

CLASSIFICATION OF THYROID CANCER DATA BY REDUCING DIMENSIONALITY

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Abstract

This analysis investigates the prediction of thyroid cancer diagnosis (benign or malignant) using various machine learning algorithms on a dataset of thyroid patient information. The study encompasses data preprocessing steps such as handling continuous variables with different scales using MinMax scaling, correlation analysis, and dimensionality reduction through Principal Component Analysis (PCA). Several machine learning algorithms were implemented, including K-Nearest Neighbors (KNN), Logistic Regression, Decision Tree, and Random Forest. Their performance is evaluated based on accuracy, precision, recall, and confusion matrices. Additionally, the impact of PCA on model performance is assessed as well.

The results indicate that Logistic Regression, Decision Tree, and Random Forest has achieved comparable high accuracy in predicting thyroid cancer diagnosis, while KNN has achieved lower accuracy. Interestingly, applying PCA to the dataset leads to improved accuracy for KNN but slightly decreased accuracy for Random Forest. The analysis concludes with a model performance comparison, highlighting the strengths and weaknesses of each approach and the effect of dimensionality reduction on prediction accuracy. Overall, this study demonstrates the efficacy of various machine learning methods in thyroid cancer diagnosis prediction and provides valuable insights into the potential benefits of using PCA in specific scenarios.

1 Introduction

Thyroid, an important gland located at the base of neck, produces hormones that regulate heart rate, blood pressure, body temperature and weight. Thyroid cancer is a growth of cells that starts in the thyroid, and it is the tenth most common cancer in Canada (Canadian Cancer Society Website, 2024). The prevalence of thyroid cancer in Canada was estimated to 6,600 new cases in 2024 with a rapidly increasing rate than any other cancer in Canada (Canadian Cancer Society Website, 2024).

The thyroid cancer dataset, simulating real-world thyroid cancer risk, is selected from Kaggle Repository (Kaggle, 2024). The dataset contains many features such as risk factors, demographic variables and thyroid hormone related variables. The risk factors are family history of thyroid cancer, exposed to radiation, iodine deficiency, smoking habit, obesity and diabetes with a response yes or no. The dataset has demographics variables age, gender, country and ethnicity with thyroid hormone related variables thyroid stimulating hormone (TSH), thyroxine (T4) and triiodothyronine (T3). The dataset also contains thyroid nodule size and thyroid cancer risk factor as low, medium or high along with the response of thyroid cancer as benign or malignant.

In this project, the goals are: (a) exploratory study of the distribution of thyroid cancer across geographical regions, race and ethnicity, (b) classify thyroid cancer as malignant or benign; several machine learning algorithms like Logistic Regression, K-Nearest Neighbour, Random Forest and Decision Tree (Hastie et al., 2013) will be used for this classification. The performance of the algorithms on test data will be compared in order to find a classification algorithm with the best prediction accuracy. The goal here is to present a machine learning algorithm with the best prediction accuracy that can be feed into test features and the model classify it as malignant or benign, (c) The third goal of the project is to explore machine learning algorithms for dimensionality reduction of feature variables. The Principal Component Analysis (Hastie et al., 2013) will be explored to transform the original thyroid cancer dataset to the selected principal component space and then perform the machine learning algorithms on transformed data. Since the dataset has both the continuous and categorical feature variables; the principal component analysis will be based on the **FAMD()** function from R-package **FactoMineR** (R-Package Repository, 2025) or Python library **Prince**. The **FAMD ()** function implements the principal component method dedicated

to explore data with both continuous and categorical variables, and (d) finally the project aims to explore how effective the dimensionality reduction than using the full set of feature variables in terms of prediction accuracy in the classification of thyroid cancer.

2 Literature Review

The research goals, in section 1, have two parts - the first part aims is to employ popular classification algorithms to classify thyroid cancer as benign or malignant, and the second part aims to explore principal component analysis algorithm for dimensionality reduction. A comparative analysis of performance based on prediction accuracy in full feature space vs reduced number of features in the transformed space will also be explored thereafter.

According to Sheta et al. (2022), the most popular and commonly used classification algorithms in machine learning are Logistic Regression, Decision Tree, Random Forest, Support Vector Machine (SVM), Naive Bayes and K-Nearest Neighbours. However, in this project only a subset of the popular algorithms is planned to implement on the thyroid cancer dataset. The article review is limited to the classification algorithms proposed in section 1. A number of relevant articles have been analysed to explore the applicability of the classification algorithms in real-life datasets, with the goal is to gain knowledge about how other authors have implemented the algorithms in classification problems.

Khalilia et al. (2011) presents a method for predicting disease risks from highly imbalanced healthcare data using random forest classification. The authors used the Nationwide Inpatient Sample dataset from the Healthcare Cost and Utilization Project to train Random Forest, Support Vector Machine, Bagging, and Boosting classifiers to predict the risk of chronic diseases. To address the class imbalance problem in the dataset, the authors employed a repeated random sub-sampling approach, where the training data is divided into balanced sub-samples. The results show that the Random Forest ensemble learning method outperformed the other classifiers in terms of the area under the receiver operating characteristic (ROC) curve. The authors also discussed the application of disease prediction in areas like risk management, health communication, and decision support systems.

Jackins et al. (2021) presents Naive Bayes and Random Forest classification algorithms to diagnose and predict the risk of diabetes, coronary heart disease, and cancer using patient data. The authors compared the performance of the two algorithms on the three

disease datasets. The results show that the Random Forest algorithm outperforms the Naive Bayes algorithm in terms of accuracy for all three diseases. The paper also compares the performance of the proposed algorithms with K-means clustering, and the Random Forest algorithm is found to be more effective. The paper concludes that the proposed model works well for both training and test data, and can be used for real-time disease diagnosis. The authors also discussed the limitations of the proposed model; the limitations are: processing time - the model uses a large amount of data to estimate the performance of the training data, and accuracy testing with different datasets - the proposed model needs to be tested with different datasets, beyond the ones used in this study, and the potential to explore other AI algorithms beyond the ones used in the study.

Sruthi et al. (2024) has studied the main purpose of the Random Forest algorithm, that is, to combine the outputs of multiple decision trees to make a single, more accurate prediction. It is an ensemble learning technique that helps overcome the overfitting problem associated with individual decision trees. The key steps involved in the Bagging (Bootstrap Aggregation) technique used in Random Forest are: select a random subset of data points and features to construct each decision tree, train individual decision trees on these bootstrap samples and combine the outputs of all the decision trees through majority voting for classification or averaging for regression. The author has demonstrated that Random Forest is better at handling overfitting compared to a single decision tree. By combining the predictions of multiple trees, the algorithm reduces the variance and improves the robustness of the model. The diversity of the trees also helps prevent overfitting. As per the article, the real-life applications of the Random Forest algorithm include customer churn prediction, fraud detection, stock price prediction, medical diagnosis and image recognition.

Boateng et al. (2019) provides a comprehensive review of the Logistic Regression model, a widely used statistical technique for modelling the relationship between multiple independent variables and a categorical dependent variable, with a focus on medical research. The review covers the concepts such as odds, odds ratio, logit transformation, logistic curve, assumptions, selecting dependent and independent variables, model fitting, including overall model evaluation, statistical significance of individual predictors, and measures of predictive accuracy and discrimination. Then, the authors highlighted the importance of adhering to recommended guidelines and best practices in the use and reporting of logistic regression, as

many studies have been found to have deficiencies in these areas. The authors also present a good example of the application of the logistic regression model using data on factors influencing the decision of expectant mothers to opt for caesarean delivery or vaginal birth.

Robust and sparse logistic regression estimator that addresses the limitations of the standard maximum likelihood estimator for logistic regression has been studied by Cornilly et al. (2024). Their proposed method uses an elastic net penalty to ensure sparsity in the regression coefficients and robustness against outlying observations. The authors show that the influence function of the proposed estimator is bounded, demonstrating its robustness properties. They also evaluate the performance of the estimator in simulations and an empirical application involving the classification of car fuel types.

Dey et al. (2025) has highlighted the methodological issues regarding the application of Logistic Regression models to complex survey data. The review emphasizes the need for greater emphasis on evaluating how well the logistic regression models fit the data. Many studies have neglected this important aspect, and the review calls for more efforts to raise awareness on proper model evaluation and performance assessment. The review underscores the importance of accounting for complex survey design features, such as: sampling weights, clusters and strata variables. The authors found that while many studies did consider these survey design factors, a significant subset did not, highlighting the need for further investigation into the implications of not properly accounting for the complex survey structure. The main approaches discussed in the review for handling survey design effects in the estimation of binary outcomes or regression coefficients are weighted logistic regression and survey-weighted logistic regression, resampling techniques (e.g., jackknife, balanced repeated replication, bootstrap) and multilevel or mixed-effects logistic regression. Finally, the review highlights that while many studies used these advanced statistical methods to account for complex survey designs, there is still room for improvement in terms of consistent and transparent reporting of the methodological approaches employed.

Syriopoulos et al. (2023) provides a comprehensive review of the K-nearest neighbors (KNN) algorithm, a popular non-parametric classifier. It covers the strengths and weaknesses of KNN, its applications in various data science tasks, available benchmarks and software, and the latest developments in the field. The review aims to serve as a valuable resource for researchers and practitioners to understand and apply KNN effectively. It discusses topics

such as anomaly detection, dimensionality reduction, and missing value imputation using KNN. The document also includes a detailed analysis of the KNN algorithm, including its theoretical foundations, distance metrics, and optimization techniques.

The theoretical foundation of nearest neighbour is covered in the article by Cover and Hart (1967). The authors focused on the analysis of the nearest neighbour pattern classification rule, which assigns an unclassified sample to the category of its nearest neighbour from a set of previously classified samples. The key results of the article are presented as: the nearest neighbour probability of error R is bounded above by $2R^*(1-R^*)$, where R^* is the Bayes probability of error (the minimum error over all decision rules). This upper bound is shown to be tight. A lower bound on R in terms of R^* has also been provided. The paper compares the nearest neighbour rule to the Bayes probability of error R^* . It shows that the nearest neighbour rule has a probability of error that is at most twice the Bayes error, indicating that a significant portion of the classification information in the sample set is contained in the nearest neighbour. The authors also analysed the convergence properties of the nearest neighbour, showing that as the sample size increases, the nearest neighbour to a given point converges to that point with probability 1. This convergence result is key to establishing the bounds on the nearest neighbour probability of error. For the multi-category case (more than 2 classes), the paper extends the analysis and provides analogous upper and lower bounds on the nearest neighbour probability of error in terms of the Bayes error rate.

Halder et al. (2024) reviews and analyzes 43 modifications to the k-Nearest Neighbors (KNN) algorithm, focusing on high-dimensional data, and provides a comprehensive overview of KNN search and join methods, including source code and future research directions. This study applies Support Vector Machine (SVM) algorithm to predict MERS-CoV risk distribution in East Java, Indonesia, utilizing 2023 data from the East Java Health Department, achieving highest accuracy of 90% with 75:25 data proportion.

Principal component analysis (PCA) as discussed by Kalantan et al. (2019) is a multivariate technique that analyzes a data table in which observations are described by several inter-correlated quantitative dependent variables, and its goal is to extract the important information from the table, to represent it as a set of new orthogonal variables called principal components, and display the pattern of similarity of the observations and of the variables as points in maps.

In a summary of the literature review, the aim is now to explore few articles that has comparatively analysed the performance of the above machine learning algorithms. With this in mind, the article by Sheta et al. (2022) is an excellent resource; in this article, the authors have compared the accuracy of four classification algorithms such as Decision Tree, Support Vector Machine, Naive Bayesian, and K-nearest Neighbour on five different datasets. The Naive Bayesian algorithm is proven to be the most effective among other algorithms. Classification of data is crucial for risk management, compliance, and data security and each data mining model has a distinct level of information; the authors have concluded that the success of a model is solely determined by the datasets being used, as there is no such thing as an excellent or a poor model.

3 Data Preprocessing

3.1 Demographic Distribution

The thyroid cancer dataset has 17 features with no missing values for any feature. This is good as it indicates a relatively clean dataset with complete data. There are 212,691 observations from different geographical regions such as Russia, Germany, Nigeria, India, UK, South Korea, Brazil, China, Japan and USA. Among the feature variables age, and thyroid hormone related features like TSH, T3, T4 and nodule size are continuous variables; all the remaining variables are categorical with a response as yes or no.

As it is important to consider the potential impact of different geographical locations on the risk of thyroid cancer and the data analysis, the distribution of thyroid cancer cases based on region, gender, and ethnicity is presented in Figure 1. This analysis reveals regional, ethnic, and gender-based disparities in thyroid cancer distribution. India, China, and Nigeria show higher rates of malignant thyroid cancer, while Asian ethnicity demonstrates a higher prevalence compared to other ethnic groups. Females also experience a higher incidence of malignant thyroid cancer, aligning with existing reports from organizations like the Canadian Cancer Society (Canadian Cancer Society Report, 2024). Further research is needed to identify the underlying factors contributing to these disparities, including genetic predisposition, environmental factors, and lifestyle choices. This information is crucial for developing targeted prevention and intervention strategies for reducing the burden of thyroid

cancer.

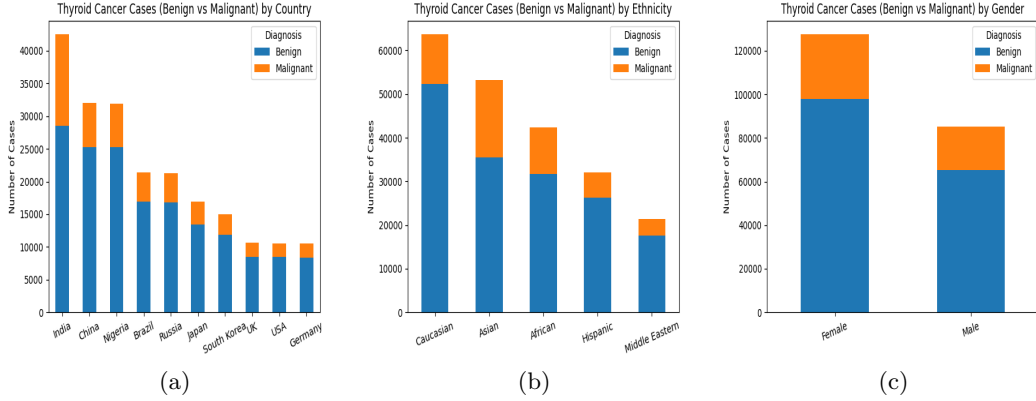


Figure 1: Distribution of Thyroid Cancer by (a) Country (b) Ethnicity, and (c) Gender.

Variable	Category	% Patient
Gender	Male	60
	Female	40
Family History	No	70
	Yes	30
Radiation Exposure	No	85
	Yes	15
Iodine Deficiency	No	75
	Yes	25
Smoking	No	80
	Yes	20
Obesity	No	70
	Yes	30
Diabetes	No	80
	Yes	20

Table 1: Percentages of patients in each attribute.

3.2 Summary Statistics

Table 1 presents the proportion of patients for each attributes, and the summary statistics of continuous attributes are shown in Table 2. From the summary statistics, it is found that the dataset has 60% female and 40% male patients. The percentages of patients to smoking and diabetes yes vs. no are 20% vs. 80% for both attributes. There are 30% patients without obesity whereas obese patients are 70% in total. The minimum age of patients in the dataset is 15 years, and maximum is 89 years with a mean age 51.92 years and standard deviation 21.63 years. The mean nodule size is 2.50 millimetres with standard deviation of

1.44 millimetres, and the range of nodule size is from 0 to 5 millimetres.

	Age	TSH	T3	T4	Nodule Size
Mean	51.92	5.05	2.00	8.25	2.50
Std	21.63	2.86	0.87	2.16	1.44
Min	15.00	0.10	0.50	4.50	0.00
Q1	33.00	2.57	1.25	6.37	1.25
Median	52.00	5.04	2.00	8.24	2.51
Q3	71.00	7.52	2.75	10.12	3.76
Max	89.00	10.00	3.50	12.00	5.00

Table 2: Summary statistics of continuous attributes.

3.3 Correlation

The correlation matrix and the heat map of continuous variables are presented in Table 3 and Figure 2. Correlation does not imply causation - it simply indicates a statistical relationship between variables. A weak negative correlation (-0.000925) exists between age and TSH levels. This suggests that as age increases, TSH levels may tend to slightly decrease as well. There is a weak negative correlation (-0.000795) is observed between TSH and T4 levels, indicating as TSH levels increase, T4 levels tend to decrease, and vice versa. This is expected, as they are part of the thyroid hormone regulation system. A weak negative correlation is found between T3 and T4 levels (-0.004069). This shows that T3 and T4 levels are closely related, likely reflecting the interconversion and interplay of these hormones. Nodule size shows a weak positive correlation with TSH (0.000416), indicating a slight tendency for larger nodules to be associated with slightly higher levels of this hormone.

	Age	TSH Level	T3 Level	T4 Level	Nodule Size
Age	1.000000	-0.000925	-0.001013	-0.002373	-0.001489
TSH Level	-0.000925	1.000000	0.000335	-0.000795	0.000416
T3 Level	-0.001013	0.000335	1.000000	-0.004069	-0.001799
T4 Level	-0.002373	-0.000795	-0.004069	1.000000	-0.001860
Nodule Size	-0.001489	0.000416	-0.001799	-0.001860	1.000000

Table 3: Correlation matrix of continuous variables; the correlation among the variables are negative with a small magnitude except a small positive correlation between TSH and T3 level, and TSH level and nodule size.

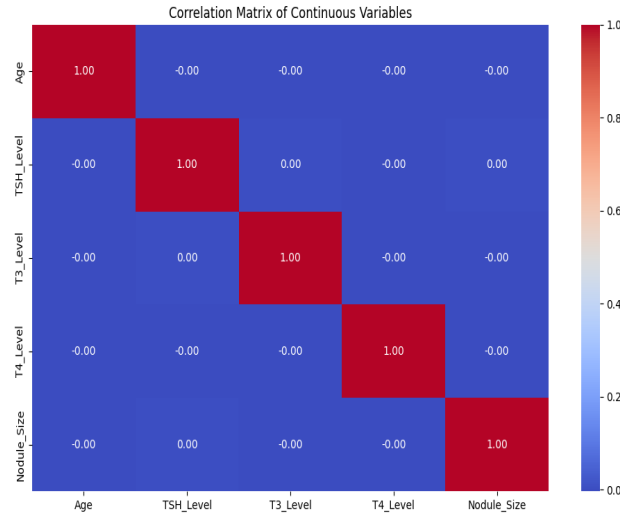


Figure 2: Heat map of continuous variables.

3.4 Dataset Scaling

The continuous attributes have different scales or units; for example, age has unit years while thyroid related hormones have unit in milliliter (ml), and the nodule size has a unit of millimetre. Thus, before we fit any machine learning algorithm, it is important to scale the attributes to have the same scale across all the attributes. The MinMax scaling function is chosen from Python library **sklearn.preprocessing**, which scales the continuous variables to have mean 0 with standard deviation 1. The mathematical formula that the MinMax

algorithm applies on each attribute is $X_{scaled} = (X - X_{min}) / (X_{max} - X_{min})$, where X is the particular attribute, and X_{min} is the minimum and X_{max} is the maximum of that attribute.

4 Predictive Analysis

The first step of predictive analysis is to divide the data into train and test datasets; the train dataset is used to train the model, while the test dataset is used to evaluate the model's performance. The second step is to choose a suitable prediction model based on the dataset; for example, Decision Trees, Logistic Regression, K-Nearest Neighbors, and Random Forests. The third step is to train the selected model on the training data, then assess the model's performance on the testing dataset. The model's performance can be assessed by using matrices like accuracy, precision, recall, F1-score, and AUC. The final step is to deploy the trained model for making predictions on new data, and monitor the model's performance over the time and retrain as needed.

As the predictive analytical steps described above, the thyroid cancer dataset is divided as train and test data using a random state for reproducibility; 80% of the data is kept a train data on which the machine learning algorithms will be fitted, and the rest of the 20% data is kept as test data for the evaluation of model performance and accuracy of prediction. The train dataset has 170,152 observation while the test dataset has 42,539 observations. Since some of the attributes are categorical, this categorical attributes are converted as factor attributes; this makes a total of 28 attributes in the dataset.

4.1 K-Nearest Neighbor

The KNN algorithm is chosen as a classification model to predict thyroid cancer diagnosis. The optimal value of K (i.e., number of nearest neighbors) is determined using **Grid-SearchCV**, which automatically tested different K values and evaluated their performance through cross-validation. In this process, the optimal K value is identified as 5. The performance of the KNN model is evaluated on a test dataset. The KNN classifier has achieved an accuracy of 72.14% on the test dataset. However, the performance varied depending on the class. The model showed reasonable performance in identifying benign thyroid cancer patients with a precision of 77%. In contrast, its performance is less satisfactory for identifying malignant cases, with a precision of only 24%. This suggests a possible class imbalance

issue, where the model is biased towards the majority class likely benign, which supports that the dataset has more benign than malignant patients (77% benign vs 23% malignant).

4.2 Logistics Regression

The logistic regression demonstrates a strong performance in predicting thyroid cancer diagnosis (benign or malignant). The logistic regression classifier has achieved 82.50% accuracy on the test dataset with a precision of 85% for benign cases and 69% for malignant cases. Logistic regression accurately classifies the majority of thyroid cancer cases in the test dataset. The model shows a higher precision in identifying benign cases compared to malignant cases. This suggests that the model is better at correctly identifying patients without thyroid cancer than those with it. The high accuracy and precision suggest that it can potentially be a valuable tool for identifying patients who may be at risk of developing thyroid cancer. The confusion matrix of logistics regression classifier is shown at Table 4.

	Predicted Benign	Predicted Malignant
Actual Benign	30657	1958
Actual Malignant	5484	4440

Table 4: Confusion Matrix for Logistic Regression Classifier.

4.3 Decision Tree

The Decision Tree classifier, utilizing entropy as the attribute selection measure and a maximum depth of 3 for pre-pruning, achieved an accuracy of 82.50% on the test dataset. The precision is 85% for benign patients and 69% for malignant patients. The recall or sensitivity value reveals how well the model can capture actual malignant cases. A higher recall indicates the model is effective at identifying all the malignant cases. The recall or sensitivity of decision tree is 44.74%. Specificity shows how well the model can correctly identify benign cases, and false positive and false negative rates show the level of error in classifying patients incorrectly as either malignant or benign. For decision tree classifier, the specificity is found to be 94.00% with false positive rate of 6.00% and false negative rate of 55.26%. All these matrices are shown in Table 5.

Metric for Decision Tree	Percentage
Recall	44.74%
Precision	69.40%
True Positive Rate (Sensitivity)	44.74%
True Negative Rate (Specificity)	94.00%
False Positive Rate	6.00%
False Negative Rate	55.26%

Table 5: Evaluation Metrics for Decision Tree.

4.4 Random Forest

First an instance of the Random forest model with the default parameters is created; then fit the model on train data. After that both the features and the target variable are passed into the model so that the model can learn to predict. The Random Forest model achieved an accuracy of 82.46% on the test data, indicating that the model correctly predicted the diagnosis (benign or malignant) for approximately 82.46% of the patients in the test dataset. Other assessment matrices like precision is also calculated for Random Forest model. The model has obtained a precision of 85% for benign cases and 70% for malignant cases. Out of all the patients predicted as benign, approximately 85% were truly benign. Similarly, out of all the patients predicted as malignant, approximately 70% were truly malignant. Overall, the Random Forest model demonstrated a good performance on this thyroid cancer dataset, achieving a competitive accuracy and reasonable precision for both benign and malignant cases. It is a robust model that can effectively distinguish between benign and malignant cases of thyroid cancer.

4.5 Principal Component Analysis

Since the dataset has both the continuous and categorical feature variables; the principal component analysis will be based on the **FAMD()** function from Python's Prince library. The FAMD () function implements the principal component method dedicated to explore data with both continuous and categorical variables. From the PCA analysis, two principal

components that explains the majority of variances are found. Then both the train and test data are transformed onto the principal component space. In the transformed space, the machine learning algorithms are fitted to evaluate model accuracy on test data.

The KNN algorithm is re-fitted on PCA transformed data and the model accuracy is evaluated on test dataset. The prediction accuracy with KNN after PCA is found to be 79.80%, which is bit higher than what is found (72.14%) found from the dataset without any PCA transformation. The other machine learning algorithms (e.g., Decision Tree and Random Forest) are also fitted on PCA transformed data. The prediction accuracy with Decision Tree on PCA transformed data is found to be the same 82.50% regardless of whether the original dataset or PCA transformed data is fitted into the model. However, the prediction accuracy with Random Forest on PCA transformed data is found to be 80.30%, which is a bit lower than what is found (82.46%) on original dataset.

5 Model Performance Comparison

The bar chart in Figure 3 visually compares the accuracy of all models, both with and without PCA. Comparing the model performance on prediction accuracy in Table 6, it is observed that KNN has the lowest prediction accuracy among all the machine learning algorithms that have been used in this analysis. Logistic regression, Decision Tree and Random Forest have almost the same prediction accuracy (Figure 3), but these prediction accuracies decrease on PCA transformed data except KNN algorithm. The KNN algorithm performs better prediction accuracy on PCA transformed dataset than the original dataset.

6 Discussion

Logistic regression, Decision Tree, and Random Forest demonstrated generally good performance on predicting thyroid cancer diagnoses, with accuracy exceeding 82%. The KNN initially suffered from lower accuracy, but PCA helped it perform better. The effect of PCA on model performance varied, highlighting the importance of considering different techniques and their potential impact on model results. The choice of a "best" model might depend on specific needs, such as the trade-off between complexity and accuracy, as well as the relative importance of correctly identifying benign and malignant cases. Further investigation into

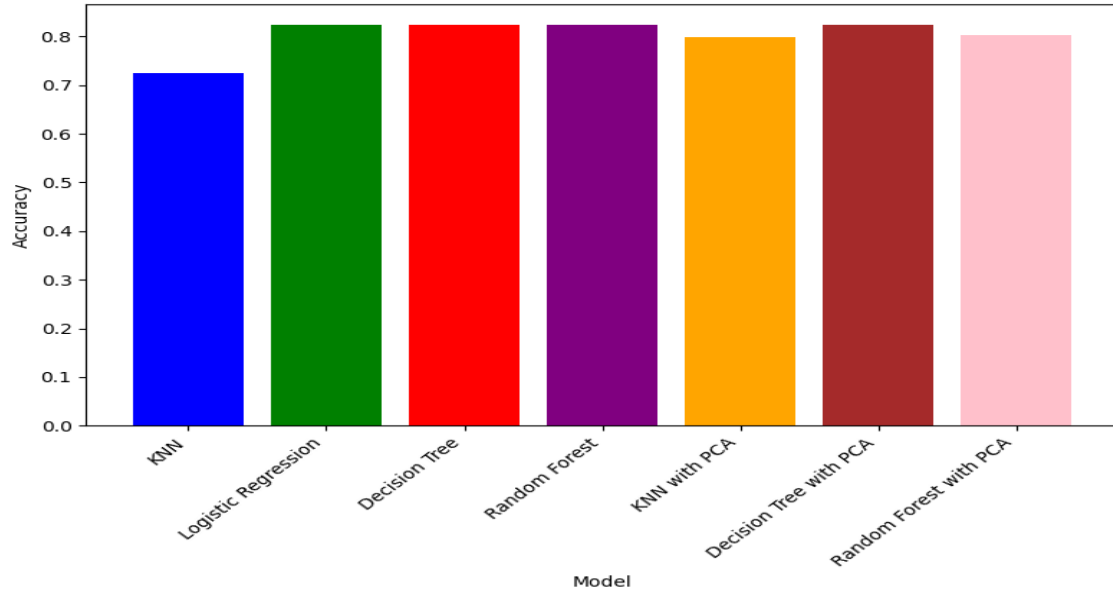


Figure 3: Bar chart of model performances.

Model	Accuracy
KNN	72.14%
Logistic Regression	82.50%
Decision Tree	82.50%
Random Forest	82.46%
KNN with PCA	79.80%
Decision Tree with PCA	82.50%
Random Forest with PCA	80.30%

Table 6: Model performance comparison of different machine learning algorithms.

hyperparameter tuning for the models can potentially improve performance. Exploring other feature engineering techniques could potentially extract more valuable information from the data. Evaluating models on different performance metrics, such as recall and F1 score, alongside accuracy would provide a more comprehensive understanding of their capabilities.

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