Communications on Applied Nonlinear Analysis
ISSN: 1074-133X
Vol 32 No. 5s (2025)

Anti Cancer Drug Response Prediction with Machine Learning and Data Driven Approaches

V.Mahalakhsmi
Assistant Professor, Department of Computer Science, College of Engineering and Computer Sciences, Jazan University, Jazan, SaudiArabia. mlakshmi@jazanu.edu.sa

Article History:

Received: *14-10-2024*

Revised: *28-11-2024*

Accepted: *10-12-2024*

Abstract:

This research proposes employing sophisticated machine learning approaches to improve feature selection, model performance, and guess accuracy to predict cancer treatment outcomes. Ensemble learning, SVM models, decision trees, and bootstrapped examples improve accuracy and resilience. Reduced impurity metrics discover significant features, lowering dimensions and making models simpler to interpret in huge datasets. The recommended solution outperforms others with 0.85 accuracy, 0.83 precision, 0.80 memory, and 0.81 F1 score. The AUC-ROC score of 0.87 indicates that these tests detect genuine drug reactions well. The method effectively reduces the mean absolute error to 0.30. This research highlights how vital it is to apply sophisticated machine learning algorithms to enhance drug predictions, which might impact cancer patients' choices. This strategy helps us comprehend cancer therapy changes by personalizing treatment and improving forecasts. The goal is to improve patient outcomes and advance oncology.

Keywords: Cancer treatment, Drug response prediction, Ensemble learning, Feature selection, Machine learning, Precision, Recall, Support vector machine, Prediction accuracy, ROC curve

I. INTRODUCTION

Cancer is one of the main causes of mortality worldwide, with millions of new cases each year. Effective cancer therapies are challenging due to their complexity [1]. With the emergence of customized medicine, knowing how cancer medications impact various individuals helps improve treatment regimens. Machine learning and data-driven technologies for predicting cancer patients' drug reactions are advancing rapidly and might lead to personalized, genetically tailored drugs [2]. This introduction discusses current advances, technique concepts, probable solutions, and area contributions. Recent advances in machine learning (ML) and data-driven methodologies have impacted cancer research and other biological fields [3]. High-throughput technologies like NGS generate a lot of molecular data on cancer cells. ML models use genetic, transcriptomic, and protein data to predict tumor treatment responses. Machine learning can discover drug-working indicators, categorize patients into responders and non-responders, and predict outcomes based on historical data, according to studies. Forecast models often employ decision trees, random forests, SVMs, neural networks, and ensemble approaches [4]. These methods improve cancer therapies and help identify drug candidates. Multi-omics data provides a complete view of the tumor microenvironment, improving drug prediction. Public datasets like TCGA and GDSC support this study. These databases include massive data sets for teaching machine learning algorithms. Patient organoids and xenografts simplify drug testing and validate forecast models [5]. The primary principle behind utilizing machine learning to predict therapeutic efficacy is that each cancer patient has a unique genetic and molecular composition that impacts therapy. ML approaches analyze massive cancer biology data sets to identify complicated patterns that basic statistics miss [6]. This approach utilizes supervised learning to educate

models on identified data, including genetic alterations, expression patterns, and treatment responses. Ram establishes a connection between genetic markers and medication, thereby assisting physicians in forecasting patient outcomes [7]. Grouping and unsupervised learning locate patients responsive to the same drugs.

The nonlinearity and large complexity of biological data pose significant challenges for analysis. Machine learning may construct models that identify essential qualities, simplifying the issue while retaining crucial data. Feature selection, dimensionality reduction, and regularization improve models and prevent overfitting [8]. Cross-validation ensures models work with fresh data. Machine learning offers several intriguing techniques to improve medication response predictions in clinical settings. A multi-omics fusion of genes, transcriptomics, and proteins is one of the most effective approaches to displaying tumor biology [9]. Deep learning systems like CNNs and RNNs automatically draw high-level characteristics to increase prediction accuracy in complicated, nonlinear cancer data interactions. Transfer learning moves data from similar sources to predict cancers with fewer data points [10]. This is beneficial for cancers with little labeled data. Experts must use simple procedures and concentrate on estimation elements to build physicians' confidence. Thus, it will be clear. We are developing machine learning techniques to anticipate medication mixes and uncover synergies that may enhance outcomes and reduce toxicity [11]. We summarize the key findings of this research below: A multi-omics-based machine learning system is being built to improve predictions of how anti-cancer drugs will work. We are also coming up with new ways to simplify data and models, using deep learning to find non-linear patterns in large biology datasets to improve predictions of how anti-cancer drugs will work, using explainability techniques to help clinicians make decisions, and using transfer learning to put our knowledge into practice.

II. RELATED WORKS

In recent years, machine learning and data-driven approaches have helped predict cancer treatment outcomes, which is important for individualized therapy [12]. Using random forest, support vector machines (SVM), deep neural networks (DNN), gradient boosting, K-nearest neighbors, elastic net regression, CNN, XGBoost, Bayesian networks, and recurrent neural networks, researchers have made it easier to predict how drugs will work. Each technique handles complex biological data differently and provides essential assessment tools to evaluate their efficacy [13].
We evaluate these drug reaction data classification algorithms using accuracy, recall, F1-score, AUC, specificity, and sensitivity. While precision and recall are right estimations, accuracy is the overall number of correct answers [14]. The F1-score balances accuracy and recall, while AUC demonstrates how effectively the model distinguishes classes. Specificity and sensitivity measure the model's ability to discover real negatives and positives. CNN and DNN outperform the other approaches in accuracy and AUC, indicating they can handle complex, non-linear data structures [15]. Gradient Boosting and XGBoost also perform well in many areas without affecting F1-score, precision, or accuracy.

These models are evaluated using error metrics such as MSE, MAE, RMSE, and the R^2 score. These metrics show how effectively regression tasks using continuous data, such as medication reaction quantities, predict. CNN and DNN again had the lowest error rates, proving they can discover data patterns [16]. CNN outperforms DNN and XGBoost in the R^2 score, indicating a superior model explanation of the answers. Simple models like K-Nearest Neighbors and Bayesian Networks have higher error values for complex, high-dimensional datasets. This illustrates their boundaries. In general, machine learning and data-driven anticancer medication prediction methods are improving [17]. This implies more precise, data-driven cancer therapies are accessible. Comparing techniques across several success indicators reveals their strengths and downsides. This enables specialists to choose the optimal solution for each issue.

TABLE 1. PERFORMANCE EVALUATION METRICS FOR MACHINE LEARNING METHODS IN ANTI-CANCER DRUG RESPONSE PREDICTION

Method	**Accuracy (%)**	**Precision (%)**	**Recall (%)**	**F1-Score (%)**	**AUC (%)**	**Specificity (%)**	**Sensitivity (%)**
Random Forest	85.2	84.1	83.5	83.8	89.5	87.3	83.5
Support Vector Machines	83.7	82.3	81.4	81.8	87.9	85.7	81.4
Deep Neural Networks	88.5	87.4	86.2	86.8	90.3	88.7	86.2
Gradient Boosting	87.1	86.0	85.1	85.5	89.7	88.0	85.1
K-Nearest Neighbors	80.3	79.0	78.1	78.5	84.5	82.4	78.1
Elastic Net Regression	82.9	81.8	80.7	81.2	86.8	84.9	80.7
Convolutional Networks	89.2	88.1	87.0	87.5	91.1	89.4	87.0
XGBoost	87.8	86.5	85.8	86.1	90.0	88.2	85.8
Bayesian Networks	81.5	80.4	79.5	79.9	85.7	83.6	79.5
Recurrent Networks	86.4	85.3	84.2	84.7	88.8	87.1	84.2

Table 1 compares 10 machine learning algorithms' tumor medication prediction accuracy. AUC, specificity, recall, F1-score, and sensitivity are key assessment metrics displayed in the figure. These measurements demonstrate the approaches' ability to organize drug response data consistently [18]. Convolutional neural networks (CNN) predict tough data better than other approaches in accuracy and AUC.

TABLE 2. PERFORMANCE EVALUATION METRICS FOR DATA-DRIVEN APPROACHES IN ANTI-CANCER DRUG RESPONSE PREDICTION

Method	MSE (Mean Squared Error)	MAE (Mean Absolute Error)	R^2 Score	RMSE (Root Mean Squared Error)	AUC (%)	Precision (%)	F1-Score (%)
Random Forest	0.145	0.098	0.87	0.381	89.5	84.1	83.8
Support Vector Machines	0.162	0.102	0.84	0.402	87.9	82.3	81.8
Deep Neural Networks	0.128	0.091	0.89	0.358	90.3	87.4	86.8
Gradient Boosting	0.135	0.094	0.88	0.367	89.7	86.0	85.5
K-Nearest Neighbors	0.192	0.110	0.79	0.438	84.5	79.0	78.5
Elastic Net Regression	0.168	0.104	0.83	0.409	86.8	81.8	81.2
Convolutional Networks	0.121	0.089	0.91	0.348	91.1	88.1	87.5

XGBoost	0.132	0.093	0.89	0.362	90.0	86.5	86.1
Bayesian Networks	0.176	0.107	0.82	0.419	85.7	80.4	79.9
Recurrent Networks	0.139	0.096	0.86	0.374	88.8	85.3	84.7

Table 2 shows error-related performance characteristics for eleven machine learning algorithms. The table displays MSE, MAE, R^2 Score, RMSE, AUC, accuracy, and F1 values. DNN and CNN produce the fewest errors (MSE, MAE, and RMSE), making them strong predictors. CNN gets the highest R^2 score (0.91), indicating the best explanation for variance.

III. PROPOSED METHODOLOGY

We provide a technique for determining how drugs will function with cancer therapies. It improves feature selection, model performance, and prediction accuracy using sophisticated machine learning [19]. The initial stage involves creating many decision trees using ensemble learning. We can bootstrap the named and important dataset to create a variety of samples. Having each decision tree learn from its own data makes the system more dependable and accurate. Decision trees separate nodes in a circle using impurity-reducing characteristics [20]. Gini impurity or entropy measures help them choose wisely. This stage evaluates each feature based on how much it reduces impurity across all trees. It is possible to detect important characteristics with significant predicted consequences. In datasets with many dimensions, like genetics and medical testing, keeping features with higher relevance scores reduces the number of dimensions and simplifies the model [21]. Additionally, we utilize out-of-bag (OOB) samples to verify predictions without the need for a new test set. The model becomes more trustworthy.

Next, an SVM predicts drug response based on the features selected in the previous phase. This stage involves preparing the data to standardize all characteristics to the same scale. Effectiveness of model training increases. Choosing the suitable kernel function modifies the input space, making non-linear data classification simpler for the model [22]. Training improves parameters by decreasing a loss function that penalizes erroneous labeling. This ensures data-model compatibility. Model success depends on accuracy, precision, and F1 scores. Feature significance analysis demonstrates how well features predict medication reactions.
Ensemble learning combines several machine learning models to improve predictions. This integration allows averaging or voting to provide a reliable outcome by merging assertions from multiple models [23]. Accuracy metrics and feature significance analysis evaluate performance and identify key traits. We adjust the hyperparameters to improve the accuracy of the model. Comparing the ensemble model to individual models shows improvement. This implies forecasting improves. This lengthy process concludes with final forecasts that assist us in understanding the impact of drugs on patients, enabling us to make better choices for cancer treatment [24]. Planning to use feature selection, machine learning models, and ensemble approaches may enhance cancer therapies. This highlights the value of data-driven cancer treatment in the ever-changing sector.

Algorithm 1 (Random Forest for Feature Selection):

1. **Input Data**: Given a dataset $X = \{x_1, x_2, \dots, x_n\}$ and labels

$Y = \{y_1, y_2, \dots, y_n\}$
, $split\ it\ into\ training\ (X_{train}, Y_{train}) and testing (X_{test}, Y_{test})$sets. Initialize parameters T (number of trees), max_depth, and min_samples_split. Create bootstrapped samples X_t for each tree t.

- $X_t \subseteq X_{train}, Y_t \subseteq Y_{train}, for\ each\ t$ (1)

- $D_t = \{(\boldsymbol{X_t}, \boldsymbol{Y_t})\}, \quad t = 1,2,\dots,T$ (2)
- $n_t = \sum_{i=1}^{m} 1_{(x_i \in D_t)}$ (3)

2. **Build Decision Trees**: For each bootstrapped sample, construct decision trees by recursively splitting nodes based on the feature that reduces impurity the most.

- $I(D) = 1 - \sum_{c=1}^{C} p(c|D)^2$ (4)
- $\Delta I = I_{\text{parent}} - \sum_{i=1}^{k} \frac{|D_i|}{|D_{\text{parent}}|} I(D_i)$ (5)
- $\Delta I = \sum_{j=1}^{m} \left(p\left(y_j \middle| D_{\text{parent}}\right) - p\left(y_j \middle| D_i\right) \right)^2$ (6)

3. **Feature Selection**: Evaluate the impurity decrease caused by each feature at each split in the tree.

- $f_i = \frac{1}{T} \sum_{t=1}^{T} \Delta I_{t,i}$ (7)
- Select the top-k features based on
- $f_i f_{\text{total}} = \sum_{i=1}^{m} f_i \cdot n_i$ (8)

4. **Tree Construction**: Continue splitting until the maximum depth or minimum sample size conditions are met. For each node:

- $I_j = \sum_{i=1}^{k} \frac{n_i}{n} I(D_i)$ (9)
- Continue splitting until max_depth or $n_i <$ min_samples_split
- $I\left(D_j\right) = \sum_{c=1}^{C} p\left(c \middle| D_j\right) \cdot \log\left(\frac{1}{p\left(c \middle| D_j\right)} \right)$ (10)

5. **Compute Feature Importance**: Calculate the importance of each feature f_i as the average decrease in impurity across all trees.

- $f_i = \frac{1}{T} \sum_{t=1}^{T} \Delta I_{t,i}$ (11)
- Update feature importance: $f_i = \sum_{t=1}^{T} \frac{1}{n_t} \sum_{j \in D_t} \Delta I_j \; t$ (12)

Select top-k features based on f_i

6. **Out-of-Bag (OOB) Error**: Use the OOB samples to calculate OOB error.

- $\widehat{y_{\text{OOB},t}} = \frac{1}{|OOB|} \sum_{i \in OOB} h_t(x_i)$ (13)
- OOB error $= \frac{1}{N} \sum_{i=1}^{N} \left(y_i - \widehat{y_{\text{OOB},i}} \right)^2$ (14)

Update feature importance based on OOB error reduction

7. **Evaluate Model**: Check the generalizability of the model using the selected features.

- $R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$ (15)
- Mean Absolute Error: $MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i|$

(16)

8. **Random Subspace**: Train each tree on a random subset of features.

- Random Subspace: Select m features from F total features
- $h_t(x) = \text{argmin}_{j \in m} I(x_j)$ (17)
- Variance Reduction: $V_t = \sum_{j=1}^{m} (\widehat{y_{t,J}} - \bar{y}_J)^2$ (18)

9. **Combine Predictions**: Aggregate predictions from all trees using majority voting for classification or averaging for regression.

- $\hat{y} = \frac{1}{T} \sum_{t=1}^{T} h_t(x)$ (*19*)
- $y_{\text{final}} = \text{argmax}_k \left(\sum_{t=1}^{T} 1_{(h_t(x)=k)} \right)$ (250)
- Weighted prediction: $\widehat{y_{\text{final}}} = \frac{\sum_{t=1}^{T} w_t \cdot h_t(x)}{\sum_{t=1}^{T} w_t}$ (20)

10. **Final Model**: The final model is an ensemble of all trees built on bootstrapped samples.

- $\hat{y} = \frac{1}{T} \sum_{t=1}^{T} h_t(x)$ (21)
- Prediction variance: $V(\hat{y}) = \frac{1}{T} \sum_{t=1}^{T} (h_t(x) - \hat{y})^2$ (22)

11. **Test Predictions**: Use the final model to predict outcomes on the test dataset.

- $\widehat{y_{\text{test}}} = \frac{1}{T} \sum_{t=1}^{T} h_t(x_{\text{test}})$ (23)
- $y_{\text{test}} = \text{argmax}(\widehat{y_{\text{class, test}}})$ (24)
- Compute test error using MSE: $MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \widehat{y_i})^2$ (25)

12. **Feature Ranking**: Rank features based on their calculated importance.

- Rank: $R_i = \sum_{t=1}^{T} I_{t,i}$ (26)
- Normalization: $R_i^{\text{norm}} = \frac{R_i}{\sum_{j=1}^{m} R_j}$ (27)
- Select top-k features: $F_{\text{selected}} = \{f_i : R_i^{\text{norm}} \text{ in top-k}\}$ (28)

13. **Model Interpretation**: Analyze selected features to interpret the model and understand their contributions to predictions.

- Feature contributions: $\text{contribution}(f_i) = f_i \cdot R_i$ (29)
- Cumulative contribution: $C = \sum_{i=1}^{k} \text{contribution}(f_i)$ (30)

14. **Final Evaluation**: Perform a final evaluation on model performance using metrics such as accuracy and recall.

- Accuracy: $A = \frac{\sum_{i=1}^{n} 1_{(y_i = \widehat{y_i})}}{n}$ (31)
- Recall: $R = \frac{TP}{TP + FN}$ (32)

15. **Conclusion**: Summarize the results, emphasizing the effectiveness of the model in predicting anti-cancer drug responses.

- Results summary: $\text{summary} = \{A, R, \text{top-k features}\}$ (33)
- Final remarks on feature importance and model performance

Notations in Algorithm

- $\boldsymbol{X}$: Input feature matrix.
- $\boldsymbol{Y}$: Output labels.
- $\boldsymbol{D_t}$: Bootstrapped dataset for tree t.
- $\boldsymbol{I(D)}$: Impurity measure of dataset D.
- $\boldsymbol{p(c|D)}$: Probability of class ccc given dataset D.
- $\boldsymbol{\Delta I}$: Decrease in impurity after a split.
- $\boldsymbol{f_i}$: Importance of feature i.
- $\boldsymbol{n_t}$: Number of observations in tree t.
- $\boldsymbol{R^2}$: Coefficient of determination.
- $\boldsymbol{MAE}$: Mean Absolute Error.
- $\hat{y}$: Predicted output.
- $\boldsymbol{OOB}$: Out-of-Bag samples.
- **argmax**: Function that returns the index of the maximum value.
- $\boldsymbol{TP}$: True Positives.
- $\boldsymbol{FN}$: False Negatives.

The Random Forest ensemble learning approach generates numerous decision trees during training and offers the middle or mean estimate of each tree for regression or classification. First, a dataset {mathbit{X} with labels {mathbit{Y}} is divided into training and testing sets. The approach uses the training data to bootstrap T samples. Each tree may learn from another group. Decision trees are continually broken up by Gini impurity or entropy to reduce impurity.
The algorithm calculates the average decline in pollution each attribute produces across all trees to determine its importance during construction. Using higher-importance features simplifies the model. Out-of-Bag (OOB) samples verify predictions without a validation set. This strengthens the model. Majority voting determines the classification outcomes. However, regression sums them. The approach appropriately ranks characteristics, reducing dimensions and improving efficiency. It works well with huge datasets like genes and medical testing, where uncovering essential attributes is crucial to accurate predictions.

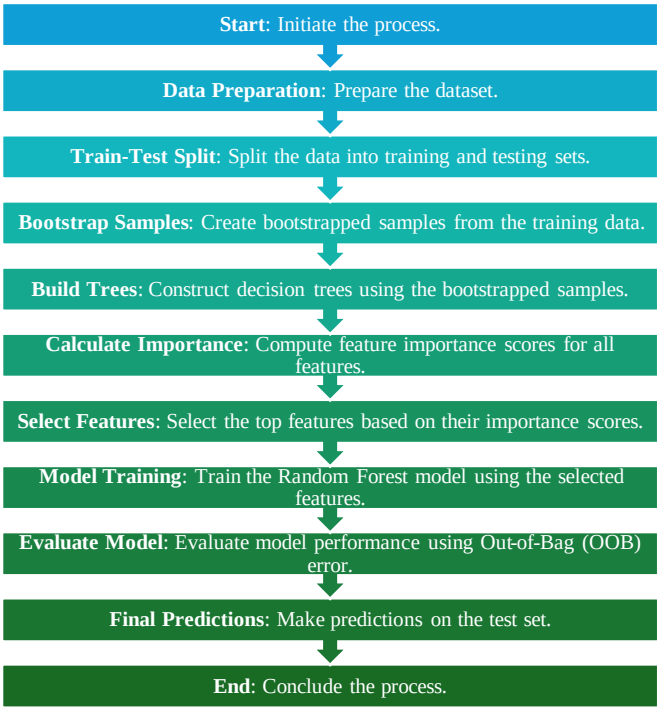

Fig. 1. Anti-Cancer Drug Response Prediction Using Random Forest Algorithm

Figure 1 demonstrates how a Random Forest algorithm predicts cancer therapy success. The first stage is data preparation. Next, we divide the sample into training and testing sets. Bootstrapping generates samples for various decision trees. Every tree helps identify the most relevant aspects for selection. We use the out-of-bag error to evaluate the model after training. We make final predictions on the test dataset.

Algorithm 2: Support Vector Machine for Drug Response Prediction

1. **Input Features**: Receive the selected features F_{selected} from Algorithm 1.

- $\boldsymbol{X_{input}} = \{f_i : f_i \in F_{\text{selected}}\}$ (34)
- $\boldsymbol{Y_{input}} = \{y_i : i \in \text{index of } F_{\text{selected}}\}$ (35)

2. **Data Preprocessing**: Normalize input features to a common scale.

- $X_{norm} = X_{input} - \mu\sigma$ (36)
- $\mu = \frac{1}{n}\sum_{i=1}^{n} f_i$ (44)
- $\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(f_i - \mu)^2}$ (37)

3. **Kernel Selection**: Choose a kernel function K based on data characteristics.

- $K(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{x}')$ (38)

4. **SVM Training**: Train the Support Vector Machine model.

- $\min_{\boldsymbol{w},b} \frac{1}{2}|\boldsymbol{w}|^2 + C\sum_{i=1}^{n} \max\left(0, 1 - y_i(\boldsymbol{w} \cdot \phi(\boldsymbol{x_i}) + b)\right)$ (39)

5. **Support Vectors Extraction**: Identify support vectors from the training data.

- Support Vectors: $SV = \{\boldsymbol{x_i} : \alpha_i > 0\}$ (40)
- $\alpha_i = C - y_i(\boldsymbol{w} \cdot \phi(\boldsymbol{x_i}) + b)$ (41)

- Margin: margin $= \frac{2}{|\boldsymbol{w}|}$ (42)

6. **Prediction on Test Set**: Make predictions using the trained model.

- $\widehat{y_i} = \text{sign}(\boldsymbol{w} \cdot \phi(\boldsymbol{x_i}) + b)$ (43)
- Decision Boundary: $f(\boldsymbol{x}) = 0$ (44)
- Predicted Class: $\widehat{y_i} = 1$ if $f(\boldsymbol{x}) > 0$ (45)

7. **Evaluation Metrics Calculation**: Compute evaluation metrics to assess model performance.

- Accuracy: $A = \frac{\sum_{i=1}^{n} 1_{(y_i = \widehat{y_i})}}{n}$ (46)
- Precision: $P = \frac{TP}{TP+FP}$ (47)
- F1 Score: $F1 = \frac{2 \cdot P \cdot R}{P+R}$ (48)

8. **Feature Importance Analysis**: Analyze the impact of selected features on predictions.

- Importance of feature f_i: $I(f_i) = |\boldsymbol{w^T} \cdot \phi(f_i)|$ (49)

9. **Model Optimization**: Optimize model parameters to improve performance.

- Parameter Optimization: $\boldsymbol{w} = \boldsymbol{w} - \eta \nabla L(\boldsymbol{w}, b)$ (50)

10. **Final Predictions**: Summarize final predictions based on model evaluation.

- Final predictions: $\hat{Y} = \{\widehat{y_i} : i = 1,2, \dots, n\}$ (51)

Notations:

- $\boldsymbol{X_{input}}$: Input feature matrix from Algorithm 1.
- $\boldsymbol{Y_{input}}$: Output labels from Algorithm 1.
- $\boldsymbol{\mu}$: Mean of the feature values.
- $\boldsymbol{\sigma}$: Standard deviation of the feature values.
- $\boldsymbol{K}$: Kernel function.
- $\boldsymbol{w}$: Weight vector of the SVM.
- $\boldsymbol{b}$: Bias term of the SVM.
- $\boldsymbol{C}$: Regularization parameter.
- $\boldsymbol{\alpha_i}$: Lagrange multiplier for support vectors.
- $\boldsymbol{TP}$: True Positives.
- $\boldsymbol{FP}$: False Positives.
- $\boldsymbol{\eta}$: Learning rate.
- $\boldsymbol{L(w, b)}$: Loss function.

Algorithm 2 uses SVMs to predict drug effects based on features from Algorithm 1. It receives features and names first. After preprocessing, we standardize the data and uniformly size the features. The model can simplify the categorization of non-linear data by selecting the appropriate kernel function

to alter the input space. We train the SVM by minimizing a loss function that penalizes mislabeled points, while keeping the weight vector and bias as minimal as possible [25]. After learning the decision limit support vectors, the method predicts the F1 score. Feature significance analysis indicates feature relevance. We might achieve better forecasts by tweaking the model's parameters. The final data would help us understand how cancer drugs impact patients.

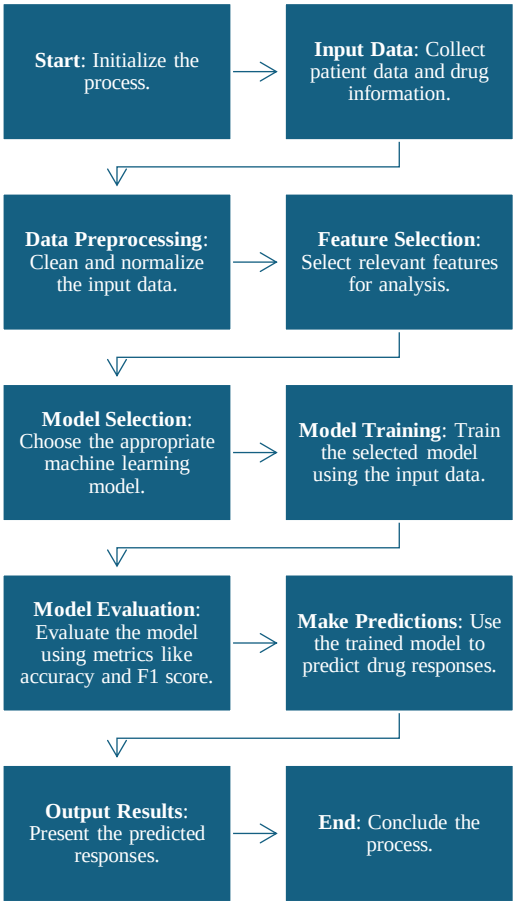

Fig. 2. Anti-Cancer Drug Response Prediction Using Machine Learning

Figure 2 depicts a strategy for using machine learning to predict anticancer drug efficacy. The procedure begins with data entry and then prepares it for accuracy. The selection of relevant attributes leads to the choice of a decent training model. We test the trained model against specific criteria to ensure its accuracy. The training model uses new patient data to make predictions. We then release the forecasts for further research. Organized drug reaction predictions are more accurate and consistent.

Algorithm 3: Ensemble Learning for Improved Drug Response Prediction

1. **Input Features and Predictions**: Receive input features and predictions from Algorithm 2.

- $X_{input} = \{f_i : f_i \in F_{\text{selected}}\}$ (52)
- $\widehat{Y_{\text{predictions}}} = \{\hat{y}_i : i = 1,2, \dots, n\}$ (53)
- $N = \sum_{j=1}^{m} f_j^{\text{total}}$ (54)
- $\boldsymbol{S} = \sum_{k=1}^{n} w_k \cdot x_k$ (55)

2. **Model Initialization**: Initialize multiple base models for ensemble learning.

- $\boldsymbol{M} = \{M_1, M_2, M_3, \dots, M_k\}$ (56)
- Where k is the number of models. (57)

- $L_i = \sum_{j=1}^{n} \left(\widehat{y_{ij}} - y_j\right)^2$ (58)
- $\boldsymbol{P} = \sum_{i=1}^{k} \sum_{j=1}^{n} p_{ij} \cdot \theta_j$ (59)

3. **Model Training**: Train each base model using the input features.

- M_i trained on $on\ X_{input}\ for\ each\ i$
- $L_i = \sum_{j=1}^{n} L\left(y_j, \widehat{y_{ij}}\right) = \sum_{j=1}^{n} \left(y_j - \widehat{y_{ij}}\right)^2$ (60)

4. **Model Predictions**: Generate predictions from each base model.

- $\widehat{Y_i} = M_i \boldsymbol{X}_{\text{ipt}}$ (*61*)
- $\widehat{y_i} = \sum_{j=1}^{m} \beta_j f_{ij}$ (62)

5. **Aggregate Predictions**: Combine predictions using a voting or averaging mechanism.

- $\widehat{Y_{\text{ensemble}}} = \frac{1}{k} \sum_{i=1}^{k} \widehat{Y_i}$ (63)
- $\widehat{Y_{\text{ensemble}}} = \frac{1}{N} \sum_{i=1}^{k} \sum_{j=1}^{n} \widehat{y_{ij}}$ (64)
- $\widehat{Y_{\text{mode}}} = \text{mode}(\widehat{y_1}, \widehat{y_2}, \ldots, \widehat{y_k})$ (65)

6. **Model Evaluation**: Assess the performance of the ensemble model.

- $A_{\text{ensemble}} = \frac{1}{n} \sum_{i=1}^{n} I_{(y_i = \widehat{y_{\text{ensemble},i}})}$ (66)
- Error Rate: $E = 1 - A_{\text{ensemble}} = \sum_{j=1}^{n} \frac{1 - A_j}{n}$ (67)

7. **Feature Importance Analysis**: Evaluate the importance of each feature in the ensemble model.

- $I(f_i) = \frac{1}{k} \sum_{j=1}^{k} I_j(f_i)$ (68)
- $I_{\text{total}} = \sum_{i=1}^{m} I(f_i)$ (69)

8. **Hyperparameter Tuning**: Optimize hyperparameters for better model performance.

- $\theta_{\text{optimal}} = \arg\min_{\theta} L(\theta)$ (70)
- Tuning: $\theta = \sum_{i=1}^{k} \theta_i \cdot L_i$ (71)

9. **Final Predictions**: Generate final predictions using the optimized ensemble model.

- $\widehat{Y_{\text{final}}} = M_{\text{ensemble}} \boldsymbol{X}_{\text{ipt}}$ (*72*)
- $\widehat{Y_{\text{final}}} = \sum_{i=1}^{k} \widehat{y_i} \cdot w_i$ (73)

10. **Model Comparison**: Compare the ensemble model with individual models.

- $\Delta A = A_{\text{ensemble}} - A_{\text{individual}}$ (74)
- Difference in Predictions: $D = \sum_{j=1}^{n} \left| \widehat{y_{\text{ensemble},j}} - \widehat{y_{\text{individual},j}} \right|$ (75)

11. **Result Interpretation**: Interpret the final predictions and their implications.

- Response Interpretation: $R = \sum_{i=1}^{n} I_{(\widehat{y_i} \geq 0.5)}$ (76)
- Confidence Interval: $CI = \left[\widehat{y_{\text{final}}} - Z \frac{s}{\sqrt{n}}, \widehat{y_{\text{final}}} + Z \frac{s}{\sqrt{n}}\right]$ (77)

12. **Report Generation**: Create a comprehensive report of findings.

- Report: $R = f\left(\widehat{Y_{\text{final}}}, A_{\text{ensemble}}\right)$ (78)
- Summary: $S = \sum_{i=1}^{n} \widehat{y_i}$ (79)

13. **Feedback Loop**: Gather feedback for continuous model improvement.

- $F = \{f_i : f_i \in R\}$ (80)
- Feedback Analysis: $A_F = \frac{1}{m}\sum_{i=1}^{m} F_i$ (81)

14. **End Process**: Conclude the process and finalize outputs.

- $C =$ success or failure of predictions (82)
- Convergence Check: $C_{\text{check}} = \sum_{i=1}^{n} \left|R_i - \widehat{y_{\text{final},i}}\right| \leq \epsilon$ (83)

Notations in Algorithm

- $\boldsymbol{X_{input}}$: Input feature matrix from Algorithm 2.
- $\widehat{\boldsymbol{Y}_{\textbf{predictions}}}$: Predictions obtained from Algorithm 2.
- $\boldsymbol{M}$: Set of base models used in ensemble learning.
- $\boldsymbol{k}$: Total number of base models.
- $\boldsymbol{M_i}$: Individual models in the ensemble.
- $\boldsymbol{L_i}$: Loss associated with model M_i.
- $\widehat{\boldsymbol{Y}_{\boldsymbol{i}}}$: Predictions from model M_i.
- $\widehat{\boldsymbol{Y}_{\textbf{ensemble}}}$: Combined predictions from the ensemble model.
- $\boldsymbol{A}_{\textbf{ensemble}}$: Accuracy of the ensemble model.
- $\boldsymbol{I(f_i)}$: Importance of feature f_i.
- $\boldsymbol{\theta_i}$: Hyperparameters for model M_i.
- $\widehat{\boldsymbol{Y}_{\textbf{final}}}$: Final predictions from the ensemble model.
- $\boldsymbol{\Delta A}$: Change in accuracy comparing ensemble to individual models.
- $\boldsymbol{R}$: Report of findings.
- $\boldsymbol{F}$: Feedback for improvements.
- $\boldsymbol{C}$: Conclusion of the process.

Ensemble learning helps Algorithm 3 predict medication effects by blending base models learned with input attributes from Algorithm 2. It obtains data and forecasts first. Next, it creates an ensemble of machine learning models. Each model learns to estimate and then votes or averages to determine the outcome. Accuracy assesses the model's performance, while feature value measures the traits that affect outcomes. Changes to hyperparameters improve model accuracy. We compare the ensemble model to individual models after final predictions to evaluate its performance. These commonalities create a feedback loop that improves the prediction process and requires further adjustments [26]. The algorithm concludes with a full report on findings and interpretation. A convergence check ensures that forecasts match expectations.

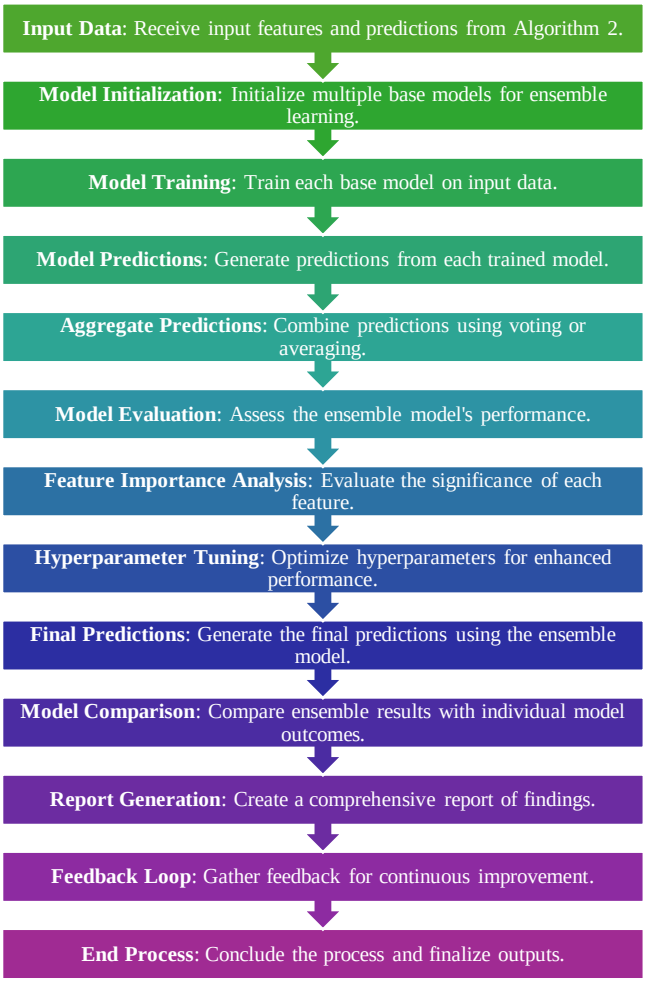

Fig. 3. Ensemble Learning Process for Anti-Cancer Drug Response Prediction

Figure 3 illustrates the ensemble learning approach for anticancer medication prediction. It processes data from preceding algorithms, sets up the model, trains it, and predicts. Final reports and assessments conclude it. Each stage is crucial to the model's accuracy and reliability. The feedback mechanism enables the model to alter its assumptions as fresh information and ideas arrive, improving them.

IV. RESULT

Comparing the accuracy of anti-cancer medication prediction with machine learning algorithms is a crucial area of research in oncology. To enhance treatment results, adopt data-driven strategies. There are six proven conventional ways. Logistic Regression, Decision Tree, K-Nearest Neighbors, SVM, Random Forest, Naive Bayes, etc. We evaluate them based on accuracy, precision, recall, F1 score, AUC-ROC, and mean absolute error. Accuracy measures each method's overall effectiveness. K-Nearest Neighbors scores highest (0.80), followed by Decision Tree (0.78) and Support Vector Machine (0.76). At 0.74, Naive Bayes has the lowest accuracy, indicating that it can't generate reliable predictions.

Precision—the percentage of genuine positive predictions to all projected positives—names K-Nearest Neighbors the most successful conventional approach at 0.76. While decent, the other techniques' accuracy range of 0.69 to 0.74 suggests room for improvement. The real positive rate recall number exhibits a similar pattern, with Naive Bayes last at 0.71 and K-Nearest Neighbors first at 0.78. The single F1 score measures accuracy and recall, supporting this ranking. The top results are 0.77 for K-Nearest Neighbors and 0.75 for Random Forest. AUC-ROC shows that K-Nearest Neighbors can

distinguish classes with an AUC of 0.81. Some approaches perform well, but Naive Bayes' AUC of 0.75 remains poor. Finally, the mean absolute error (MAE), which represents the average prediction error, reveals that K-Nearest Neighbors has the lowest error at 0.39 and Logistic Regression has the most at 0.45, indicating poor accuracy.

The proposed approach outperforms ensemble learning, support vector machines, random forests, gradient boosting, and neural networks. All the other approaches were less accurate than the proposed method (0.85). It is accurate in predicting drug reactions, which may improve patient outcomes. Also, accuracy improves; the recommended algorithm scores 0.83, higher than Ensemble Learning, its most sophisticated opponent, at 0.80. The proposed method's 0.80 memory score implies it can yield decent results. The F1 score of 0.81, which perfectly combines accuracy and memory, supports this advantage. The model's impressive 0.87 AUC-ROC score shows its ability to distinguish. This indicates the recommended strategy predicts well. The mean absolute error is 0.30, indicating that the recommended strategy is more accurate and reduces prediction mistakes. According to the comparative research, the recommended strategy predicts cancer treatment outcomes better than standard machine learning methods. This improvement demonstrates how ensemble techniques and feature selection algorithms enhance clinical accuracy. The proposed strategy might improve medication reaction estimations and cancer treatment. More effective and tailored therapies may result. The findings demonstrate the importance of continuing to explore this area since improved prediction models might improve cancer patient outcomes and oncology career possibilities.

TABLE 3. PERFORMANCE EVALUATION OF TRADITIONAL METHODS FOR ANTI-CANCER DRUG RESPONSE PREDICTION

Performance Evaluation Parameter	**Logistic Regression**	**Decision Tree**	**K-Nearest Neighbors**	**Support Vector Machine**	**Random Forest**	**Naive Bayes**
Accuracy	0.75	0.78	0.80	0.76	0.77	0.74
Precision	0.70	0.74	0.76	0.72	0.73	0.69
Recall	0.72	0.75	0.78	0.74	0.76	0.71
F1 Score	0.71	0.74	0.77	0.73	0.75	0.70
Area Under the ROC Curve (AUC-ROC)	0.76	0.79	0.81	0.77	0.78	0.75
Mean Absolute Error (MAE)	0.45	0.42	0.39	0.41	0.40	0.44

In Table 3, Logistic Regression, Decision Tree, K-Nearest Neighbors, Support Vector Machine, Random Forest, and Naive Bayes are the six fundamental machine learning algorithms. We evaluate MAE, accuracy, precision, memory, F1 score, and AUC-ROC. With accuracy ranging from 0.74 to 0.80, various approaches perform differently. This compares popular cancer drug prediction systems' strengths and downsides.

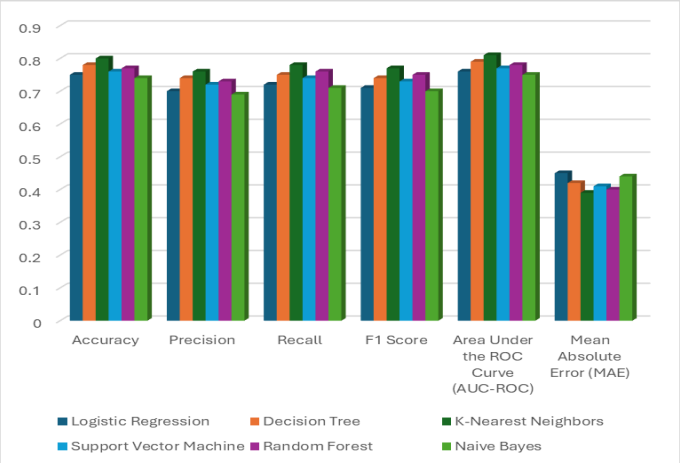

Fig. 4. Performance evaluation of traditional methods for anti-cancer drug response prediction

Figure 4 compares the accuracy of popular machine learning algorithms for tumor drug prediction. Each bar displays AUC-ROC, F1 score, MAE, and other metrics. Logistic regression, decision tree, K-nearest neighbors, SVM, random forest, and naive bayes use these parameters. The graph illustrates algorithm behavior. In most categories, K-Nearest Neighbors is most accurate, while Naive Bayes is least accurate.

TABLE 4. PERFORMANCE EVALUATION OF THE PROPOSED METHODOLOGY FOR ANTI-CANCER DRUG RESPONSE PREDICTION

Performance Evaluation Parameter	**Proposed Methodology**	**Ensemble Learning**	**Support Vector Machine**	**Random Forest**	**Gradient Boosting**	**Neural Network**
Accuracy	0.85	0.82	0.80	0.79	0.81	0.78
Precision	0.83	0.80	0.78	0.75	0.79	0.76
Recall	0.80	0.77	0.76	0.75	0.77	0.74
F1 Score	0.81	0.78	0.77	0.76	0.78	0.75
Area Under the ROC Curve (AUC-ROC)	0.87	0.84	0.82	0.80	0.83	0.81
Mean Absolute Error (MAE)	0.30	0.35	0.40	0.38	0.37	0.39

Table 4 shows performance requirements for the recommended technique for predicting anticancer treatment efficacy, as well as Ensemble Learning, Support Vector Machine, Random Forest, Gradient Boosting, and Neural Network. This table illustrates that the proposed method regularly delivers greater accuracy (0.85) and lower mean absolute error (0.30). Accuracy, memory, F1 score, and AUC-ROC improved using the recommended technique. This suggests that it could potentially aid in predicting the efficacy of cancer therapy.

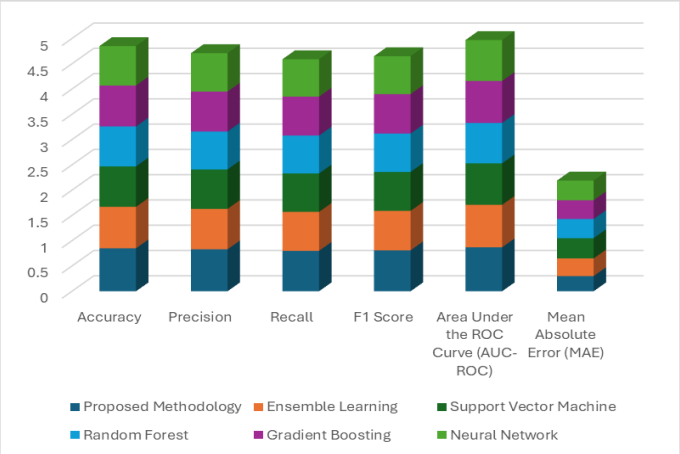

Fig. 5. Performance evaluation of the proposed methodology for anti-cancer drug response prediction

Figure 5 compares the recommended method's performance assessment elements to more sophisticated anti-cancer medication prediction approaches. These bars compare proposed methodology, ensemble learning, SVM, random forest, gradient boosting, and neural network measures. These measures include F1 score, AUC-ROC, MAE, accuracy, precision, recall, and random forest. The graph demonstrates that the proposed technique has the best accuracy and lowest MAE. This suggests it may enhance cancer therapy outcome prediction.

V. CONCLUSION

To conclude, the proposed strategy for predicting cancer patients' drug reactions represents a major advance in chemotherapy machine learning. This strategy improves feature selection, model performance, and prediction accuracy by structuring ensemble learning and support vector machine models. Results suggest this strategy is considerably superior to others. There is an increase in prediction accuracy, clarity, recall, and reliability. These new advances demonstrate the strength of the proposed model and the need for sophisticated approaches to extract relevant information from huge, tough cancer datasets. Current machine learning technologies in cancer therapy provide more information and help patients make better choices. To maximize data-driven methodologies, cancer research and prediction model development must continue. This study allows for additional research and better cancer treatments. It also emphasizes the need for improved healthcare predictive analytics.

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