Special Issue – AI-Driven and Multimodal Innovations in Biomedical Imaging and Sensing

An Optimized Predictive Machine Learning Model for Lung Cancer Diagnosis

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https://dx.doi.org/10.13005/bpj/3075

(Received: 30 November 2024; accepted: 06 February 2025)

Lung cancer is one of the leading causes of death worldwide. Increasing patient survival rates requires early detection. Traditional methods of diagnosis often result in late-stage detection, necessitating the development of more advanced and accurate predictive models. This paper has proposed a methodology for lung cancer prediction using machine learning models. Synthetic minority over-sampling technique (SMOTE) is used before classification to resolve the problem of class imbalance. Bayesian optimization is used to enhance model's performance. Performance of three classifiers adaptive boosting (AdaBoost), random forest (RF), and extreme gradient boosting (XGBoost) is evaluated both with and without hyperparameter optimization. Optimized models of RF, AdaBoost and XGBoost achieved accuracies of 96.11%, 95.74% and 95.92% respectively. Results demonstrate the effectiveness of combining machine learning classifiers, SMOTE, and hyperparameter tuning in improving prediction accuracy.

Keywords: AdaBoost, Lung Cancer, Machine Learning, Random Forest, XGBoost.

Lung cancer causes a significant portion of cancer-related fatalities. It causes more deaths than the total deaths from breast, colon, and cervical cancers. Cancer arises when cells in the body begin to proliferate uncontrollably. Lung cancer usually develops gradually and predominantly affects those aged 55 to 65. Lung cancer can be non-small cell (NSCLC) or small cell (SCLC) lung cancer. Eighty to eighty five percent of cases of lung cancer are of NSCLC. Ten to fifteen percent of cases are of SCLC. NSCLC is more commonly developed by smokers or ex-smokers. In cigarette smokers, there is a high chance of developing SCLC.¹

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The most typical sign of lung cancer is coughing, which can worsen with time, become more severe, and can even produce bloody sputum. Additional symptoms include haemoptysis, anorexia, weight loss, chest pain, and shortness of breath. Improving patient outcomes requires detection of lung cancer at early stage.² Traditional methods of diagnosis can lead to diagnosis at late stage. Early-stage diagnosis can help in providing better treatment to patients. The diverse and complex characteristics of lung cancer make it challenging to identify early indicators using conventional clinical approaches.^{3,4}

In recent decades, advent of machine learning has brought revolution in numerous fields by offering different tools for analysing patterns in large datasets. It has a big impact on the medical field as well.⁵

Authors evaluated three machine learning algorithms RF, AdaBoost, and XGBoost regarding their performance in lung cancer prediction. This paper introduced a novel approach for lung cancer detection by combining SMOTE for class imbalance handling and Bayesian optimization for hyperparameter tuning, ensuring enhanced accuracy for lung cancer detection. The aim of this research is to improve early-stage diagnosis of lung cancer by harnessing machine learning techniques. **The objectives of this research are as follows**

1. To perform comparative analysis of performance of three classifiers RF, AdaBoost, and XGBoost in lung cancer prediction. This research sheds light on the classifiers' initial performance as well as areas for improvement by assessing them both with and without optimization.

2. To address the problem of imbalanced datasets using SMOTE. Class imbalance is a common problem in datasets involving medical diagnosis. By training the models on balanced dataset, this phase helps to minimize bias and improves the models' capacity to generalize across various patient populations.

3. To fine-tune the hyperparameters of the RF, AdaBoost, and XGBoost using bayesian optimization.

Section 2 of literature survey reviews existing research to establish the relevance of the study. Section 3 methodology describes proposed methodology. Section 4 presents the key findings. Section 5 discusses the results. After that paper is concluded in Section 6 by summarizing key insights and discussing future scope.

Literature Review

In recent decades, extensive research has been conducted on using various machine learning techniques for predicting lung cancer. Various classifiers have been used by researchers to improve diagnostic accuracy. Numerous studies have analysed how different models perform on various datasets. This literature survey highlights the key findings from recent research efforts.

Radhika evaluated the performance of four traditional classifiers, including SVM, NB, LR, and DT. The study utilized datasets from the UCI Repository and found that SVM attained the highest accuracy of 99.2%, outperforming other classifiers. It highlighted the potential of SVM in handling complex data typical in medical imaging.⁶ Patra performed lung cancer classification using the dataset available on Kaggle. Weka tool was used to perform experiments with different classifiers. Experiments were done with KNN, NB, RF and J48 classifiers. KNN achieved 75% accuracy, NB achieved 78.12% accuracy, RBF achieved 81.25% accuracy, and J48 achieved 78.12% accuracy.7 Dritsas evaluated the performance of various classifiers, including artificial neural network (ANN), support vector machine (SVM), K-nearest neighbour (KNN), decision tree (DT), naive bayes (NB), and Rotation Forest, achieving accuracies of 94.6%, 95.4%, 95.2%, 93.7%, 95%, and 97.1%, respectively. Rotation Forest demonstrated the highest accuracy at 97.1%.8

Mamun performed lung cancer prediction using the dataset available on kaggle. Dataset was balanced using SMOTE. Experiments were done using XGBoost, AdaBoost, LightGBM and Bagging attaining accuracies of 94.42%, 90.70%, 92.55, and 89.76% respectively.⁹ Sachdeva performed lung cancer prediction using the dataset of 59 records available on kaggle. Performance of DT, KNN, RF, Adaboost, SVM, LR, NB and Xgboost was evaluated. NB outperformed other classifiers with 98.33% accuracy.¹⁰

Ojha performed lung cancer prediction using SVM, NB, AdaBoost, KNN, logistic regression (LR), and J48, yielding accuracies of 92.6%, 91.6%, 90.5%, 90.5%, 94.7%, and 90.5%, respectively, with LR outperforming the other models.¹¹ Riktapresented XML-GBM model, which combined gradient boosting with explainable AI to enhance lung cancer diagnosis. Random Oversampling method was used for class balancing. Training used 65% of data and testing used 35%. Principal component analysis and hypertuning were also used to improve the accuracy. GBM obtained accuracy of 98.76%.¹²

Maurya evaluated the performance of twelve classifier including LR, Bernoulli NB, Gaussian NB, RF, SVM, XGBoost, KNN, AdaBoost, Extra Tree, Ensemble of XGB and AdaBoost, Voting Classifier and multilayer perceptron (MLP). KNN achieved maximum accuracy of 92.86%.¹³ Prakasha focused on feature extraction techniques like Gray-Level Co-occurrence Matrix (GLCM) and Principal Component Analysis (PCA) to enhance performance of classifiers. After comparing performance of NB, DT, and SVM for lung cancer classification it was found that SVM, when combined with GLCM features, achieved the highest accuracy of 96.1%. It demonstrated the importance of integrating effective feature extraction techniques with machine learning models for improved classification accuracy.14

In reviewing the existing literature, several demerits have been identified. Some studies faced challenges with class imbalance leading to biased predictions. Additionally, limited emphasis on hyperparameter optimization in models can prevent achieving optimal performance. Many studies also rely on very small datasets such as 59 records dataset of kaggle which may not generalize well. To address these gaps, the proposed work incorporated SMOTE to handle class imbalance and applied bayesian optimization for hyperparameter tuning. Authors evaluated classifiers on a larger, balanced dataset and provided a comparison of RF, AdaBoost, and XGBoost classifiers. The proposed work integrated class balancing with optimization techniques ensuring improved model performance.

MATERIALS AND METHODS

Proposed methodology for lung cancer prediction is presented in Figure 1. The methodology includes following steps: data acquisition, class balancing, model implementation, hyper parameter optimization, and model evaluation.

Dataset

The dataset used in this research is acquired from Kaggle.¹⁵ It has a total of 15 predictive attributes: Age, Gender, Smoking, PeerPressure, Anxiety, Yellow Fingers, Allergy, Fatigue, Chronic Disease, Coughing, Alcohol Consuming, Wheezing, Chest Pain, Swallowing Difficulty and Shortness of Breath. Comprehensive details about the dataset are shown in Table 1. Figure 2 illustrates a two-sided bar chart displaying the distribution of features for patients with Lung Cancer and without Lung Cancer.

Dataset Link	https://www.kaggle.com/datasets/shuvojitdas/lung-cancer-dataset
Number of Records	309
Attribute Name	Description
Age	Age of the individual
Gender	Gender of the individual (e.g., Male/Female)
Smoking	Whether the individual smokes
PeerPressure	Influence of peer pressure
Anxiety	Presence of anxiety
Yellow Fingers	Observed yellow fingers (potentially due to smoking)
Allergy	Any allergies reported
Fatigue	Feeling of fatigue
Chronic Disease	Presence of any chronic disease
Coughing	Frequency or severity of coughing
Alcohol Consuming	Alcohol consumption habits
Wheezing	Presence of wheezing sounds
Chest Pain	Reported chest pain
Swallowing Difficulty	Difficulty in swallowing
Shortness of Breath	Experience of breathlessness

Table 1. Comprehensive details about the dataset



Fig. 1. Methodology for Lung Cancer Prediction

Correlation of each predictive feature with target feature is shown in Figure 3. It helps in finding the most relevant features and improving model performance by focusing on impactful variables. It also helps domain experts to better understand which factors influence the target outcome that increase model interpretability. Initially, the dataset was imbalanced. It comprised 309 instances, with 39 instances of Class 0 (non-cancerous) and 270 instances of Class 1 (cancerous). After balancing both the classes have 270 instances. Number of instances before balancing and after balancing is shown in Figure 4.

Class Balancing

To resolve the class imbalance problem, SMOTE was used. SMOTE generates artficial samples in minority class by performing interpolation between existing instances.¹⁶ It works by identifying the k-nearest neighbours of each minority class instance, then creating new samples by interpolating between the original instance and its neighbours. This process generates diverse, synthetic data points that balance the dataset. It resulted in balanced dataset with equal number of 270 instances for both classes.



Fig. 2. Two-Sided Bar Chart Showing Feature Distributions for Lung Cancer and No Lung Cancer



Fig. 3. Correlation of predictive feature with target feature



Fig. 4. (a) Class distribution before balancing (b) Class distribution after balancing

Table 2. Performance metrics of classification algorithms before hyperparameter tuning	ROC- AUC (%)	1.89 97.8 0.09		ROC- AUC (%)	0.66	98.8	98.8
	.0g s (%)	75 76 3.33		Log Loss (%)	15.73	13.70	45.60
	L Los	61 18 18		Cohen's Kappa (%)	92.22	91.85	91.48
	Cohen's Kappa (%	91.11 89.62 89.25		MCC (%)	92.22	91.85	91.48
	MCC (%)	91.12 89.65 89.25	l optimization	F-Measure (%)	96.11	95.91	95.73
	easure %)	5.58 4.87 4.63	ained through	Specificity (%)	95.92	96.29	95.92
	, F-M (36 7 7 7 7 7	eters obta	Recall (%)	96.97	95.55	95.99
	Specificity (%)	94.81 93.70 94.44	Hyperparam	Precision (%)	95.94	96.26	95.91
	Recall (%)	96.92 95.91 94.81	 Values of 	Accuracy (%)	96.11	95.92	95.74
	scision (%)	4.89 3.84 4.46	Table	Value	gini True 1 10 10	0.59 1 1	0.68 10
	Accuracy Pre (%) (95.55 9 94.81 9 94.62 9		Hyperparameter	criterion bootstrap max_features random_state min_samples_leaf n_estimators max_denth	learning_rate max_depth oanma	learning_rate n_estimators
	Classification Algorithm	RF AdaBoost XGBoost		Classifier	RF	XGB	AdaBoost

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Classification Algorithms

Three machine learning classifiers named RF, XGBoost and AdaBoost are applied to the balanced dataset. Random Forest is an ensemble learning algorithm in which multiple decision trees are constructed and merged to produce a more robust prediction. It operates by selecting random subsets of the features and data points to construct each tree, which reduces overfitting and improves generalizability of the model. AdaBoost is a boosting ensemble method that combines multiple weak learners to create a strong model.

It works by adjusting the weights of incorrectly predicted samples, placing more



Fig. 5. Enhancement in Accuracy after Optimization



Fig. 6. Enhancement in Precision after Optimization

emphasis on these points in subsequent iterations. Multiple models are trained and each new model tries to correct the errors made by the previous model. In XGBoost, ensemble of decision trees is constructed. Each next tree corrects the errors of the previous tree.

Optimization of Classifiers

The performance of the classifiers is further enhanced through hyperparameter optimization. Bayesian optimization method is utilized for optimization. This method helped in finding the optimal hyperparameters for each classifier, improving their performance.¹⁷ Bayesian optimization is computationally intensive and may not find the global optimum due to suboptimal configuration. To address this challenge, optimization settings are carefully tuned such as the choice of acquisition function and number of iterations.







Fig. 8. Enhancement in Specificity after Optimization

Model Evaluation

The classifiers' performance is evaluated based on standard metrics accuracy, precision, recall, specificity and F1-Measure, MCC (Matthews Correlation Coefficient), Cohen's Kappa, Log-Loss and receiver operating characteristics (ROC) curve.^{18,19} Validation is done using k fold crossvalidation method. It involves splitting the dataset into k subsets and using each subset for testing while the remaining K-1 subsets are used for training.²⁰



Classifier





Fig. 10. ROC before Optimization

RESULTS

Performance of RF, AdaBoost and XGBoost classifiers is evaluated without optimization and with optimization to assess the impact of hyperparameter tuning on classification accuracy. Table 2 demonstrates the performance before hyperparameter tuning illustrating how these algorithms perform initially. RF, AdaBoost and XGBoost achieved accuracies of 95.55%, 94.81%, and 94.62% respectively.

Performance of the classifiers is improved by tuning the hyperparameters using bayesian optimization. This optimization process aimed to identify the best combination of hyperparameters that could maximize the classifiers' performance. Table 3 shows values of hyperparameters obtained through optimization, highlighting the adjustments made to improve model performance. It also shows the performance of classifiers after optimization. Figures 5 to 9 show the enhancement in the classifier's performance after optimization.



Fig. 11. ROC after Optimization



Fig. 12. RF Confusion Matrix

Fig. 13. AdaBoost Confusion Matrix

Figure 10 and 11 illustrates the ROC curve of the classifier before and after the optimization process.

Both XGBoost and AdaBoost have shown an improvement in value of area under the ROC (AUROC) after optimization. However, RF exhibits no change in its AUROC value. Confusion matrix for the three classifiers is demonstrated in Figure 13 to 15. Results indicate that RF has given the best performance with 96.11 % accuracy. Comparison of classifiers' accuracy is shown in Figure 16.

AdaBoost, RF, and XGBoost are complex models and less interpretable as compared to simpler models. To resolve this problem, SHAP





(Shapley Additive Explanations) tool is used. This tool helps in visualizing the contribution of each feature to the predictions of model. It helps in making the results more transparent and easier for clinicians to interpret. Figure 16 shows the SHAP value of each feature.

DISCUSSION

Results demonstrate the effectiveness of hyperparameter optimization in boosting the classifiers' predictive power. All three classifiers showed enhanced accuracy after optimization, AdaBoost and XGBoost benefited significantly from tuning, underscoring the importance of tailored hyperparameter adjustments for specific algorithms. RF has given the best performance with 96.11% accuracy, further increasing its reliability as a robust classification model in this study.

 Table 4. Comparison between proposed work and existing studies

Year	Authors	Classification Method	Accuracy
2022	Mamun ¹⁰	XGBoost	94.82%
2023	Ojha ¹²	LR	94.7%
2024	Maurya ¹⁴	KNN	92.86%
2024	Proposed	RF	96.11%



Fig. 15. Comparison of Classifiers' Accuracy







Fig. 17. Comparison of Proposed Work with Existing Studies

A detailed comparison between the proposed work and existing studies is outlined in Table 4. Comparison in graphical manner is shown in Figure 17. To make the evaluation consistent and fair, comparison is done with studies using the same dataset. This comparison highlights the competitive edge of the proposed work in terms of accuracy and robustness. Such evaluations ensure a fair and consistent benchmarking process, further validating the efficacy of the optimized model in lung cancer prediction task.

Proposed work has certain limitations also. SMOTE method is used for balancing. This method generates synthetic samples through interpolation, which may not fully represent the complexity of real-world data. This could introduce the problem of overfitting in model when applied on new data. Dataset size is small, region-specific and derived from a particular demographic. It may limit the generalizability of findings to diverse populations. This limitation can be resolved by validating the model on large datasets in future. Another limitation of this research work is that it primarily focuses on computational performance. This limitation can be removed by validating the model on real-world clinical datasets in future to assess its performance in diverse and practical settings. Kaggle lung cancer dataset provides a degree of clinical relevance as it is derived from patient data but for full clinical validation there is a need of involving diverse datasets and real-world clinical collaboration.

CONCLUSION

This research work presented a method for predicting lung cancer employing machine learning algorithms. Methods of SMOTE and bayesian optimization are used to improve performance of classifiers. RF, AdaBoost and XGBoost achieved accuracies of 96.11%, 95.74%, and 95.92% respectively. RF has shown the highest accuracy. The integration of explainability technique of SHAP has enhanced model interpretability, making the predictions more transparent for clinicians. There are several possibilities of improvement in future. Dataset can be expanded to include more patient parameters. Collaboration with medical professionals in future can validate the model in real-world clinical settings. Testing the model on more diverse populations could improve its generalizability across different demographic groups. More methods of optimization can be investigated to further improve the performance. Deep leaning methods can be used on the dataset of images.

ACKNOWLEDGEMENT

The authors would like to express their gratitude to Maharishi Markandeshwar (Deemed to be University), Mullana-Ambala, for supporting and facilitating this research work.

Funding Sources

The author(s) received no financial support for the research, authorship, and/or publication of this article.

Conflict of Interest

The author(s) do not have any conflict of interest.

Data Availability Statement

This statement does not apply to this article.

Ethics Statement

This research did not involve human participants, animal subjects, or any material that requires ethical approval.

Informed Consent Statement

This study did not involve human participants, and therefore, informed consent was not required.

Clinical Trial Registration

This research does not involve any clinical trials

Permission to reproduce material from other sources

Not Applicable

Authors' Contribution

Conceptualization & Methodology: Rohit Lamba; Visualization & Supervision: Pooja Rani and Ravi Kumar Sachdeva; Analysis and Writing – Original Draft: Priyanka Bhatla, Karan Kumar, Kapil Joshi; Visualization & Reviewing: Vikas Mittal; All authors made a significant and equal contribution to this work.

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