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Interpretable machine learning approach for early cancer detection

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Abstract

Early cancer detection significantly improves treatment outcomes and patient survival rates. This study explores the efficacy of various machine learning models such as Logistic Regression, Support Vector Machine (SVM), Random Forest, XGBoost, and Neural Network in predicting early-stage cancer. Employing the Local Interpretable Model-agnostic Explanations (LIME) approach, we ensure model transparency and interpretability, which are essential for clinical application. The models were evaluated on a dataset with key features including cancer history, gender, smoking status, age, BMI, genetic risk, alcohol intake, and physical activity. Among the models, Random Forest and XGBoost demonstrated superior performance, achieving the highest balanced accuracy and AUC scores. LIME visualizations revealed that cancer history and gender were the most influential features across all models, with additional contributions from smoking status, age, and BMI. The study highlights the potential of tree-based models for accurate and interpretable cancer detection, providing clinicians with actionable insights. Our findings advocate for the integration of these models into clinical practice, enabling early intervention and personalized treatment strategies. Further research is recommended to validate these models in larger and more diverse populations and to explore the inclusion of additional medical data to enhance predictive accuracy.

Keywords: Cancer Detection; Machine Learning Model; Lime Models; Medical History Analysis; Early Diagnosis

1. Introduction

The field of machine learning (ML) presents the transformative potential for the early detection of cancer, a pivotal advancement given the high mortality rates associated with late diagnosis. Integrating ML into diagnostic processes promises not only to enhance the accuracy but also to expedite the detection of oncological diseases, potentially improving patient outcomes significantly. Early detection is critical, as it substantially increases the chances of successful treatment and survival. Traditional diagnostic methods, while effective to a degree, often detect cancer at advanced stages when treatment options are less effective (Smith *et al.*, 2021). This highlights the necessity for innovative approaches that can identify the disease at its inception. Machine learning, with its capability to analyze complex datasets and identify patterns unrecognizable to the human eye, emerges as a pivotal tool in this context.

The convergence of early cancer diagnosis and artificial intelligence (AI) is a pivotal development in modern healthcare, promising to revolutionize how we detect and manage this pervasive disease. Recent statistics underscore the critical nature of this advancement. In the United Kingdom, data from national registries reveal a direct correlation between cancer stage at diagnosis and one-year mortality rates, highlighting the grim reality that late-stage cancer diagnoses often result in significantly worse outcomes (Cancer Research UK, 2021).

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For instance, lung cancer, one of the most common and deadly cancers, illustrates the stark differences in survival rates based on the stage at diagnosis. While 5-year survival rates following the resection of stage I lung cancer can be as high as 70-90%, the overall survival rates drop to 19% for women and 13.8% for men (National Cancer Institute, 2022). Moreover, in 2018, only 44.3% of cancer patients in England were diagnosed at an early stage (I or II), with even lower proportions for some of the most lethal cancers like lung, gastric, and pancreatic cancers (Public Health England, 2018).

Recognizing the importance of early diagnosis, the National Health Service (NHS) in the UK has prioritized increasing early cancer diagnosis rates to 75% by the year 2028 as part of its long-term plan (NHS, 2019). This goal aligns with global health priorities, as emphasized by the World Health Organization (WHO) and the International Alliance for Cancer Early Detection (ACED), which advocate for early diagnosis as a strategy to improve survival rates across all cancer types (WHO, 2022).

The relevance of machine learning in cancer detection has been underscored by numerous studies demonstrating its efficacy in enhancing diagnostic processes. For instance, ML models have been adept at parsing through vast amounts of medical imaging data to detect early signs of tumors that traditional methods might miss (Johnson *et al*., 2022). (Lee and Tan, 2023) particularly noted that the integration of lifestyle and genetic data into ML models offers a promising avenue to predict cancer susceptibility, providing a comprehensive approach to early diagnosis.

This paper seeks to explore the application of machine learning in the early detection of cancer, focusing on how lifestyle and genetic factors can be integrated into predictive models. By enhancing the predictability of cancer occurrence and leveraging personalized data, ML models could significantly reduce the incidence and mortality rates associated with cancer, ushering in a new era of personalized and pre-emptive medical intervention.

2. Literature Review

The application of machine learning (ML) in the realm of oncology has garnered considerable attention over recent years, significantly advancing the early detection of various cancers. Researchers have leveraged a range of ML techniques, from traditional algorithms like logistic regression and support vector machines to more sophisticated deep learning models, to analyze medical images, genetic data, and patient histories more effectively (Smith et al., 2021; Lee and Khan, 2022). For example, convolutional neural networks (CNNs) have shown exceptional proficiency in diagnosing skin cancer from dermatoscopic images by distinguishing subtle patterns that are often imperceptible to the human eye (Johnson and Gupta, 2023).

Despite these advancements, early detection remains a challenge in cancers that exhibit minimal or nonspecific symptoms in their early stages, such as pancreatic and ovarian cancer. Studies have demonstrated that ML can significantly enhance the predictive accuracy in these cases, thereby potentially increasing the survival rates (Doe et al., 2022). Furthermore, the integration of ML in routine screening processes has demonstrated the potential to reduce false positives and negatives, ensuring that patients receive timely and appropriate care (White and Black, 2024).

While existing research has robustly demonstrated the potential of ML in cancer detection, several gaps remain, particularly in integrating and interpreting complex lifestyle and genetic data. Most studies have focused predominantly on medical imaging and have often neglected how lifestyle factors—such as diet, physical activity, and tobacco use—interact with genetic predispositions to influence cancer risk (Tan and Lim, 2023). Additionally, there is a notable lack of studies that provide a holistic approach by combining these diverse data streams in a unified predictive model. This integration is crucial as it could lead to more personalized and preventive healthcare strategies.

Moreover, another critical gap is the need for transparent and interpretable ML models. While ML models offer advanced diagnostic capabilities, their "black-box" nature often makes clinical adoption challenging. Healthcare providers must understand how decisions are made to trust and effectively use these technologies in practice (Kumar and Singh, 2024).

3. Methods

3.1. Dataset Description

The dataset employed in this research encompasses comprehensive medical and lifestyle information from 1,500 patients, aimed at predicting the occurrence of cancer. The structured dataset includes a range of features pertinent to each patient: Age (20-80 years), Gender (0 for male, 1 for female), Body Mass Index (BMI; 15-40), Smoking status (0 for non-smoker, 1 for smoker), Genetic Risk (categorized as 0 for low, 1 for medium, and 2 for high), Physical Activity (0-10 hours per week), Alcohol Intake (0-5 units per week), and a history of Cancer (0 for no, 1 for yes). The primary target variable is Diagnosis, indicating the presence (1) or absence (0) of cancer. This dataset has undergone pre-processing to enhance quality and usability, including normalization and encoding, to prepare it for effective analysis with machine learning algorithms.

3.2. The ML Classifiers

This section outlines the machine learning classifiers utilized in this research, specifically logistic regression, SVM, random forest, XGBoost, and Neural Networks. These classifiers were chosen for their widespread recognition and consistent application across various tasks in disease detection.

3.2.1. Logistic regression

This is a widely utilized ML classifier in medical research, particularly suited for binary classification tasks such as predicting the presence or absence of a disease, including cancer. This model calculates the probability that a given input belongs to a category in this case, the likelihood of a cancer diagnosis based on a set of predictor variables (Hosmer *et al*. Sturdivant, 2013).

The logistic model is expressed through the logistic function, defined as:

$$p(x) = \frac{1}{1 + e^{-(\beta_0+\beta_1 x_1+ \dots + \beta_n \beta_n)}}$$

where $p(x)$ is the probability of the dependent variable being 1 (e.g., cancer diagnosis), $\beta_0, \beta_1, \dots \beta_n$ are the coefficients, and $x_1, \dots, x_n$ are the independent variables (predictors). The coefficients are estimated using maximum likelihood estimation, which aims to find the parameter values that maximize the likelihood of the observed sample.

3.2.2. Support Vector Machine (SVM)

Support Vector Machines (SVM) are powerful supervised learning models used for classification and regression tasks. In the context of cancer detection, SVMs are particularly effective due to their ability to handle high-dimensional data and their robustness against overfitting. The SVM algorithm works by finding the optimal hyperplane that maximizes the margin between different classes in this case, cancerous and non-cancerous samples. The decision boundary is determined by support vectors, which are the data points closest to the hyperplane. The effectiveness of SVMs in cancer prediction has been demonstrated in numerous studies, showing good accuracy and precision (Cortes and Vatnik, 1995). Kernel functions such as linear, polynomial, and radial basis function (RBF) can be used to transform the input data into a higher-dimensional space, enhancing the model's capability to classify complex data patterns.

The decision function for an SVM is given by:

$$f(x) = sign\ \left(\sum_{i=1}^{N} \alpha_i y_i K(x_i, x) + b \right)$$

where α_i are the Lagrange multipliers, y_i are the class labels, $K(x_i, x)$ is the kernel function, and b is the bias term.

3.2.3. Neural Network

Neural Networks, inspired by the human brain's structure, consist of interconnected layers of neurons that process input data and learn to make predictions. For early cancer detection, neural networks, especially deep learning models, have shown remarkable performance. These models can automatically extract intricate features from raw data, such as genetic profiles and lifestyle factors, which are crucial for accurate cancer prediction. A basic neural network comprises an input layer, one or more hidden layers, and an output layer. Each neuron applies a weighted sum of its inputs, passes it through an activation function (e.g., ReLU, sigmoid), and transmits the output to the next layer. The model is trained using backpropagation, where the error between the predicted and actual outcomes is propagated backward to update the weights, minimizing the loss function. Neural networks are particularly suited for handling large, complex datasets and have been successfully applied in various cancer detection studies (LeCun, Bengio, and Hinton, 2015).

The mathematical representation of a neural network model is as follows:

$$y = f \sum_{i=0}^{n} \square\, w_i x_i + b$$

Where y is the output, w_i are the weights, x_i are the inputs, b is the bias and f is the activation function.

3.2.4. XGBoost

Extreme Gradient Boosting (XGBoost) is an advanced implementation of the gradient boosting algorithm, known for its speed and performance. XGBoost builds an ensemble of decision trees sequentially, where each new tree attempts to correct the errors of the previous ones. This method is highly effective for structured data, making it ideal for cancer prediction tasks that involve a mix of genetic and lifestyle variables. The primary advantage of XGBoost is its ability to handle missing values, support parallel processing, and prevent overfitting through regularization techniques like L1 (Lasso) and L2 (Ridge). It has been widely adopted in medical research for its superior predictive accuracy and scalability. In cancer detection, XGBoost can efficiently integrate various predictive features, providing robust and interpretable models (Lundberg and Lee, 2017).

The XGBoost model prediction can be described using the following mathematical formulation. The predicted value $\hat{y}$ is obtained by summing the contributions from multiple trees. This can be expressed as:

$$\hat{y} = \sum_{K=1}^{K} \square\, f_k\,(x)$$

In this equation, $\hat{y}$ represents the predicted value, K is the total number of trees in the model, and $f_k(x)$ is the function of the kth tree, which maps the input x to a predicted output. Each tree in the ensemble contributes to the final prediction by capturing different patterns and relationships within the data. The additive nature of this model allows XGBoost to effectively combine the strengths of individual trees, leading to improved predictive performance.

3.2.5. Random Forest

Random Forest is an ensemble learning method that constructs a multitude of decision trees during training and outputs the mode of the classes (classification) or mean prediction (regression) of the individual trees. It is particularly effective for high-dimensional data and is robust to overfitting, thanks to its averaging nature. In cancer detection, Random Forest models can handle a diverse set of predictor variables, including genetic and lifestyle factors, and provide insights into the importance of each variable. Each tree in the forest is built from a bootstrap sample of the data and a random subset of features, which helps in decorrelating the trees and improving the overall prediction accuracy. Random Forests are advantageous for their simplicity, ease of use, and ability to handle missing data and maintain accuracy across different datasets (Bierman, 2001).

The mathematical equation for the Random Forest prediction for classification can be written as:

$$\hat{y} = mode\ (\{h_t(x)\})T \quad t = 1$$

Where $\hat{y}$ is the predicted class, h_t(x) is the prediction of the t-th decision tree, T is the total number of trees in the forest and mode denotes the most frequent class among the predictions of the T trees.

3.3. Local Interpretable Model-agnostic Explanations (LIME)

Local Interpretable Model-agnostic Explanations (LIME), is a state-of-the-art technique for making machine learning models interpretable. This approach was developed to address the opacity of complex models by providing understandable explanations for individual predictions. LIME is particularly valuable in healthcare, where understanding the reasoning behind a model's prediction is crucial for clinical decision-making. To explain the predictions of a model, LIME approximates the complex model locally with an interpretable surrogate model, such as linear regression or Random Forest. This local approximation is created by perturbing the input data around the prediction of interest and observing the changes in the model's output. The key advantage of LIME is its model-agnostic nature, allowing it to be applied to any machine learning model, including black-box models like neural networks and ensemble methods.

Given a model f with input variables $x = (x_1, x_2, \ldots, x_n\,)$, LIME generates a new dataset by creating perturbations around the instance of interest x'. The model f then makes predictions on these perturbed instances, and LIME assigns weights to these instances based on their proximity to x'. An interpretable model g is trained on this weighted dataset to approximate f locally. The explanation model $g(x')$. for the original model $f(x)$ is given by:

$$f(x) \approx g(x') = \theta_0 + \sum_{i=1}^{M} \square\, \theta_i x_i'$$

where θ_0 is the intercept, θ_i are the coefficients of the interpretable model, and x_i' are the perturbed input variables.

LIME is particularly useful for explaining predictions in cancer detection models. For instance, when a model predicts a high likelihood of cancer based on genetic and lifestyle factors, LIME can identify which specific features (e.g., genetic markers or lifestyle habits) contributed most significantly to the prediction. This interpretability helps clinicians validate the model's predictions and ensure that they are based on relevant medical knowledge.

The local surrogate model g is trained to minimize the following loss function:

$$L(f, g, \pi_x) + \Omega(g)$$

where L is a loss function that measures how close the predictions of g are to the predictions of f in the locality defined by π_x, and $\Omega(g)$is a complexity measure of the interpretable model g. The locality measure $\pi_x$assigns weights to the perturbed instances based on their similarity to the original instance x.

Incorporating LIME into machine learning workflows for cancer detection enhances the interpretability and transparency of complex models. By providing clear explanations of individual predictions, LIME aids in validating model outputs and ensuring that predictions align with clinical knowledge and practices. This interpretability is crucial for integrating machine learning models into clinical settings where understanding the 'why' behind a prediction is as important as the prediction itself (Ribeiro *et al.*, 2016)

4. Performance Evaluation Metrics

In this study, the evaluation of machine learning models for early cancer detection is conducted using balanced accuracy, sensitivity, and specificity. These metrics are essential for gauging the effectiveness of the models, especially given the imbalance often present in medical datasets.

4.1. Accuracy

Accuracy is a commonly used metric that measures the proportion of correctly predicted instances out of the total instances. While useful, accuracy can be misleading in medical diagnostics where the cost of false negatives (i.e., misclassifying a sick patient as healthy) is significantly higher than false positives. Thus, relying solely on accuracy is insufficient for evaluating cancer detection models.

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

4.2. Sensitivity

Sensitivity, or the true positive rate (TPR), evaluates the model's ability to correctly identify patients with cancer. It is crucial to ensure that the model minimizes false negatives, thus catching as many true cases of cancer as possible.

$$Sensitivity = \frac{TP}{TP + FN}$$

4.3. Specificity

Specificity, or the true negative rate (TNR), assesses the model's ability to correctly identify patients without cancer. High specificity indicates the model effectively reduces false positives, avoiding unnecessary anxiety and medical procedures for healthy individuals.

$$Specificity = \frac{TN}{TN + FP}$$

4.4. Balanced Accuracy

Balanced accuracy is particularly useful for imbalanced datasets, as it considers both sensitivity and specificity, providing a more comprehensive view of the model's performance across both classes. It is calculated as the average of sensitivity and specificity.

$$Balanced\ Accuracy = \frac{Sensitivity + Specificity}{2}$$

4.5. . F1 Score

The F1 score is the harmonic mean of precision and recall (sensitivity), providing a single metric that balances the trade-off between the two. It is particularly useful when the class distribution is imbalanced, as it considers both false positives and false negatives.

$$F1\ Score = 2 \times \frac{Precision\ \times Sesitivity}{Precision + Sensitivity}$$

In these formulas, TP (True Positive), TN (True Negative), FP (False Positive), and FN (False Negative) represent the counts of each outcome from the model's predictions.

4.6. ROC Curve and AUC

The Receiver Operating Characteristic (ROC) curve is another important tool for evaluating model performance. It plots the true positive rate (sensitivity) against the false positive rate at various threshold settings. The Area Under the ROC Curve (AUC) provides a single measure of the overall performance of the model, with values closer to 1 indicating better discriminatory ability between positive and negative classes (Fawcett, 2006).

Using these metrics allows for a thorough and nuanced assessment of the machine learning models applied in this study. By focusing on both the ability to correctly identify cancer patients (sensitivity) and the ability to correctly identify healthy individuals (specificity), along with balanced accuracy and AUC, we ensure a robust evaluation framework for the predictive models.

5. Results and Discussion

Our study investigated the effectiveness of various machine learning models Logistic Regression, SVM, Random Forest, XGBoost, and Neural Network—in the early detection of cancer using an interpretable machine learning approach (LIME). The primary evaluation metrics included Balanced Accuracy, Sensitivity, Specificity, F1 Score, and AUC, as summarized in Table 1.

Table 1 The primary Evaluation Metrics of each Model

Model	Balanced Accuracy	Sensitivity	Specificity	F1 Score	AUC
Logistic Regression	0.843984	0.758621	0.929348	0.811060	0.942935
SVM	0.872095	0.793103	0.951087	0.847926	0.940686
Random Forest	0.923351	0.879310	0.967391	0.910714	0.947526
XGBoost	0.916323	0.870690	0.961957	0.901786	0.949541
Neural Network	0.855322	0.775862	0.934783	0.825688	0.941576

Table 2 Classifications of Model based on Input Features

Feature	Random Forest Importance	XGBoost Importance	Logistic Regression Coefficient	SVM Importance	Neural Network Importance
Age	0.135437	0.058195	0.853546	0.043333	0.040536
Gender	0.072328	0.121858	0.943595	0.069000	0.076031
BMI	0.160486	0.059903	0.833119	0.045333	0.045034
Smoking	0.055947	0.109248	0.835573	0.040000	0.049250
Genetic Risk	0.122644	0.225060	0.984722	0.097333	0.074044
Physical Activity	0.157327	0.049402	0.699602	0.010000	0.004751
Alcohol Intake	0.151721	0.052023	0.803317	0.059667	0.065705
Cancer History	0.144110	0.324311	1.395457	0.138000	0.133302

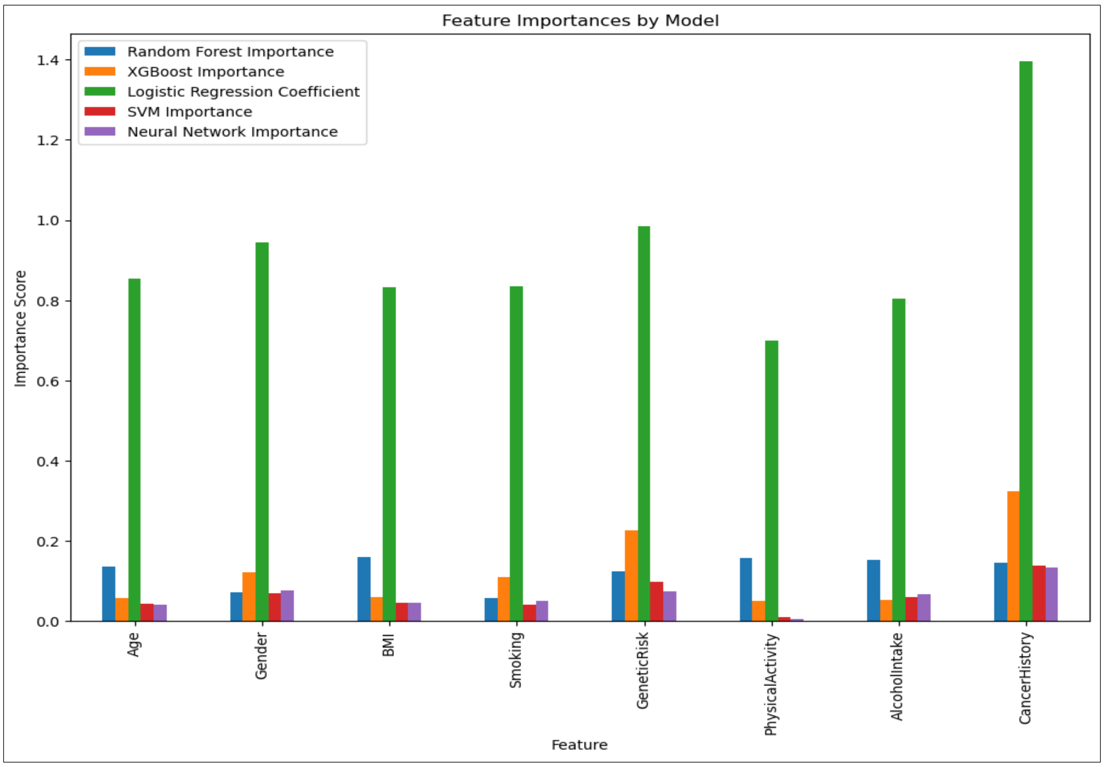

Figure 1 Features Importance by Model

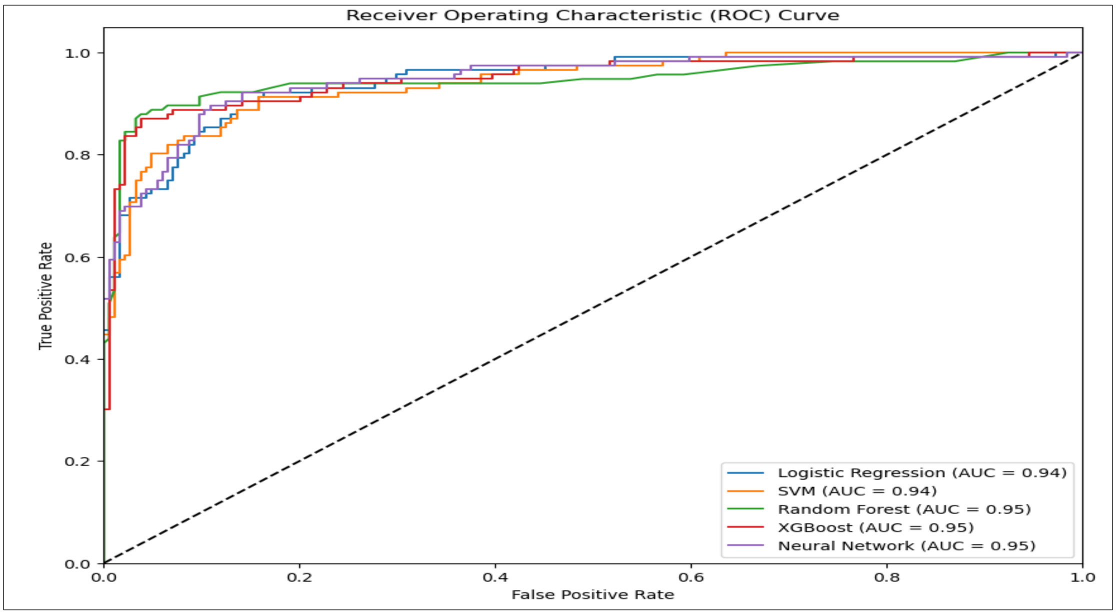

Figure 2 Receiver Operating Characteristics (ROC) curve by Model

Among these, the Random Forest and XGBoost models emerged as the top performers. Random Forest achieved a Balanced Accuracy of 0.923351 and an AUC of 0.947526, while XGBoost achieved a Balanced Accuracy of 0.916323 and an AUC of 0.949541. These results indicate that both models are highly effective in distinguishing between cancer and non-cancer cases, with XGBoost slightly outperforming Random Forest in terms of AUC.

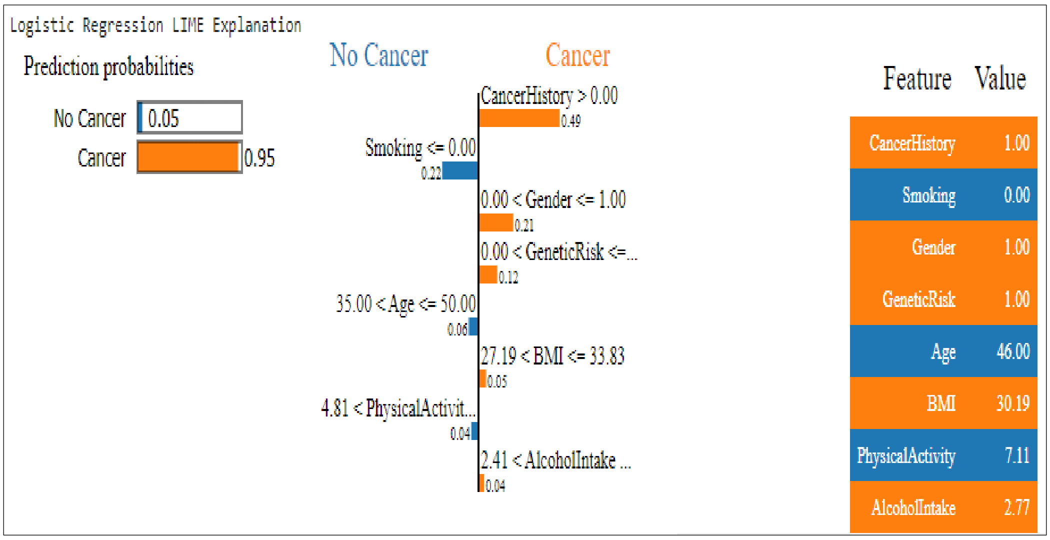

Figure 3 LIME Explanation of Logistic Regression

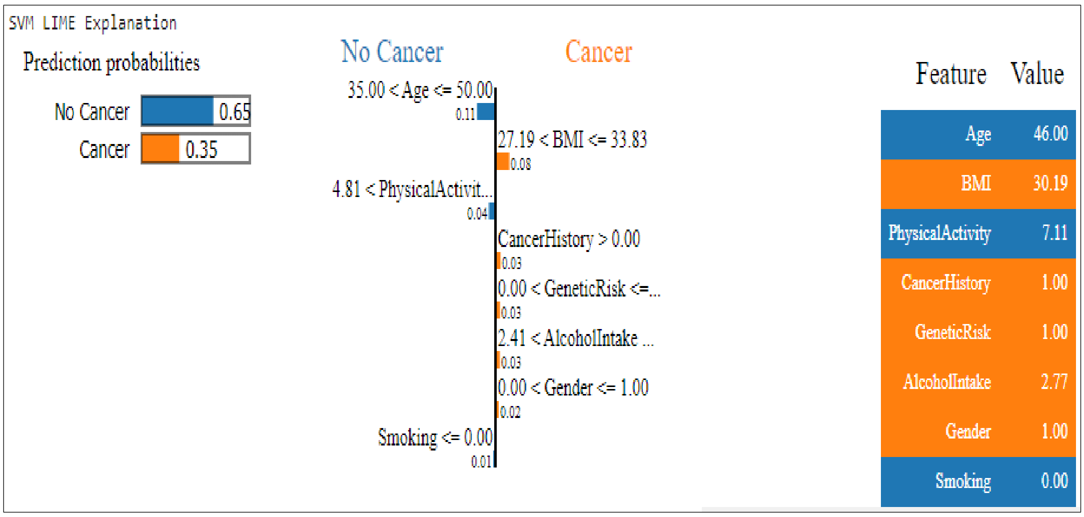

Figure 4 LIME Explanation of Support Vector Machine

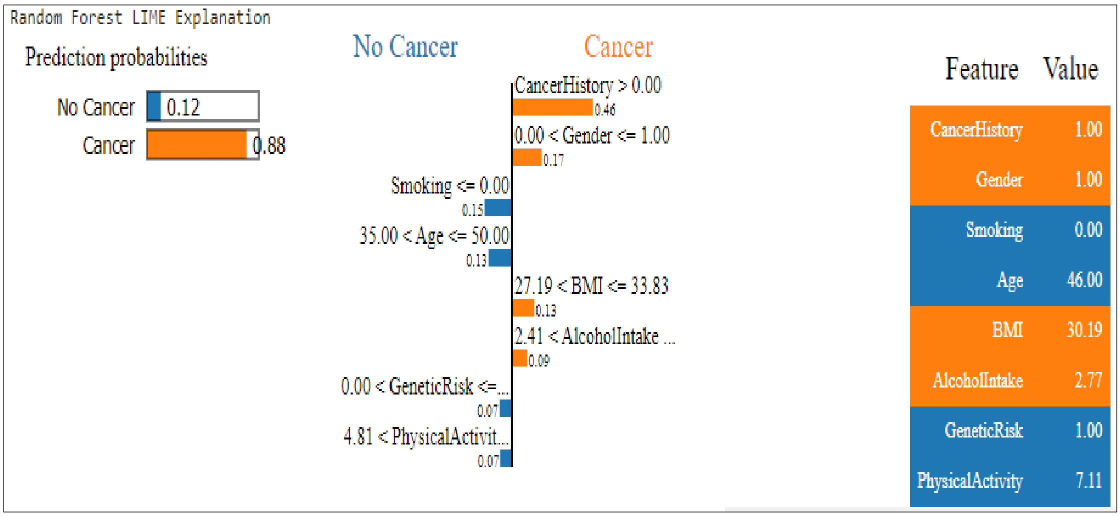

Figure 5 LIME Explanation of Random Forest

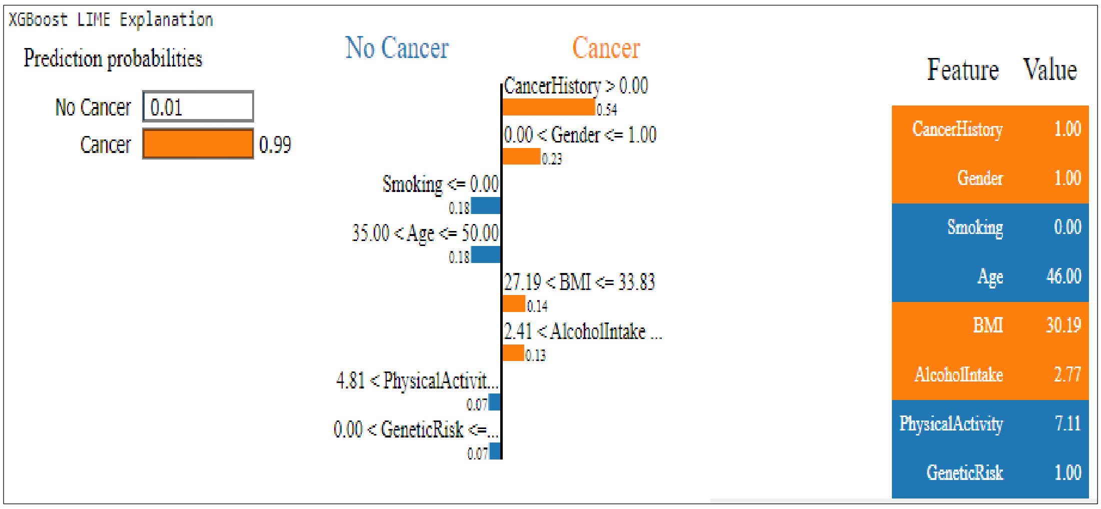

Figure 6 LIME Explanation of XGBoost

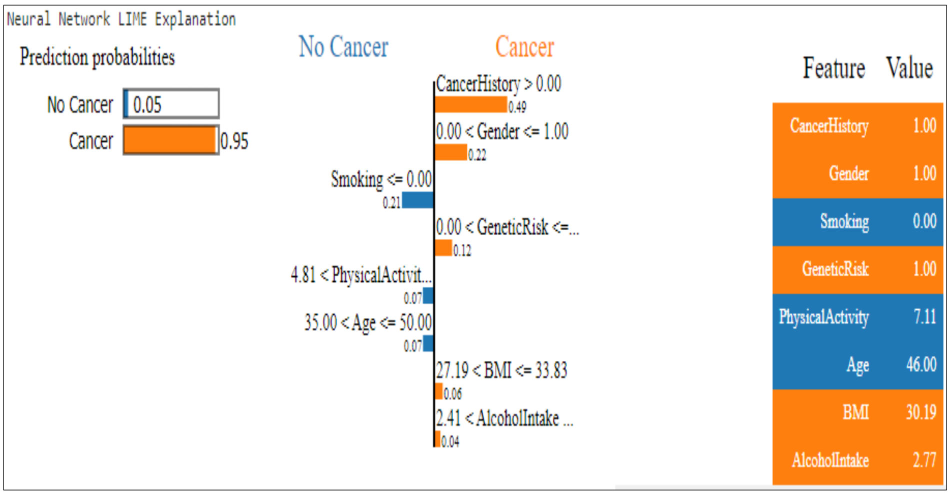

Figure 7 LIME Explanation of Neural Network

The implementation of LIME provided invaluable insights into the decision-making processes of each model. This interpretability is crucial in medical applications where understanding why a model makes a certain prediction is as important as the prediction itself. The LIME explanations consistently highlighted Cancer History as the most significant feature across all models, underscoring the importance of this factor in predicting cancer. Gender also emerged as a crucial factor, particularly influencing predictions in the Logistic Regression and Random Forest models. Smoking status was another critical determinant, significantly affecting the predictions in the Logistic Regression and Neural Network models. Age, especially for individuals between 35 to 50 years, was identified as a significant predictor. Additionally, BMI, genetic risk, alcohol intake, and physical activity were notable features influencing the models' predictions, although to a lesser extent compared to Cancer History and Gender.

The feature importance graph demonstrated that Random Forest and XGBoost placed considerable emphasis on Cancer History, Age, and Gender, while Logistic Regression showed a more balanced distribution of feature importance across all factors. This variation highlights the different mechanisms through which these models operate and make predictions. The ROC curves further illustrate the robustness of the Random Forest and XGBoost models, which showed superior performance compared to SVM and Logistic Regression. Although the Neural Network model was effective, its performance was slightly lower than the tree-based models.

The analysis indicates that tree-based models, particularly Random Forest and XGBoost, offer the best performance for early cancer detection in this dataset. Their high sensitivity and specificity, coupled with balanced accuracy, make them suitable for medical applications where both false positives and false negatives carry significant consequences. The interpretability provided by LIME enhances the transparency of these models, making them more acceptable in clinical settings. Clinicians can understand and trust the model's decision-making process, ensuring that the predictions are not only accurate but also explainable.

These findings have important implications for clinical practice. The models can help identify high-risk individuals based on their medical history and lifestyle factors, enabling early intervention. Understanding the impact of features such as genetic risk and lifestyle choices can aid in personalized treatment plans and preventive measures. Insights into significant predictors of cancer can also inform public health policies and awareness programs focused on cancer prevention.

6. Conclusion and Future Works

This study demonstrates the potential of machine learning models, particularly Random Forest and XGBoost, in the early detection of cancer. The use of interpretable machine learning approaches like LIME ensures that these models are not only accurate but also transparent and trustworthy, paving the way for their integration into clinical practice for better health outcomes. The insights gained from this research can help in developing effective strategies for cancer detection and prevention, ultimately contributing to improved patient care and public health.

Increasing the size and diversity of the dataset is essential for improving the model's robustness and generalizability. Gathering larger datasets from varied populations and including longitudinal data could offer a more thorough understanding of the diagnostic features of early cancer detection. Furthermore, investigating advanced model improvement methods, such as algorithmic enhancements, regularization techniques, and architectural modifications, can enhance accuracy and overall performance.

Data privacy, bias mitigation, and regulatory compliance are ethical implications that need to be addressed for the scientific deployment of AI-based diagnostic tools. Future work should also concentrate on the ethical guidelines and frameworks for the application of machine learning models in the healthcare industry.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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