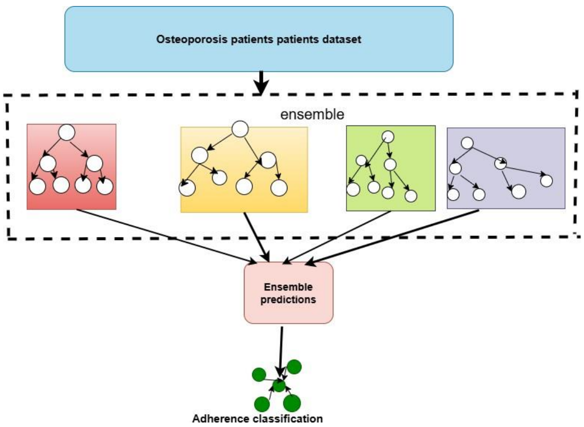


Figure 3.15: A Conceptual architecture of a Gradient Boosting Classifier applied to the osteoporosis patients dataset for therapeutic adherence classification showcasing multiple sequential decision trees form an ensemble and each tree corrects errors from the previous learners, and their combined predictions enhance the final adherence classification outcome.

Mathematically, the prediction function after M iterations can be represented as:

$$F_M(x) = F_{M-1}(x) + \eta h_M(x) \tag{25}$$

where $F_{M-1}(x)$ denotes the current prediction of the ensemble, $h_M(x)$ represents the new weak learner fitted to the residuals, and η is the learning rate that controls the contribution of each new tree.

The residuals for each iteration m were computed by taking the negative gradient of the loss function $L(y, F(x))$ with respect to the current prediction:

$$r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)} \tag{26}$$

For binary classification tasks, the logistic loss function is commonly used. By iteratively minimizing this loss, the model incrementally improves its predictions.

3.2.10 Recurrent Neural Networks (RNN)

RNNs were implemented for their ability to model complex non-linear relationships in the data, which makes them effective in dictating therapeutic adherence.RNN is Showcased in the Figure 3.16

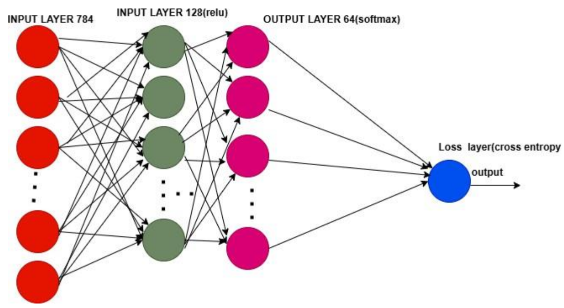


Figure 3.16: RNN architecture:RNNs are made of neurons: data-processing nodes that work together to perform complex tasks. The neurons were organized as input, output, and hidden layers. The input layer receives the information to process, and the output layer provides the result.

3.2.11 Gated Recurrent Units (GRU)

GRU were selected as part of this study for their proven efficiency in modeling sequential dependencies within time series or ordered data. Compared to traditional recurrent neural networks (RNNs) or long-short-term memory (LSTM) networks, GRUs offered a simpler architecture with fewer parameters while retaining the ability to capture long-term dependencies. This made them computationally faster and less prone to overfitting on small or medium data sets. For this study, therapeutic adherence, GRUs help capture sequential or temporal patterns in patient-related factors such as treatment history, behavioral trends, or periodic follow-ups that can influence adherence outcomes over time.

3.2.12 Long Short-Term Memory (LSTM)

LSTM were used for their ability to capture long-term dependencies and temporal patterns in sequential data, making them ideal for modeling patient adherence behavior over time. These deep learning models were chosen to capture intricate patterns in data that traditional machine learning models may not identify.An illustration shown in Figure 3.17

3.2.13 The LSTM + XGBoost hybrid model

This hybrid combined the strengths of Recurrent Neural Networks (RNNs) and Extreme Gradient Boosting (XGBoost). The LSTM component processed sequential data,

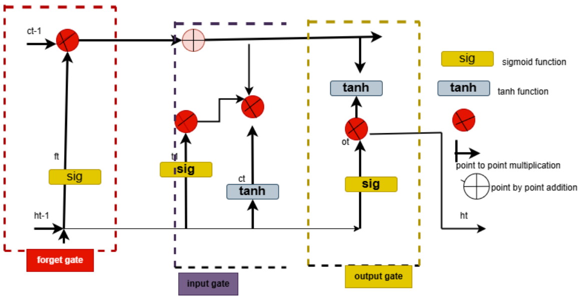


Figure 3.17: lstm architecture

capturing temporal relationships and patterns. The output provided by the LSTM is then fed into the XGBoost component, which further refines the predictions by identifying complex interactions between features. The XGBoost algorithm's ability to handle high-dimensional data and nonlinear relationships complemented the LSTM's sequential processing capabilities, resulting in a powerful hybrid model that excels in tasks such as time series forecasting and sequential data classification.

3.2.14 KNN + SVM Hybrid Model

This combined the strengths of closest neighbors (KNN) and support vector machines (SVMs) to create a robust and accurate classification model. The KNN component provided a local, instance-based approach to classification, while the SVM component offered a global, discriminative approach. The KNN output was used as input to the SVM, which further refined the predictions by identifying the optimal hyperplane that maximally separates the classes.

3.2.15 CNN + RNN Hybrid Model

This combines the strengths of Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs) to process data with spatial and temporal hierarchies. The CNN component extracts local features and patterns from the input data, while the RNN component models the sequential relationships and temporal dynamics. The output from the CNN is fed into the RNN, which further processes the information to generate predictions. This hybrid architecture is particularly effective in tasks such as image captioning, video analysis, and speech recognition, where both spatial and temporal information are crucial.

Chapter 4

Model Evaluation and Results and Discussion

This chapter presents the study findings and provides a clear and comprehensive overview of the study . The results are presented using tables, figures, and text to facilitate understanding and interpretation.

4.1 Model Evaluation

To assess the performance of models, a number of evaluation metrics such as accuracy, precision, recall, F1 score, and AUC score were used as seen in Table 4.1 and Table 4.2 before hyperparameter tuning and in Figure 4.1 and Figure 4.2 shown in bar graphs for both validation and test metrics respectively. These metrics provided a comprehensive understanding of how well each model predicted the outcomes, considering both positive and negative class performance. Accuracy gave an overall measure of correct predictions, while precision and recall focused on the model's ability to identify positive instances and minimize false positives and false negatives. The F1 score balanced precision and recall.

Table 4.1: Validation Metrics Comparison Before Hyperparameter Tuning

Model	Accuracy (%)	Precision (%)	Recall (%)	F1 Score (%)	AUC-ROC (%)
LogReg	61.6	59.9	70.3	64.7	66.7
NBayes	51.1	57.8	8.4	14.7	56.9
SVM	63.6	63.4	64.2	63.8	68.5
DTree	65.1	70.8	51.4	59.5	68.4
KNN	64.7	65.9	61.0	63.4	68.0
RanForest	68.2	71.0	61.4	65.9	71.5
XGBoost	67.1	70.0	60.1	64.6	73.8
Stacking	67.6	70.6	60.3	65.0	73.3
Bagging	68.0	70.8	61.4	65.8	73.6
RNN	64.5	62.3	73.3	67.4	70.0
GRU	61.6	59.6	72.6	65.4	70.0
LSTM	65.3	64.7	67.4	66.0	71.8
XGBoost + LSTM	67.1	68.9	62.3	65.5	71.5
KNN + SVM	57.9	60.6	45.2	51.8	55.6

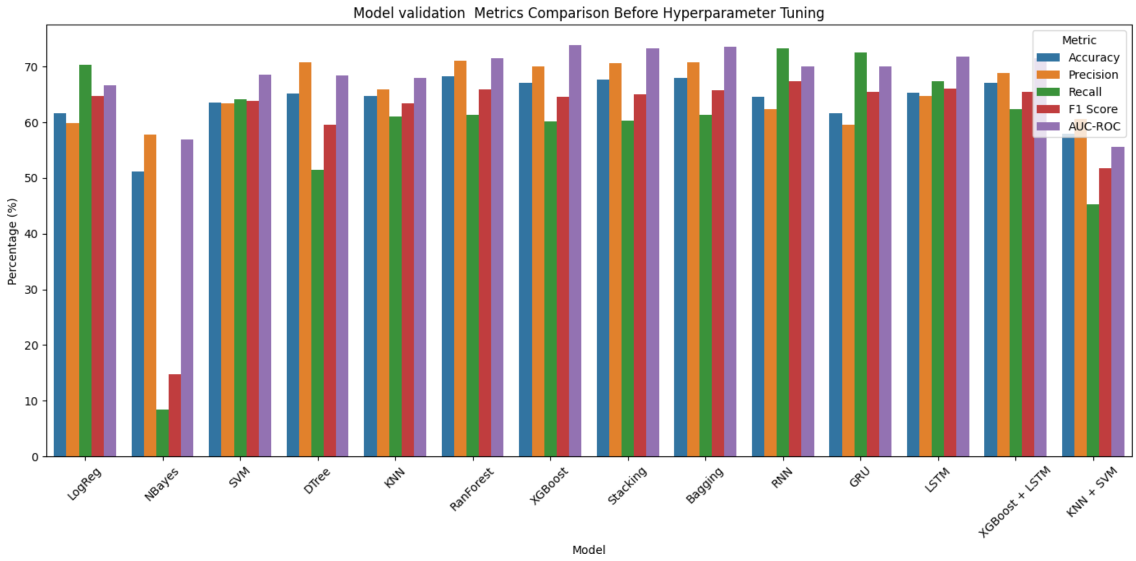


Figure 4.1: A bar graph showing validation metrics before hyperparameter tuning

Table 4.2: Test Metrics Comparison Before Hyperparameter Tuning

Model	**Accuracy (%)**	**Precision (%)**	**Recall (%)**	**F1 Score (%)**	**AUC-ROC (%)**
Logistic Regression	62.0	60.6	68.5	64.3	68.8
Naive Bayes	53.1	66.7	12.3	20.8	56.0
SVM	61.0	61.0	61.0	61.0	68.1
Decision Tree	66.4	71.1	55.5	62.3	71.3
KNN	64.7	65.3	63.0	64.1	67.6
Random Forest	68.2	71.0	61.4	65.9	71.5
XGBoost	66.1	68.5	59.6	63.7	75.1
Stacking	66.4	69.1	59.6	63.9	74.8
Bagging	66.1	68.5	59.6	63.7	74.6
RNN	66.1	63.3	76.7	69.3	70.6
GRU	61.6	59.6	72.6	65.4	70.0
LSTM	66.1	65.2	69.2	67.1	71.8
XGBoost + LSTM	66.4	67.6	63.0	65.2	73.0
KNN + SVM	58.6	61.5	45.9	52.5	56.8

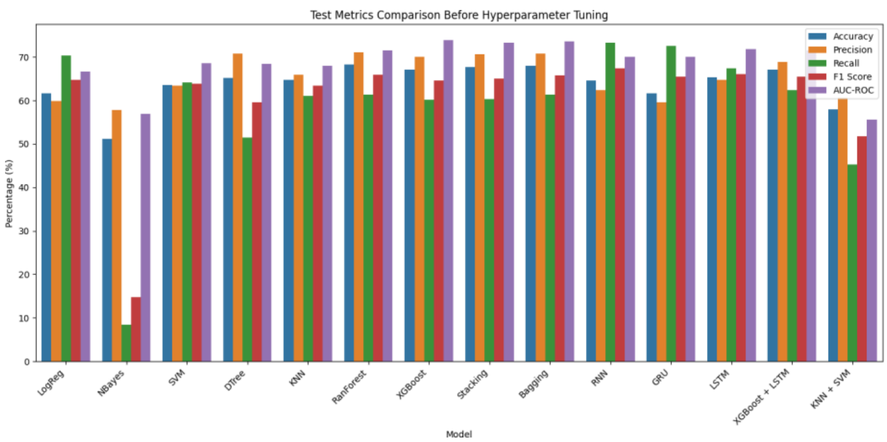


Figure 4.2: A bar graph showing test metrics before hyperparameter tuning

Hyperparameter tuning

Hyperparameter tuning was done systematically for all trained models to optimize model performance and ensure robust, generalizable predictions of therapeutic adherence among osteoporosis patients using Grid search and random search strategies while adjusting key parameters such as learning rates, maximum tree depth, number of estimators, regularization strengths, and kernel parameters,batch sizes,sub sampling rates and dropout rates. The tuning phase resulted in improved accuracy,precision, recall, and AUC-ROC scores across both validation and test datasets .Results are shown in

Table 4.3,Table 4.4 and visually represented in bar graphs Figure 4.3 and Figure 4.4 for both validation and test metrics respectively.

Table 4.3: Validation Metrics Comparison After Hyperparameter Tuning

Model	**Accuracy (%)**	**Precision (%)**	**Recall (%)**	**F1 Score (%)**	**AUC-ROC (%)**
SVM	65.4	66.0	63.7	64.8	70.7
Decision Tree	65.2	70.3	52.5	60.1	68.5
KNN	65.1	68.9	54.8	61.1	68.5
Random Forest	67.4	69.1	62.8	65.8	72.1
Logistic Regression	61.99	59.8	73.3	65.8	66.7
Naive Bayes	51.3	58.5	8.7	15.1	56.9
XGBoost	68.3	70.6	62.6	66.3	73.4
Stacking Ensemble	68.3	71.3	61.2	65.8	72.4
Bagging	68.2	70.9	61.6	65.9	71.7
Gradient Boosting	68.3	70.3	63.2	66.6	73.7
RNN	63.4	66.5	53.9	59.5	69.3
GRU	64.7	62.9	71.7	67.0	71.5
KNN + SVM	64.0	64.1	64.0	63.9	68.6
XGBoost + LSTM	67.7	69.7	62.6	65.9	71.5

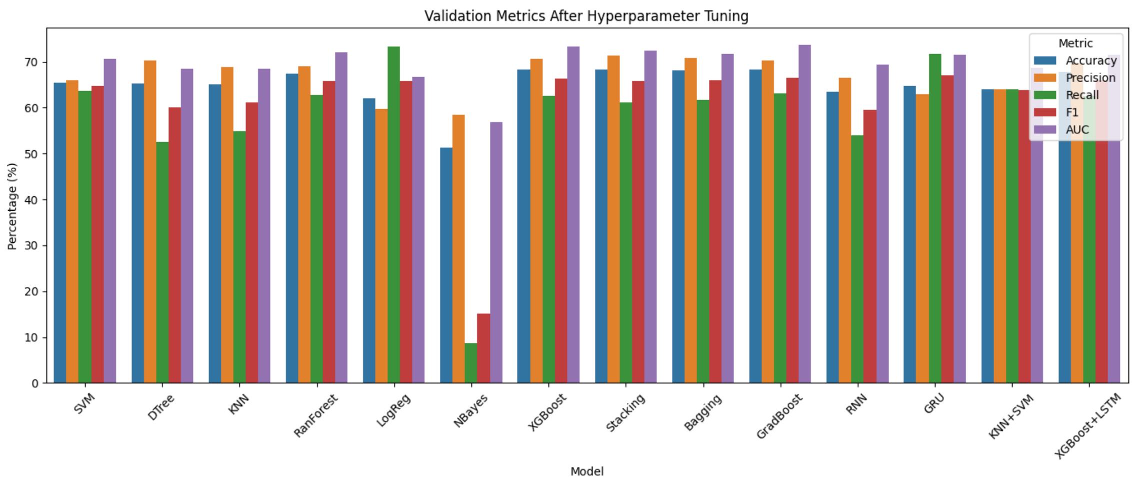


Figure 4.3: A bar graph showing Validation Metrics Comparison After Hyperparameter Tuning

Table 4.4: Test Metrics Comparison After Hyperparameter Tuning

Model	Accuracy (%)	Precision (%)	Recall (%)	F1 Score (%)	AUC-ROC (%)
SVM	67.1	67.9	65.1	66.4	72.4
Decision Tree	66.8	72.1	54.8	62.3	71.7
KNN	66.4	69.7	58.2	63.4	72.2
Random Forest	67.4	69.1	62.8	65.8	72.1
Logistic Regression	64.7	62.4	73.9	67.7	69.1
Naive Bayes	53.1	66.7	12.3	20.8	56.0
XGBoost	67.1	69.5	60.9	64.9	74.7
Stacking Ensemble	66.1	68.2	60.3	64.0	73.9
Bagging	68.5	72.6	59.4	65.3	72.1
Gradient Boosting	67.1	68.7	63.0	65.7	75.1
RNN	64.4	69.4	51.4	59.1	70.97
GRU	64.7	62.9	71.7	67.0	71.5
KNN + SVM	63.0	63.1	63.0	62.9	66.8
XGBoost + LSTM	66.1	67.9	60.9	64.3	73.6

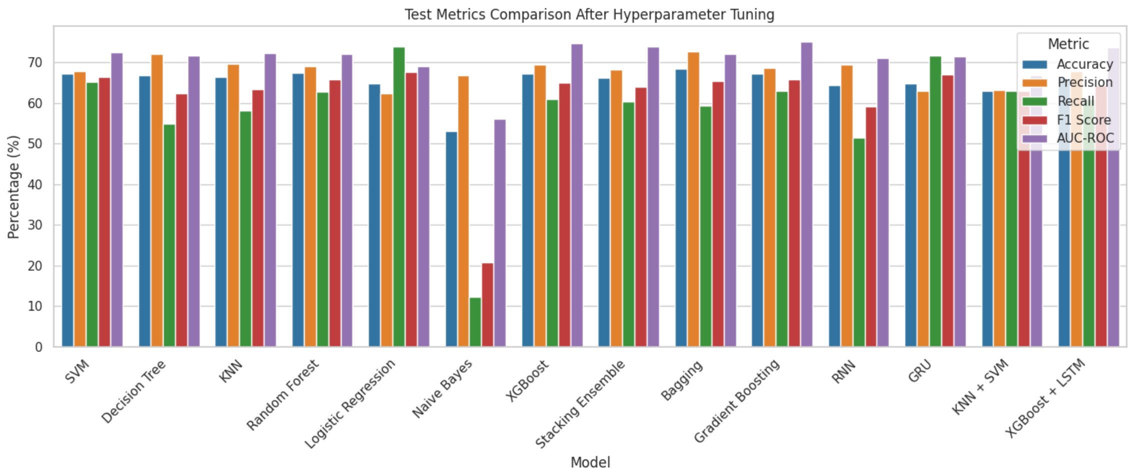
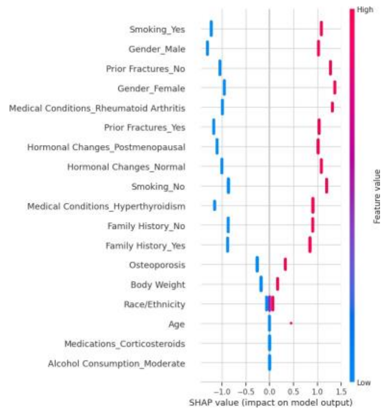


Figure 4.4: A bar graph showing Test Metrics Comparison After Hyperparameter Tuning

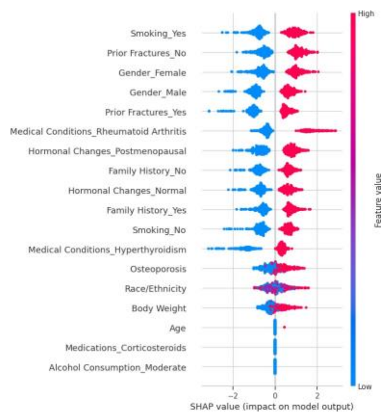
4.2 Application of Explainable Artificial Intelligence (XAI)

Multiple XAI including SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-Agnostic Explanations), and Permutation Feature Importance (PFI) were implemented to enhance the interpretability of the predictive models. While SHAP and LIME provided local and global insights into how individual features contributed to each prediction, the PFI graphs quantified the impact of each feature on the model's performance by measuring the decrease in prediction accuracy when a feature's values were randomly shuffled. Together, these explanations allowed for a complete understanding of the factors that influence therapeutic adherence, ensuring that model decisions are transparent and clinically interpretable, as shown in Figures 4.5a, 4.5b, 4.5c, 4.6a, 4.6b, 4.6c, 4.6f, 4.6e 4.6d.



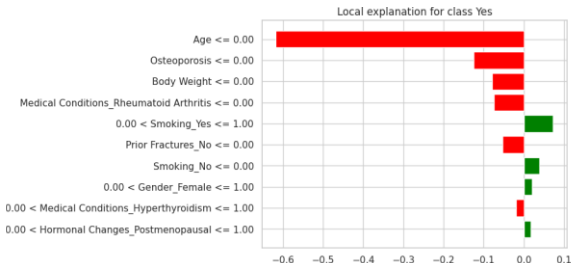
(a) SHAP for Logistic Regression

(b) SHAP for Decision Tree

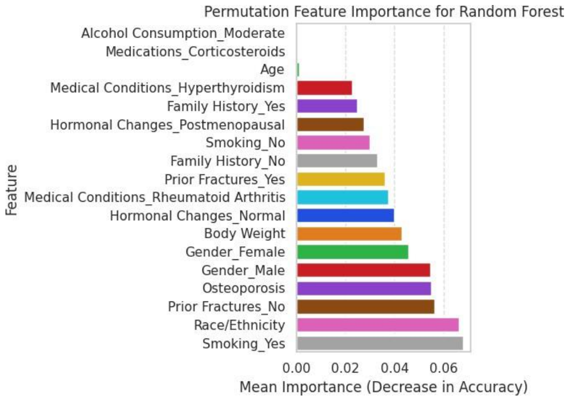


(c) SHAP for XGBoost

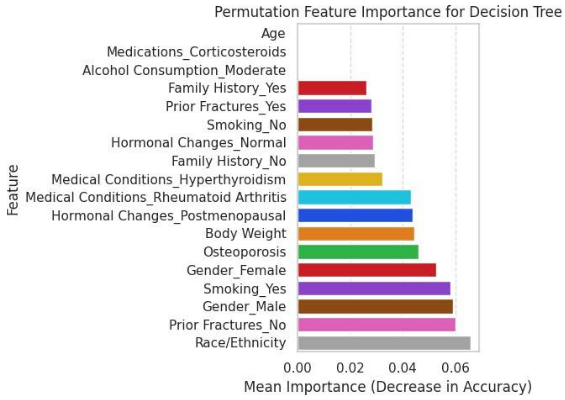
Figure 4.5: SHAP summary plots for different models illustrating feature contributions to therapeutic adherence prediction.



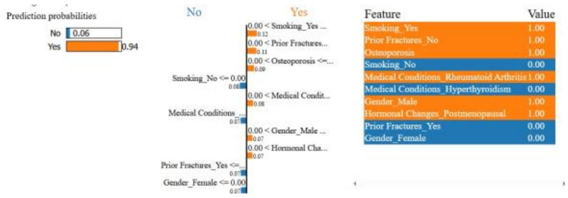
(a) LIME plot for Naive Bayes.



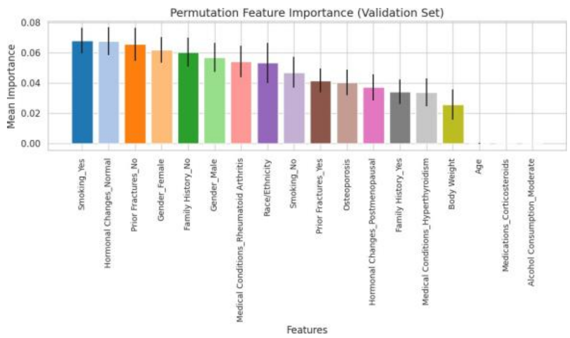
(b) Permutation Feature Importance for Decision Tree.



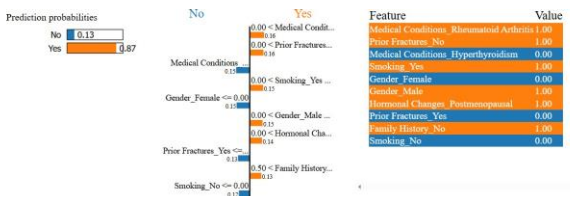
(c) Permutation Feature Importance for Decision Tree.



(d) LIME plot for Random Forest.



(e) Permutation Feature Importance graph for xgboost



(f) LIME plot for xgboost

Figure 4.6: Comparison of remaining interpretability plots (LIME and Permutation Feature Importance) for different models.

Interpretation of Explainable AI Plots and Clinical Insights

Table 4.5 summarizes the interpretability plots by detailing each image's meaning, the interpretation provided, and the clinical insights derived. This comparison ensures that model predictions are transparent and actionable for clinicians and decision-makers. By understanding how features like smoking, prior fractures, or gender impact adherence predictions, healthcare providers can design personalized interventions and better communicate treatment plans, ultimately improving patient adherence and outcomes.

Table 4.5: Interpretability plots summary: image label, interpretation, and clinical insights

Image Label	**Interpretation**	**Explanation and Clinical Insights**
SHAP for Logistic Regression Figure 4.5a,	Shows how various features contribute to adherence prediction	Smoking , male gender, No prior fractures are shown as top key predictors that contribute positively to adherence.
shap for descision tree in Figure 4.5b	visualizes how Race/Ethnicity and Age interact and contribute together to the model's prediction of osteoporosis treatment adherence.	Indicates that Age has a more concentrated and wider spread of interaction impact, plays a stronger role in modifying the effect of Race/Ethnicity on adherence predictions.The influence of a patient's race/ethnicity on adherence depends partly on their age group.
SHAP for XGBoost in Figure 4.5c	Shows feature impact across boosting stages	smoking status, prior fractures, hormonal changes, and age play significant roles in shaping the prediction.
Permutation Feature Importance for Decision Tree 4.6c	Features influencing adherence ranked	Not smoking,having pior fractures,family history to osteoporosis fractures are the top ranking features in predicting adherence.
Permutation Feature Importance for XGBoost 4.6e	Measures feature effect by permutation	smoking,hormonal changes,gender female as the top most features influencing adherence prediction
LIME for XGBoost Figure 4.6f	Local explanation for individual XGBoost prediction	Reveals that medical conditions,smoking, positively influence the XGBoost model's high adherence prediction for this patient, guiding clinicians on personalized support needs.
LIME for Random Forest 4.6d	Local explanation for Random Forest output	Not having prior fractures, rheumatoid condition,male gender positively influence adherence whereas having prior fractures,female gender medical condition hyperthyroidism negatively influence in this study adherence.

4.2.1 Model selection

Based on the comparative evaluation shown in Table 4.3, the XGBoost model was selected as the primary model to predict therapeutic adherence to osteoporosis treatment among chronic patients due to its consistency in high performance in all key metrics, giving a precision of 68. 3%, a precision of 70. 6%, a recall of 62.6%, an F1 score of 66.3%, and a robust AUC-ROC of 73.4%. Compared to other models, XGBoost showed strong generalization with competitive precision and recall balance, which is critical for correctly identifying adherent and non adherent patients. In addition to that,in the medical domain, accurate prediction of therapeutic adherence is crucial for patient outcomes. Given the class imbalance in adherence data, XGBoost's robustness to overfitting and its ability to handle imbalanced datasets made it a top choice. Its high AUC-ROC score (73.4%) indicates strong discrimination between adherent and non-adherent patients. Additionally, XGBoost's compatibility with SHAP and LIME enables interpretable predictions, aligning with the study's goal of providing actionable insights for healthcare professionals.

4.2.2 Deployment pipeline

After model selection, XGBoost model was deployed using a containerized architecture to ensure accessible, scalable, and secure delivery of adherence predictions. As illustrated in Figure 4.7, the deployment process began by storing the Flask application and trained model files in a GitHub repository. Continuous integration was achieved using GitHub Actions, which automated the building of a Docker image and its upload to Docker Hub. The Render web service was then used to pull this Docker image, run the container, and expose the Flask web user interface. Through this pipeline, raw osteoporosis patient input data could be submitted via the Flask interface to generate real-time adherence predictions, demonstrating an end-to-end practical application of the developed XGBoost model for supporting clinicians and patients.

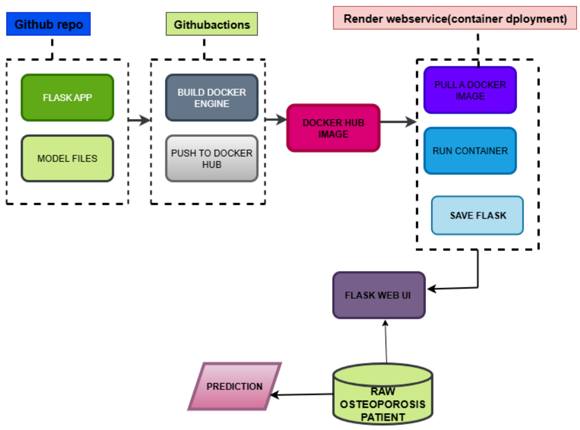
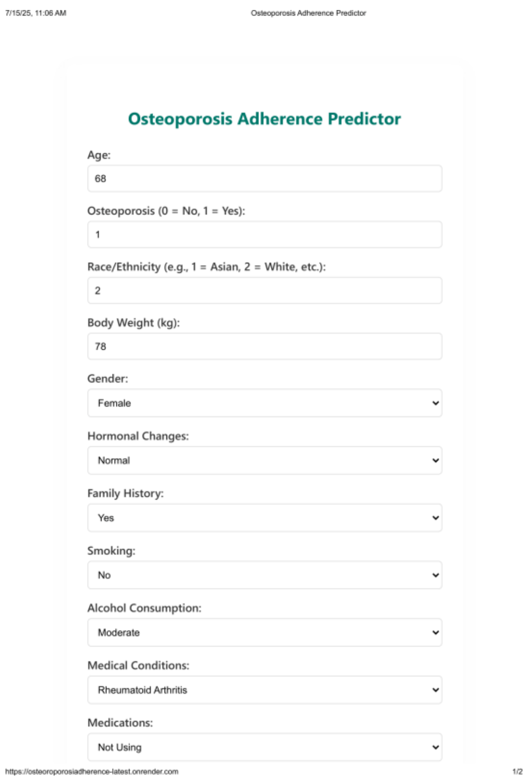


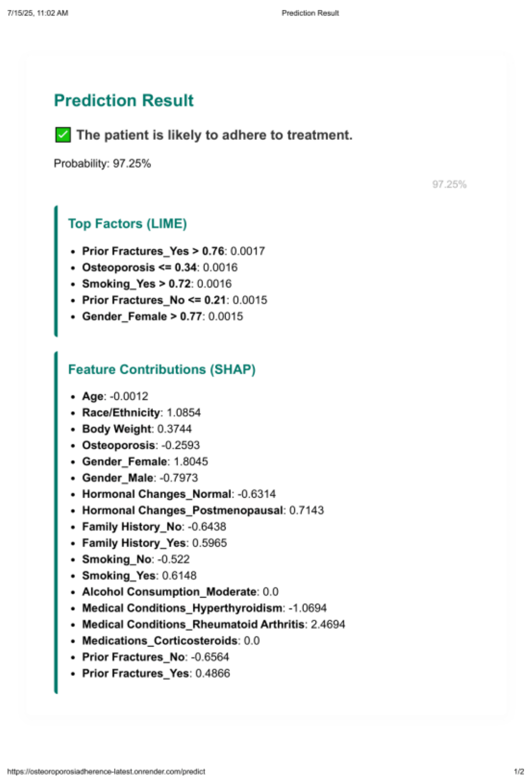
Figure 4.7: System architecture diagram illustrating the deployment workflow for the XGBoost predictive model. The figure shows how patient input data is processed through the web interface, passed to the trained XGBoost model hosted on the backend, and returns adherence predictions to end-users via the deployed application.

4.2.2.1 *Deployed User facing Prediction Interface and Explainability*

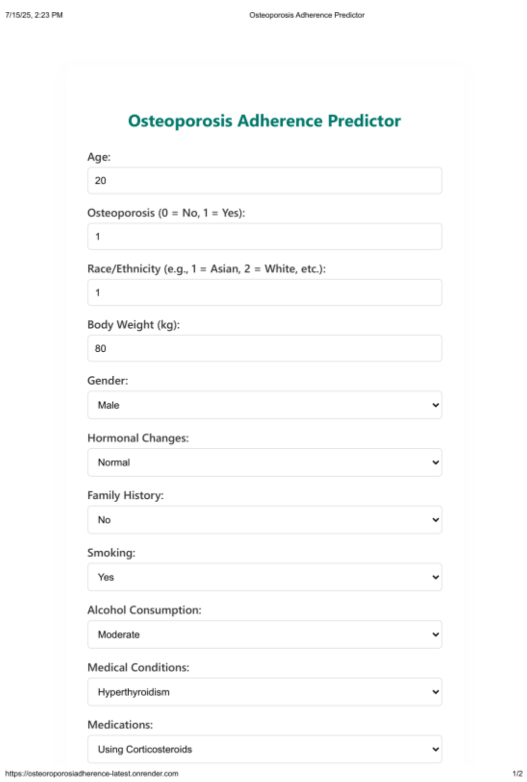
The final predictive model was deployed as a simple web application where users can input patient data . After submission, the app preprocesses and scales the data, then generates an adherence prediction with a probability score. To support interpretability, the interface presents local explanations using LIME, identifying which factors influenced the specific prediction, and SHAP values to show the contribution of each feature. This ensures users see not only the prediction but also understand the key factors behind it as shown in Figure 4.8a, 4.8b, 4.8b, 4.8c, 4.8d



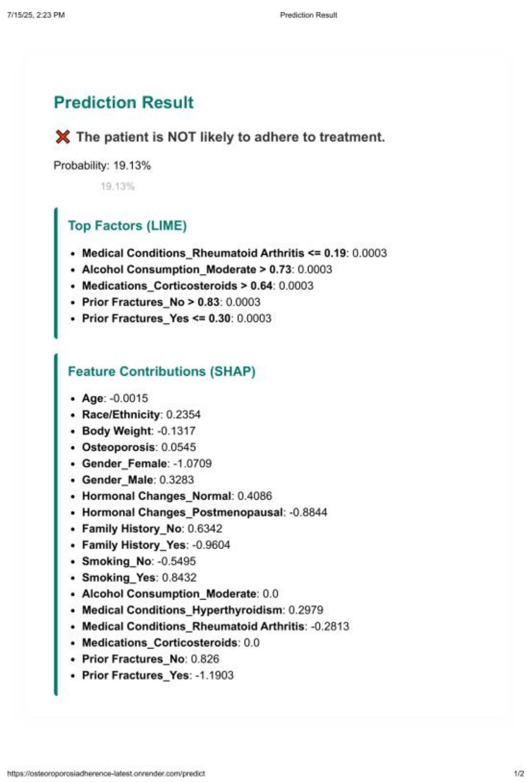
(a) Web-based input form for collecting patient demographic and clinical information for adherence prediction.



(b) Web interface showing predicted adherence result with probability and LIME/SHAP explanations.



(c) Web-based input form for collecting patient demographic and clinical information for adherence prediction.



(d) Web interface showing predicted non-adherence result with probability and LIME/SHAP explanations

Figure 4.8: Deployed web application showing patient input, prediction results, and interpretability for adherent and non-adherent scenarios.

4.3 Result discussion

The results indicated that the XGBoost model outperformed most other models across key metrics after hyperparameter tuning, achieving an accuracy of 68.3%, an F1-score of 66.3%, and an AUC-ROC of 73.4%, confirming its strong predictive capability in classifying therapeutic adherence.Compared to traditional models like Logistic Regression, which achieved higher recall (73.3%) but lower accuracy (62.0%) and AUC-ROC (66.7%), XGBoost offered a better balance between precision and recall, making it more reliable for real-world adherence prediction where both false positives and false negatives must be minimized. Tree-based models such as Decision Tree and Random Forest showed good performance, Random Forest with an accuracy of 67.4% and AUC-ROC of 72.1%), yet XGBoost provided a marginal improvement, demonstrating the value of boosting in reducing bias and variance. Ensemble methods like Stacking and Bagging also performed well, with Stacking matching XGBoost in accuracy but showing slightly lower AUC-ROC, indicating slightly less discrimination power between adherent and non-adherent cases. Deep learning models such as GRU and RNN showed reasonable F1-scores but lower overall accuracy and discrimination power compared to XGBoost, likely due to the dataset size and tabular nature of the features which favor tree-based models. These results demonstrate that XGBoost, with its robust gradient boost mechanism and compatibility with SHAP explanations, is well suited for the aim of this study: to provide accurate predictions while providing clear, interpretable insights into the factors at the patient level that influence the adherence to osteoporosis treatment. On the side of XAI, Table 4.5 explains that the SHAP graphs for logistic regression, decision tree, and XGBoost provide a global understanding of which patient factors contribute the most to the overall output of the model. The Permutation Feature Importance plots rank the most influential features by measuring prediction impact when each feature is permuted, showing the significance of lifestyle and medical factors. The LIME plots complement this by giving local explanations for individual predictions, showing how combinations of characteristics increase or reduce the probability of adherence for a specific patient. These interpretability results give clinicians and decision makers confidence in the model predictions by making the decision pathways transparent and clinically meaningful, supporting personalized intervention strategies to improve adherence to osteoporosis treatment.

4.3.1 User-facing Prediction Interface and Explainability

The final predictive model was deployed as a simple web application where users can input patient data such as age, race/ethnicity, body weight, osteoporosis status, gender, hormonal changes, family history, alcohol consumption and previous fractures. After submission, the app preprocesses and scales the data, then generates an adherence prediction with a probability score. To support interpretability, the interface presents local explanations using LIME, highlighting which factors influenced the specific prediction, and SHAP values to show the contribution of each feature. This ensures that users see not only the prediction but also understand the key factors behind it.

Chapter 5

Conclusion and future works

5.1 Conclusion

Conclusively, this study successfully developed an interpretable multi-strategy learning framework for predicting therapeutic adherence to osteoporosis treatment among chronic patients. Traditional, ensemble, and hybrid models were all evaluated, XGBoost emerged as the best-performing model, demonstrating high predictive accuracy and strong AUC-ROC, while providing compatibility with advanced explainable AI techniques. The integration of LIME, SHAP, and permutation feature importance enabled transparent interpretation of the key patient factors influencing adherence behaviors. The final model has been deployed as an accessible web-based tool for clinicians and researchers, with potential for integration into mobile applications to support patients with personalized adherence insights. These findings contribute toward actionable, explainable, and data-driven support for improving therapeutic outcomes in osteoporosis care.Medically, this study provides an interpretable AI framework for predicting osteoporosis treatment adherence. Key factors such as smoking, gender, age, prior fractures, hormonal changes, medical conditions, and family history were identified, enabling personalized adherence interventions. This framework supports clinicians in tailoring patient care and demonstrates a reproducible approach for applying explainable AI in chronic disease management.

5.2 Future Work

This research recommends expanding the dataset to include more diverse patient demographics and additional longitudinal adherence data. Incorporating real-time patient feedback and monitoring could further refine the model's predictive power and personalization. Exploring advanced interpretability methods and interactive XAI dashboards will strengthen end-user trust and practical adoption. Integrating the deployed system with electronic health records and patient management platforms can enhance its impact, supporting both clinicians and patients in making informed, personalized treatment decisions for better osteoporosis management.

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