

Model Optimization and Tuning Phase Template

Date	July 2024
Team ID	739675
Project Title	Drug classification using machine learning
Maximum Marks	10 Marks

Model Optimization and Tuning Phase

The Model Optimization and Tuning Phase involves refining machine learning models for peak performance. It includes optimized model code, fine-tuning hyperparameters, comparing performance metrics, and justifying the final model selection for enhanced predictive accuracy and efficiency.

Hyperparameter Tuning Documentation (6 Marks):

Model	Tuned Hyperparameters
Decision tree	<pre>def decisionTree(x_train, x_test, y_train, y_test): dt=DecisionTreeClassifier() dt.fit(x_train,y_train) yPred = dt.predict(x_test) print('***DecisionTreeClassifier***') print('Confusion matrix') print(confusion_matrix(y_test,yPred)) print('Classification report') print(classification_report(y_test,yPred))</pre>

Random forest	<pre>def randomForest(x_train, x_test, y_train, y_test): rf = RandomForestClassifier() rf.fit(x_train,y_train) yPred = rf.predict(x_test) print('***RandomForestClassifier***') print('Confusion matrix') print(confusion_matrix(y_test,yPred)) print('Classification report') print(classification_report(y_test,yPred))</pre>
Kneighbors	<pre>def KNN(x_train, x_test, y_train, y_test): knn = KNeighborsClassifier() knn.fit(x_train,y_train) yPred = knn.predict(x_test) print('***KNeighborsClassifier***') print('Confusion matrix') print(confusion_matrix(y_test,yPred)) print('Classification report') print(classification_report(y_test,yPred))</pre>
Gradient boosting	<pre>def xgboost (x_train, x_test, y_train, y_test): xg = GradientBoostingClassifier() xg.fit(x_train,y_train) yPred = xg.predict(x_test) print('***Gradient BoostingClassifier***') print('Confusion matrix') print(confusion_matrix(y_test,yPred)) print('Classification report') print(classification_report (y_test, yPred))</pre>

Performance Metrics Comparison Report (2 Marks):

Model	Baseline Metric	Optimized Metric

Decision tree	<table><tr><td>accuracy</td><td></td><td></td><td>0.97</td><td>60</td></tr><tr><td>macro avg</td><td>0.96</td><td>0.93</td><td>0.93</td><td>60</td></tr><tr><td>weighted avg</td><td>0.97</td><td>0.97</td><td>0.97</td><td>60</td></tr></table>	accuracy			0.97	60	macro avg	0.96	0.93	0.93	60	weighted avg	0.97	0.97	0.97	60	<pre>***DecisionTreeClassifier*** Confusion matrix [[25 0 0 0 0] [0 7 0 0 0] [0 2 4 0 0] [0 0 0 7 0] [0 0 0 0 15]] Classification report precision recall f1-score support DrugY 1.00 1.00 1.00 25 drugA 0.78 1.00 0.88 7 drugB 1.00 0.67 0.80 6 drugC 1.00 1.00 1.00 7 drugX 1.00 1.00 1.00 15</pre>
accuracy			0.97	60													
macro avg	0.96	0.93	0.93	60													
weighted avg	0.97	0.97	0.97	60													
Random forest	<table><tr><td>accuracy</td><td></td><td></td><td>0.95</td><td>60</td></tr><tr><td>macro avg</td><td>0.94</td><td>0.90</td><td>0.91</td><td>60</td></tr><tr><td>weighted avg</td><td>0.96</td><td>0.95</td><td>0.95</td><td>60</td></tr></table>	accuracy			0.95	60	macro avg	0.94	0.90	0.91	60	weighted avg	0.96	0.95	0.95	60	<pre>***RandomForestClassifier*** Confusion matrix [[25 0 0 0 0] [0 7 0 0 0] [0 2 4 0 0] [0 0 0 6 1] [0 0 0 0 15]] Classification report precision recall f1-score support DrugY 1.00 1.00 1.00 25 drugA 0.78 1.00 0.88 7 drugB 1.00 0.67 0.80 6 drugC 1.00 0.86 0.92 7 drugX 0.94 1.00 0.97 15</pre>
accuracy			0.95	60													
macro avg	0.94	0.90	0.91	60													
weighted avg	0.96	0.95	0.95	60													
Kneighbors	<table><tr><td>accuracy</td><td></td><td></td><td>0.37</td><td>60</td></tr><tr><td>macro avg</td><td>0.23</td><td>0.24</td><td>0.22</td><td>60</td></tr><tr><td>weighted avg</td><td>0.28</td><td>0.37</td><td>0.30</td><td>60</td></tr></table>	accuracy			0.37	60	macro avg	0.23	0.24	0.22	60	weighted avg	0.28	0.37	0.30	60	<pre>***KNeighborsClassifier*** Confusion matrix [[18 2 1 0 4] [6 0 0 0 1] [3 0 2 0 1] [5 0 0 0 2] [10 1 1 1 2]] Classification report precision recall f1-score support DrugY 0.43 0.72 0.54 25 drugA 0.00 0.00 0.00 7 drugB 0.50 0.33 0.40 6 drugC 0.00 0.00 0.00 7 drugX 0.20 0.13 0.16 15</pre>
accuracy			0.37	60													
macro avg	0.23	0.24	0.22	60													
weighted avg	0.28	0.37	0.30	60													
Gradient boosting	<table><tr><td>accuracy</td><td></td><td></td><td>0.93</td><td>60</td></tr><tr><td>macro avg</td><td>0.93</td><td>0.87</td><td>0.88</td><td>60</td></tr><tr><td>weighted avg</td><td>0.94</td><td>0.93</td><td>0.93</td><td>60</td></tr></table>	accuracy			0.93	60	macro avg	0.93	0.87	0.88	60	weighted avg	0.94	0.93	0.93	60	<pre>***Gradient BoostingClassifier*** Confusion matrix [[25 0 0 0 0] [0 7 0 0 0] [0 2 3 0 1] [0 0 0 6 1] [0 0 0 0 15]] Classification report precision recall f1-score support DrugY 1.00 1.00 1.00 25 drugA 0.78 1.00 0.88 7 drugB 1.00 0.50 0.67 6 drugC 1.00 0.86 0.92 7 drugX 0.88 1.00 0.94 15</pre>
accuracy			0.93	60													
macro avg	0.93	0.87	0.88	60													
weighted avg	0.94	0.93	0.93	60													

Final Model Selection Justification (2 Marks):

Final Model	Reasoning
Random forest	<p>The Random forest model was selected for its superior performance, exhibiting high accuracy during hyperparameter tuning. Its ability to handle complex relationships, minimize overfitting, and optimize predictive accuracy aligns with project objectives, justifying its selection as the final model</p> <pre> # Decision tree and Random forest performs well from sklearn.model_selection import cross_val_score # Random forest model is selected rf = RandomForestClassifier() rf.fit(x_train,y_train) yPred=rf.predict(x_test) f1_score (yPred, y_test, average='weighted') 0.9516222084367246 cv = cross_val_score(rf,x,y,cv=5) np.mean(cv) 0.985 </pre>