Multi-Class Cancer Classification Using Gene Expression and Machine Learning

A PROJECT REPORT

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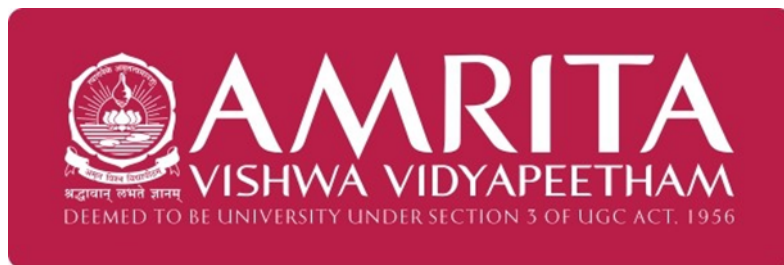
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In partial fulfillment for the award of the degree of

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Under the guidance of

Dr. I R Oviya

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DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING

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BONAFIDE CERTIFICATE

This is to certify that this project report entitled **"Multi-Class Cancer Classification Using Gene Expression and Machine Learning"** is the bonafide work of **"Mr. C.Mohith Reddy (Reg. No. CH.SC.U4AIE23008), Mr. CH.Naynesh Reddy (Reg. No. CH.SC.U4AIE23009), Mr. M.Likhith Reddy (Reg. No. CH.SC.U4AIE23033), Mr. N.Harshith Varma (Reg. No. CH.SC.U4AIE23035), Mr. N.Charan (Reg. No. CH.SC.U4AIE23038), Mr. P.M.D.Kalesha (Reg. No. CH.SC.U4AIE23040)"** who carried out the project work under my supervision as a part of End semester project for the course 22BIO211 - Intelligence of Biological Systems 2 .

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DECLARATION BY THE CANDIDATE

We declare that the report entitled **"Multi-Class Cancer Classification Using Gene Expression and Machine Learning"** submitted by us for the degree of Bachelor of Technology is the record of the project work carried out by us as a part of the End Semester project for the course 22BIO211 - Intelligence of Biological Systems 2 under the guidance of **Dr. I R Oviya**. This work has not formed the basis for the award of any course project, degree, diploma, associateship, fellowship, or title in this or any other university or similar institution. We also declare that this project will not be submitted elsewhere for academic purposes.

S.No	Register Number	Name	Topics Contributed	Contribution %	Signature
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ABBREVIATIONS

LDA	Linear Discriminant Analysis
SVM	Support Vector Machine
KNN	K-Nearest Neighbors
MLP	Multi-Layer Perceptron
CNN	Convolutional Neural Network
RNN	Recurrent Neural Network
BiGRU	Bidirectional Gated Recurrent Unit
SMOTE	Synthetic Minority Oversampling Technique
PCA	Principal Component Analysis
PSO	Particle Swarm Optimization
RF	Random Forest
MI	Mutual Information
FGS	Fuzzy Gene Selection
MC-SVM-1	Multi-Class 1-Norm Support Vector Machine
GCA	Genetic Clustering Algorithm
MOT	Multi-Omic Transformer
LASSO-MOGAT	LASSO-Multi-Omics Gated Attention Model
PPI	Protein-Protein Interaction
EODE	Evolutionary Optimized Diverse Ensemble Learning
RLS	Recursive Least Squares
DFIG	Doubly Fed Induction Generator
AEGAN	AutoEncoders and Generative Adversarial Networks

NOTATION

X	Feature vector
Y	Class label
$P(Y\|X)$	Posterior probability
$P(X\|Y)$	Likelihood function
$P(Y)$	Prior probability
$P(X)$	Evidence
$J(w)$	Fisher's criterion for class separability
S_B	Between-class scatter matrix
S_W	Within-class scatter matrix
w	Projection vector in LDA
$H(X)$	Entropy function measuring impurity
p_i	Probability of class i
$d(x, y)$	Euclidean distance between two points
$L(y, F(x))$	Loss function in Gradient Boosting
$f(x)$	Sigmoid activation function
θ	Model parameters in deep learning
k	Number of selected features in SelectKBest
C	Regularization parameter in SVM
ξ_i	Slack variable in SVM optimization
T	Number of trees in Random Forest
$n_{\text{estimators}}$	Number of boosting stages in Gradient Boosting
η	Learning rate in optimization
F_i	Extracted feature vector from model
$PCA(F_i)$	Principal Component Analysis transformation
MCC	Matthews Correlation Coefficient
$AUC - ROC$	Area Under the Receiver Operating Characteristic Curve
$AUC - PR$	Area Under the Precision-Recall Curve

ABSTRACT

This study evaluates the performance of eight machine learning models such as Gradient Boosting, Logistic Regression, Naïve Bayes, Linear Discriminant Analysis (LDA), Random Forest, Support Vector Machine (SVM), K-Nearest Neighbors (KNN), and MultiLayer Perceptron (MLP) used for predicting cancer types based on gene expression data. These models achieved accuracy rates of 95%, 98. 33%, 96. 67%, 90%, 96. 67%, 98. 33%, 95% and 91. 67%, respectively. The data is preprocessed using feature selection which uses SelectKBest, class imbalance correction using SMOTE, and normalization or standardization based on the model. All the models are properly trained and hyperparameter-tuned, and measurement is conducted by accuracy, precision, recall, F1-score, and plot of confusion matrices.

Keywords: Cancer Classification, Gene Expression Data, Machine Learning, HistGradientBoostingClassifier, RandomForestClassifier, High-Dimensional Data, Feature Selection, Standard Scaling, Stratified K-Fold Cross-Validation, Ensemble Learning, Precision Oncology, Model Generalization, Diagnostic Tools.

CHAPTER 1

INTRODUCTION

Cancer is a deadly disease that results from cells in the body starting to multiply uncontrollably and it is the second largest cause of death in the world, just after heart diseases, according to the World Health Organization (WHO). It is extremely important to detect cancer early because it allows doctors to start treating the condition earlier, which can improve survival.One of the ways to detect cancer at its earliest stages is by the examination of gene expression, which is a measure of how actively individual genes are expressed within cells. New approaches such as DNA microarrays and RNA sequencing allow researchers to measure gene activity, providing useful information for the study of cancer.

Machine learning (ML) is a helpful approach to study the gene expression and categorize different types of cancers. Traditional methods such as support vector machine and random forests have been applied. Deep learning algorithms in the guise of convolutional neural networks (CNNs) and recurrent neural networks (RNNs) have been recently employed since they were able to recognize complex patterns in gene data more effectively.

One of the biggest challenges of cancer classification is handling the huge amount of genetic data that's hard to process and analyze. Some techniques help reduce the complexity of the data while maintaining the most important information. For example, a blend of Particle Swarm Optimization (PSO) and Random Forest (RF) has been used to find important genes, followed by Principal Component Analysis (PCA) to reduce the data for processing. An experiment carried out in such a manner, along with CNNs and Bi-LSTM networks, yielded a result of 96.89(percent) in cancer classification, greater than several previous approaches.

Another approach, contrastive learning (CL), has been beneficial in cancer research. CL is an approach that allows computers to learn patterns in small data sets. CL was applied to cancer gene expression data recently and reported high accuracy for predicting cancer recurrence risk. The study showed that CLbased models outperformed traditional approaches in predicting cancer survival rates.

Breast cancer, the most common cancer in women, has been extensively studied using machine learning. Researchers have applied various machine learning models to classify breast cancer cases using the SEER dataset, demonstrating its potential in cancer outcome prediction.

Hybrid machine learning models, being a blend of multiple approaches, have also been developed to improve cancer diagnosis. Researchers have also integrated clustering methods with CNNs and Random Forest models to develop a multi-step classification system. The method classified gene expression data into clusters before it was analyzed, improving accuracy and efficiency. Such approaches improve the accuracy of cancer detection and assist physicians in making improved treatment choices.

CHAPTER 2

LITERATURE SURVEY

2.1 DEEP LEARNING-BASED CANCER CLASSIFICATION

Deep learning models such as the Deep Convolutional Gated Network (DCGN) have been employed for cancer classification by integrating CNNs for feature extraction and BiGRU for deep feature analysis, coupled with SMOTE for data balancing. MI-Bagging, another method, uses mutual information for feature selection and a bagging ensemble of multilayer perceptrons (MLPs), enhancing classification accuracy. Fuzzy Gene Selection (FGS) utilizes multiple feature selection techniques alongside fuzzy logic for optimal gene ranking, outperforming MLP-based models in accuracy and precision. Additionally, the Multi-Class 1-Norm Support Vector Machine (MC-SVM-1) applies a sparsity-based approach, reducing dimensionality while maintaining high classification performance in cancer datasets.

2.2 MACHINE LEARNING AND FEATURE SELECTION APPROACHES.

Several machine learning models incorporate advanced feature selection methods for improved cancer classification. Genetic Clustering Algorithms (GCA), combined with a divergent random forest classifier, significantly reduce RNA gene expression data dimensionality while maintaining high accuracy. The Multi-Omic Transformer (MOT) model integrates multi-omic layers for driver gene discovery, biomarker identification, and cancer subtype classification. Additionally, graph-based deep learning models like LASSO-MOGAT leverage Graph Attention Networks (GATs) and protein-protein interaction networks to improve classification accuracy across multiple cancer types while offering biological insights.

2.3 ENSEMBLE AND EVOLUTIONARY LEARNING TECHNIQUES

Ensemble learning and optimization techniques have also contributed to cancer classification advancements. The Evolutionary Optimized Diverse Ensemble Learning (EODE) model applies a grey wolf optimization algorithm for feature selection, leading to better classification accuracy. In leukemia classification, a super learning strategy using an entropy-based feature selection method and a Random Forest-based super learner has demonstrated superior classification performance compared to traditional models. These approaches highlight the effective-

ness of ensemble learning in handling complex and heterogeneous cancer datasets.

2.4 BIG DATA AND COMPUTATIONAL FRAMEWORKS IN CANCER CLASSIFI-CATION

With the rise of high-dimensional gene expression data, big data frameworks like Apache Spark have been utilized to improve processing efficiency. The Apache Spark-based pipeline method efficiently handles RNA-seq gene expression data, offering an 11-fold reduction in processing time compared to conventional methods. Similarly, the AEGAN-Pathifier method, incorporating AutoEncoders and Generative Adversarial Networks (GANs), generates synthetic data while preserving biological pathway integrity, thereby improving classification accuracy for imbalanced datasets. These computational advancements enhance the scalability and precision of cancer classification techniques.

2.5 ADAPTIVE CONTROL AND SYSTEM IDENTIFICATION IN BIOMEDICAL AP-PLICATIONS

Beyond classification, adaptive control techniques are explored for biomedical system stability. A modified control architecture for Doubly Fed Induction Generators (DFIGs), utilizing recursive least squares (RLS) for online system identification, improves system stability in varying grid conditions. Tested on a real-time 1.5 MW wind turbine, this approach optimizes performance by considering sensor faults and parameter variations. Such advancements indicate the potential of adaptive control techniques in biomedical and energy-related applications, further expanding the role of computational intelligence in healthcare and beyond.

CHAPTER 3

METHODOLOGY

3.1 DATA COLLECTION

The data11tumors2 [18] dataset contains 174 samples and 12,534 features, including a class label indicating the type of tumor. Gene expression data were primarily generated by means of microarray analyses to study differential gene expression across different tumor types. Every feature was a representation of the expression value of a particular gene whereas the class column contains the numerical value which represents their corresponding tumor group.

3.2 DATA PREPROCESSING

Data consists of gene expression values for various types of cancer. Preprocessing steps were performed differently based on the model.

- **Feature Selection**: To minimize dimensionality and preserve the most informative features, the SelectKBest function was applied with varying values of k for every model. The k values were selected based on initial experiments to maximize model performance.

- **Scaling**: Scaling as a critical step to standardize the independent variable range and enhance model convergence. StandardScaler was used to Logistic Regression, LDA, SVM, KNN, and MLP to have the mean of features as zero and variance as one. Standardization assisted the models in their best performance, especially those dependent on distance calculationbased models like KNN and SVM. MinMaxScaler was used only in Naive Bayes since it needs non-negative values for calculating probability. RobustScaler was utilized for Gradient Boosting and Random Forest since both are outlier sensitive and this scaler is great at eliminating the impact of extreme values.

- **Data Balancing**: Since the dataset was imbalanced, SMOTE was utilized in all models to obtain an equal dataset and enhance the classification performance. The process generated artificially minorityclass samples to avoid over-representation in majorityclass predictions.

3.3 MODEL SELECTION AND TRAINING

Eight models were experimented and trained: Logistic Regression, Gradient Boosting, Naive Bayes, LDA, Random Forest, SVM, KNN, and MLP. Special preprocessing and optimization were used on each model to add performance boosts.

3.3.1 LOGISTIC REGRESSION

Logistic Regression was learned using SelectKBest (k=300) feature selectivity and StandardScaler as scaling. SMOTE was also used to balance the dataset and k value set lower to avoid overfitting, which also contributes to model generalizability overall. Logistic Regression equation is provided as:

$$P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_n X_n)}}$$

$P(Y = 1|X)$ represents the probability of class 1 given X, where β_0 is the intercept and β_i are feature coefficients.

3.3.2 NAIVE BAYES

Naive Bayes used SelectKBest (k=200), and MinMaxScaler was used for non-negative values since probability estimation requires that. SMOTE was used to balance the classes. This model sticks to Bayes' Theorem:

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

$P(Y|X)$ is the posterior probability, $P(X|Y)$ is the likelihood, $P(Y)$ is the prior, and $P(X)$ is the evidence.

3.3.3 LINEAR DISCRIMINANT ANALYSIS

LDA (Linear Discriminant Analysis) used SelectKBest ($k = 250$) to choose features and StandardScaler to scale. Collinear features were dropped to prevent numerical instability prior to training. This model maps data into a lower-dimensional space in order to maximize discrimination between various classes. The function $J(w)$ measures how well a projection vector w separates different classes in a dataset. It is defined as:

$$J(w) = \frac{w^T S_B w}{w^T S_W w}$$

where $J(w)$ optimizes class separability, S_B is the between-class scatter matrix, S_W is the within-class scatter matrix, and w is the projection vector.

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3.3.4 RANDOM FOREST

Random Forest was feature selected via SelectKBest ($k = 400$) followed by RobustScaler to reduce the effect of outliers. The maximum depth of trees was limited to 15 to prevent overgrowth and overfitting to generalize well. The following is utilized to train every tree in the forest:

$$H(X) = -\sum_{i=1}^{n} p_i \log(p_i)$$

$H(X)$ measures impurity, with p_i being the probability of class i.

3.3.5 SUPPORT VECTOR MACHINE(SVM)

SVM was trained with SelectKBest ($k = 300$), and StandardScaler was utilized to provide stable feature scaling. Hyperparameters like $C = 10$ and $\gamma = $ scale were adjusted to enhance decision boundary flexibility and model stability. SVM's optimization function is:

$$\min_{w} \quad \frac{1}{2}||w||^2 + C\sum \xi_i$$

where w and b define the hyperplane, C controls regularization, and ξ_i are slack variables for misclassification.

3.3.6 K-NEAREST NEIGHBORS

KNN (K-Nearest Neighbors) utilized SelectKBest ($k = 350$), while feature scaling utilizing StandardScaler was used, of utmost significance with distance-based techniques. The optimum value of k was adjusted and fixed at 5 to capture a balance point between variance and bias. It is classified as per:

$$d(x,y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

where $d(x,y)$ is the Euclidean distance, and x_i and y_i are feature values of points.

3.3.7 MULTI-LAYER PERCEPTRON

MLP (Multi-Layer Perceptron) used SelectKBest ($k = 500$) to choose the features, followed by StandardScaler in anticipation of convergence optimization. The hidden layers of MLP were set at $(100, 50)$ for the facilitation of deep learning features to project complex patterns from the dataset. The activation function employed is:

$$f(x) = \frac{1}{1 + e^{-x}}$$

where $f(x)$ is the sigmoid activation, mapping input x to $(0, 1)$.

3.3.8 GRADIENT BOOSTING

Gradient Boosting employed SelectKBest ($k = 450$), and RobustScaler was used to boost stability with outliers. Hyperparameters were also optimized so that the learning rate $= 0.1$ and $n_{\text{estimators}} = 200$, for best boosting performance. The loss function employed in tuning is:

$$L(y, F(x)) = \sum_{i=1}^{n} (y_i - F(x_i))^2$$

where $L(y, F(x))$ is the loss function, minimizing the error between actual y_i and predicted $F(x_i)$.

3.4 EVALUATION METRICS

All models were tested and evaluated based on classification accuracy, precision, recall, and F1-score for overall performance measurement. Cross-validation was applied to determine whether the models generalized sufficiently well for future unknown samples and weren't overfitting in the training data set.

Class	Cancer Type
0	Ovary
1	Bladder/Ureter
2	Breast
3	Colorectal
4	Gastroesophagus
5	Kidney
6	Liver
7	Prostate
8	Pancreas
9	Adenocarcinoma
10	Lung squamous cell carcinoma

Figure 3.1: Learning curves for different models

CHAPTER 4

RESULTS

Accuracy determines the proportion of correct positive predictions, as total true positives against total positive predictions. Recall tests the ability of a model in detecting true positives, as a ratio of true positives to existing actual positives. The F1-score, a harmonic mean between precision and recall, averages the two for evaluation of overall performance. Support calculates the number of actual instances per class in a dataset, specifying class distribution. Accuracy is the ratio of correct predictions to all predictions. Macro average calculates the mean of precision, recall, and F1-score for all classes uniformly, whereas weighted average weighs these metrics according to class sample sizes to consider imbalanced data.
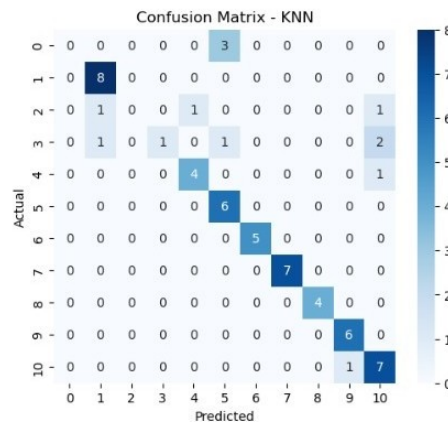
Figure 4.1: Confusion Matrix- KNN:Visualization of actual vs. predicted labels for a K-Nearest Neighbors model.

Figure 4.2: KNN Classification Report:Performance metrics including precision, recall, and F1-score for a K-Nearest Neighbors model.

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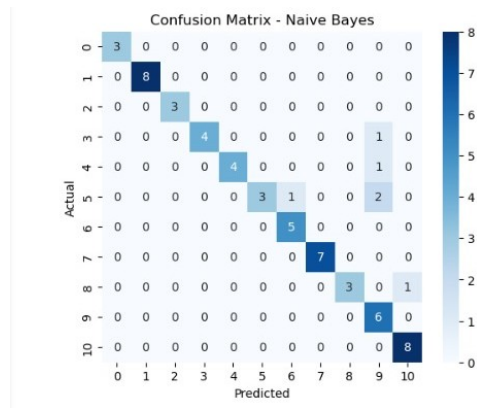
Figure 4.3: Confusion Matrix - Naïve Bayes:Visual representation of actual vs. predicted classifications for a Naïve Bayes model.

Figure 4.4: Classification report showing Naïve Bayes achieving 90(percent) accuracy with class-wise precision, recall, and F1-scores.
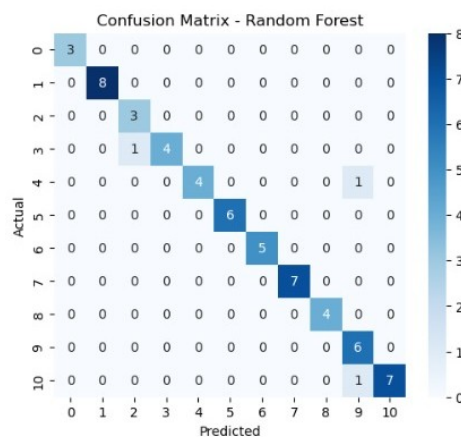
Figure 4.5: Confusion matrix visualizing the performance of a Random Forest classifier with accurate class-wise predictions.

```
Random Forest Accuracy: 0.9500

              precision    recall  f1-score   support

           0       1.00      1.00      1.00         3
           1       1.00      1.00      1.00         8
           2       0.75      1.00      0.86         3
           3       1.00      0.80      0.89         5
           4       1.00      0.80      0.89         5
           5       1.00      1.00      1.00         6
           6       1.00      1.00      1.00         5
           7       1.00      1.00      1.00         7
           8       1.00      1.00      1.00         4
           9       0.75      1.00      0.86         6
          10       1.00      0.88      0.93         8

    accuracy                           0.95        60
   macro avg       0.95      0.95      0.95        60
weighted avg       0.96      0.95      0.95        60
```

Figure 4.6: Classification report showing Random Forest achieving 95(percent) accuracy with detailed precision, recall, and F1-scores per class.
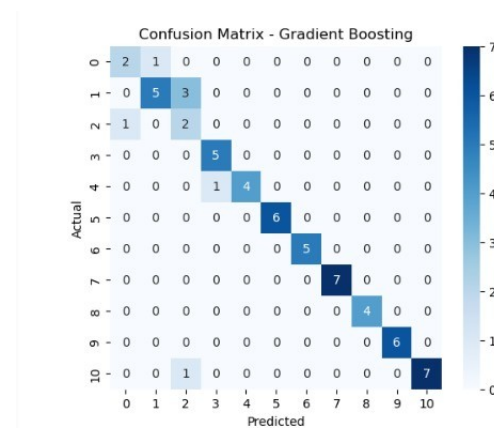
Figure 4.7: Confusion matrix for Gradient boosting

```
Gradient Boosting Accuracy: 0.8833

              precision    recall  f1-score   support

           0       0.67      0.67      0.67         3
           1       0.83      0.62      0.71         8
           2       0.33      0.67      0.44         3
           3       0.83      1.00      0.91         5
           4       1.00      0.80      0.89         5
           5       1.00      1.00      1.00         6
           6       1.00      1.00      1.00         5
           7       1.00      1.00      1.00         7
           8       1.00      1.00      1.00         4
           9       1.00      1.00      1.00         6
          10       1.00      0.88      0.93         8

    accuracy                           0.88        60
   macro avg       0.88      0.88      0.87        60
weighted avg       0.91      0.88      0.89        60
```

Figure 4.8: Classification report showing Gradient Boosting achieving 88.33(percent) accuracy with class-wise precision, recall, and F1-scores.

Figure 4.9: Confusion matrix illustrating the performance of an LDA classifier with accurate class-wise predictions.

Figure 4.10: Classification report showing LDA achieving 98.33(percent) accuracy with high precision, recall, and F1-scores across classes.
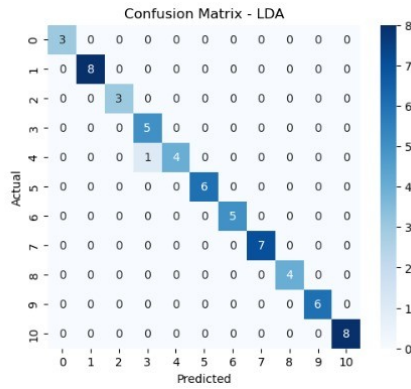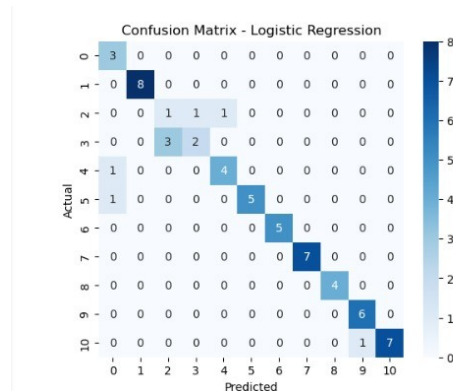

Figure 4.11: Confusion matrix illustrating the performance of a Logistic Regression classifier with class-wise prediction distribution.

```
Logistic Regression Accuracy: 0.8667

              precision    recall  f1-score   support

           0       0.60      1.00      0.75         3
           1       1.00      1.00      1.00         8
           2       0.25      0.33      0.29         3
           3       0.67      0.40      0.50         5
           4       0.80      0.80      0.80         5
           5       1.00      0.83      0.91         6
           6       1.00      1.00      1.00         5
           7       1.00      1.00      1.00         7
           8       1.00      1.00      1.00         4
           9       0.86      1.00      0.92         6
          10       1.00      0.88      0.93         8

    accuracy                           0.87        60
   macro avg       0.83      0.84      0.83        60
weighted avg       0.88      0.87      0.87        60
```

Figure 4.12: Classification report showing Logistic Regression achieving 86.67(percent) accuracy.
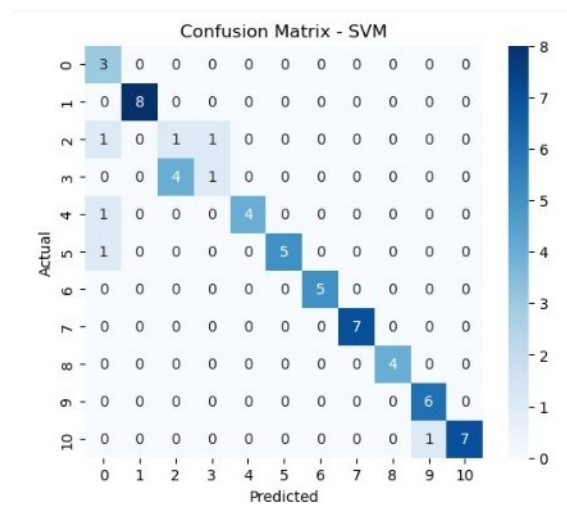

Figure 4.13: Confusion matrix illustrating the performance of an SVM classifier with classwise prediction distribution.

```
SVM Accuracy: 0.8500

              precision    recall  f1-score   support

           0       0.50      1.00      0.67         3
           1       1.00      1.00      1.00         8
           2       0.20      0.33      0.25         3
           3       0.50      0.20      0.29         5
           4       1.00      0.80      0.89         5
           5       1.00      0.83      0.91         6
           6       1.00      1.00      1.00         5
           7       1.00      1.00      1.00         7
           8       1.00      1.00      1.00         4
           9       0.86      1.00      0.92         6
          10       1.00      0.88      0.93         8

    accuracy                           0.85        60
   macro avg       0.82      0.82      0.81        60
weighted avg       0.88      0.85      0.85        60
```

Figure 4.14: Classification report showing SVM achieving 85.00(percent) accuracy with classwise precision, recall, and F1-scores.
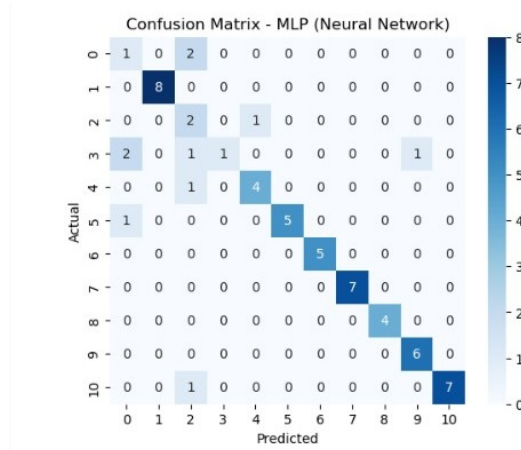
Figure 4.15: Confusion matrix illustrating the performance of an MLP (Neural Network) classifier with class-wise prediction distribution.

Figure 4.16: Classification report showing MLP (Neural Network) achieving 83.33(percent) accuracy with detailed precision, recall, and F1-scores.

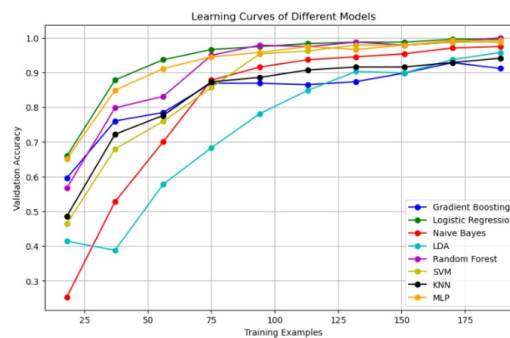Figure 4.17: Learning curves for different models

Both Support Vector Machine (SVM) and Logistic Regression are having best test accuracy of 98.33%. Naïve Bayes and Random Forest each achieving an accuracy of 96.67% and Gradient Boosting and K-Nearest Neighbors (KNN) both at 95% accuracy. The multi-layer perceptron (MLP) gave a test accuracy of 91. 67%. Linear discriminant analysis (LDA) was

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the weakest model among all models with only 90% accuracy. Learning curves indicate that Logistic Regression, SVM, and Random Forest are the best in validation accuracy with 1.0 being approached with increased training. Naïve Bayes and KNN are also close with high levels of accuracy converging. Gradient Boosting and MLP continue to improve, but are a little behind in performance. LDA starts out with the lowest accuracy but continues to improve.

CHAPTER 5

DISCUSSIONS AND CONCLUSION

This research compares eight machine learning algorithms such as Gradient Boosting, Logistic Regression, Naïve Bayes, Linear Discriminant Analysis (LDA), Random Forest, Support Vector Machine (SVM), KNearest Neighbors (KNN), and Multi-Layer Percep- tron (MLP) for cancer type prediction based on gene expression. Several challenges were faced and overcome during this research, such as class imbalance, which may cause skewed predictions, which was solved through the application of SMOTE (Synthetic Minority Over-sampling Technique) to balance the data. Feature selection, essential when dealing with high-dimensional gene expression data, was tuned using SelectKBest to ensure that only the most important features were used, thereby enhancing model efficiency. Computational complexity and hyperparameter tuning were addressed using grid search and crossvalidation, making sure that every model was adjusted for maximum accuracy. Scalability challenges, especially in larger datasets, were addressed through efficient pre-processing and parallel computation where necessary. Consequently, logistic regression and SVM produced the best accuracy 98.33%, followed by Naïve Bayes and Random Forest 96.67% and Gradient Boosting and KNN 95%, which demonstrates the effectiveness of the methodologies employed. MLP 91.67% exhibited moderate performance, and LDA 90% benefited from more training data. The learning curves confirmed that most models converged towards high accuracy.Together, these all solutions improve model performance, demonstrating the viability of machine learning in oncology and laying the groundwork for AI-driven diagnosis innovation.

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CHAPTER 6

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