

Model Optimization and Tuning Phase Template

Date	19 June 2025
Team ID	SWTID174971392
Project Title	Early prediction for chronic kidney disease detection: A progressive approach to health management
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	Optimal Values
Random Forest	<pre>'Random Forest': { 'model': RandomForestClassifier(random_state=42, class_weight='balanced'), 'params': { 'n_estimators': [10, 25, 50, 100], 'max_depth': [3, 5, 7, 10, None], 'min_samples_split': [20, 40, 60, 80], 'min_samples_leaf': [10, 20, 30, 40], 'max_features': ['sqrt', 'log2', 0.3, 0.5], 'max_samples': [0.6, 0.7, 0.8, 0.9], 'min_impurity_decrease': [0.0, 0.01, 0.02, 0.05], 'ccp_alpha': [0.0, 0.01, 0.02, 0.05] } },</pre>	<p>BEST HYPERPARAMETERS:</p> <pre>n_estimators: 10 min_samples_split: 80 min_samples_leaf: 40 min_impurity_decrease: 0.05 max_samples: 0.6 max_features: 0.3 max_depth: 7 ccp_alpha: 0.05</pre> <p>Random Forest: Successfully tuned</p>
Decision Tree	<pre>'Decision Tree': { 'model': DecisionTreeClassifier(random_state=42, class_weight='balanced'), 'params': { 'max_depth': [3, 5, 7, 10], 'min_samples_split': [40, 60, 80, 100], 'min_samples_leaf': [20, 30, 40, 50], 'max_features': ['sqrt', 'log2', 0.3, 0.5, None], 'min_impurity_decrease': [0.01, 0.02, 0.05, 0.1], 'ccp_alpha': [0.01, 0.02, 0.05, 0.1, 0.2] } },</pre>	<p>BEST HYPERPARAMETERS:</p> <pre>min_samples_split: 40 min_samples_leaf: 40 min_impurity_decrease: 0.05 max_features: None max_depth: 10 ccp_alpha: 0.05</pre> <p>Decision Tree: Successfully tuned</p>

Gradient Boosting	<pre>'Gradient Boosting': { 'model': GradientBoostingClassifier(random_state=42), 'params': { 'n_estimators': [10, 25, 50, 100], 'learning_rate': [0.01, 0.05, 0.1, 0.2], 'max_depth': [2, 3, 4, 5], 'min_samples_split': [40, 60, 80], 'min_samples_leaf': [20, 30, 40], 'subsample': [0.6, 0.7, 0.8, 0.9], 'max_features': ['sqrt', 'log2', 0.3, 0.5], 'min_impurity_decrease': [0.01, 0.02, 0.05], 'ccp_alpha': [0.0, 0.01, 0.02] } },</pre>	<p>BEST HYPERPARAMETERS:</p> <pre>subsample: 0.6 n_estimators: 100 min_samples_split: 80 min_samples_leaf: 40 min_impurity_decrease: 0.05 max_features: log2 max_depth: 2 learning_rate: 0.01 ccp_alpha: 0.0 Gradient Boosting: Successfully tuned</pre>
XGBoost	<pre>'XGBoost': { 'model': xgb.XGBClassifier(random_state=42, eval_metric='logloss'), 'params': { 'n_estimators': [50, 100, 150, 200], 'learning_rate': [0.1, 0.15, 0.2, 0.3], 'max_depth': [5, 6, 7, 8], 'min_child_weight': [3, 5, 7, 10], 'subsample': [0.7, 0.8, 0.9, 1], 'colsample_bytree': [0.6, 0.7, 0.8, 0.9], 'reg_alpha': [0, 0.01, 0.1, 1], 'reg_lambda': [0.1, 1, 5, 10], 'gamma': [0, 0.1, 0.5, 1], 'scale_pos_weight': [1, 2, 3] # Handle class imbalance } },</pre>	<p>BEST HYPERPARAMETERS:</p> <pre>subsample: 0.9 scale_pos_weight: 1 reg_lambda: 10 reg_alpha: 0 n_estimators: 200 min_child_weight: 7 max_depth: 8 learning_rate: 0.15 gamma: 0.5 colsample_bytree: 0.6 XGBoost: Successfully tuned</pre>
LightGBM	<pre>'LightGBM': { 'model': lgb.LGBMClassifier(random_state=42, verbose=-1), 'params': { 'n_estimators': [10, 25, 50, 100], 'learning_rate': [0.01, 0.05, 0.1, 0.2], 'max_depth': [2, 3, 4, 5], 'num_leaves': [7, 15, 31, 63], 'min_child_samples': [10, 20, 30, 40], 'min_split_gain': [0.01, 0.1, 0.5, 1], 'subsample': [0.6, 0.7, 0.8, 0.9], 'colsample_bytree': [0.3, 0.5, 0.7, 0.9], 'reg_alpha': [0, 0.01, 0.1, 1], 'reg_lambda': [0.1, 1, 5, 10], 'min_child_weight': [0.001, 0.01, 0.1, 1], 'class_weight': ['balanced', None] } },</pre>	<p>BEST HYPERPARAMETERS:</p> <pre>subsample: 0.6 reg_lambda: 0.1 reg_alpha: 0.01 num_leaves: 15 n_estimators: 10 min_split_gain: 1 min_child_weight: 0.001 min_child_samples: 30 max_depth: 2 learning_rate: 0.2 colsample_bytree: 0.5 class_weight: balanced LightGBM: Successfully tuned</pre>

CatBoost	<pre> 'CatBoost': { 'model': CatBoostClassifier(random_state=42, verbose=False), 'params': { 'iterations': [10, 25, 50, 100], 'learning_rate': [0.01, 0.05, 0.1, 0.2], 'depth': [2, 3, 4, 5], 'min_data_in_leaf': [10, 20, 30, 40], 'l2_leaf_reg': [1, 3, 5, 10, 20], 'subsample': [0.6, 0.7, 0.8, 0.9], 'colsample_bylevel': [0.3, 0.5, 0.7, 0.9], 'border_count': [32, 64, 128], 'bagging_temperature': [0, 0.5, 1], 'class_weights': [[1, 1], [1, 2], [1, 3]] # Handle imbalance } }, </pre>	<p>BEST HYPERPARAMETERS:</p> <pre> subsample: 0.6 min_data_in_leaf: 40 learning_rate: 0.2 l2_leaf_reg: 5 iterations: 10 depth: 4 colsample_bylevel: 0.5 class_weights: [1, 3] border_count: 64 bagging_temperature: 0 CatBoost: Successfully tuned </pre>
AdaBoost	<pre> # ADABOOST 'AdaBoost': { 'model': AdaBoostClassifier(random_state=42), 'params': { 'n_estimators': [10, 25, 50, 100], 'learning_rate': [0.01, 0.1, 0.5, 1.0, 2.0], 'algorithm': ['SAMME', 'SAMME.R'] } }, </pre>	<p>BEST HYPERPARAMETERS:</p> <pre> algorithm: SAMME learning_rate: 0.01 n_estimators: 10 AdaBoost: Successfully tuned </pre>
Logistic Regression	<pre> 'Logistic Regression': { 'model': LogisticRegression(random_state=42, max_iter=1000, class_weight='balanced'), 'params': { 'C': [0.001, 0.01, 0.1, 1, 10, 100], 'penalty': ['l1', 'l2', 'elasticnet'], 'solver': ['liblinear', 'saga'], 'l1_ratio': [0.1, 0.3, 0.5, 0.7, 0.9], 'fit_intercept': [True, False] } }, </pre>	<p>BEST HYPERPARAMETERS:</p> <pre> solver: liblinear penalty: l2 l1_ratio: 0.5 fit_intercept: False C: 1 Logistic Regression: Successfully tuned </pre>
SGD Classifier	<pre> 'SGD Classifier': { 'model': SGDClassifier(random_state=42, max_iter=1000, class_weight='balanced'), 'params': { 'alpha': [0.0001, 0.001, 0.01, 0.1, 1], 'penalty': ['l1', 'l2', 'elasticnet'], 'l1_ratio': [0.1, 0.3, 0.5, 0.7, 0.9], 'learning_rate': ['constant', 'optimal', 'invscaling', 'adaptive'], 'eta0': [0.001, 0.01, 0.1, 1], 'early_stopping': [True, False], 'validation_fraction': [0.1, 0.2, 0.3] } }, </pre>	<p>BEST HYPERPARAMETERS:</p> <pre> validation_fraction: 0.3 penalty: l1 learning_rate: constant l1_ratio: 0.3 eta0: 0.01 early_stopping: True alpha: 0.01 SGD Classifier: Successfully tuned </pre>

SVM (RBF)	<pre>'SVM (RBF)': { 'model': SVC(random_state=42, probability=True, class_weight='balanced'), 'params': { 'C': [0.001, 0.01, 0.1, 1, 10, 100], 'gamma': ['scale', 'auto', 0.001, 0.01, 0.1, 1], 'kernel': ['rbf'], 'shrinking': [True, False], 'cache_size': [200, 500, 1000] } },</pre>	<p>BEST HYPERPARAMETERS:</p> <p>shrinking: False kernel: rbf gamma: 0.1 cache_size: 500 C: 100 SVM (RBF): Successfully tuned</p>
KNN	<pre>'K-Nearest Neighbors': { 'model': KNeighborsClassifier(), 'params': { 'n_neighbors': [3, 5, 7, 9, 11, 15, 21, 31], 'weights': ['uniform', 'distance'], 'algorithm': ['auto', 'ball_tree', 'kd_tree', 'brute'], 'metric': ['euclidean', 'manhattan', 'minkowski'], 'p': [1, 2, 3], 'leaf_size': [10, 20, 30, 40, 50] } },</pre>	<p>BEST HYPERPARAMETERS:</p> <p>weights: distance p: 2 n_neighbors: 21 metric: euclidean leaf_size: 40 algorithm: auto K-Nearest Neighbors: Successfully tuned</p>
Linear	<pre>'Linear Discriminant Analysis': { 'model': LinearDiscriminantAnalysis(), 'params': { 'solver': ['svd', 'lsqr', 'eigen'], 'shrinkage': [None, 'auto', 0.1, 0.3, 0.5, 0.7, 0.9], 'priors': [None], 'n_components': [None, 1, 2, 3] } },</pre>	<p>BEST HYPERPARAMETERS:</p> <p>n_components: None priors: None shrinkage: 0.3 solver: lsqr</p>

Performance Metrics Comparison Report (2 Marks):

Model	Optimized Metric				
Random Forest		precision	recall	f1-score	support
	0	1.00	0.88	0.94	50
	1	0.83	1.00	0.91	30
	accuracy			0.93	80
	macro avg	0.92	0.94	0.92	80
	weighted avg	0.94	0.93	0.93	80
	Test Accuracy: 0.9250				
	Precision: 0.9375				
	Recall: 0.9250				
	F1 Score: 0.9260				
XGBoost		precision	recall	f1-score	support
	0	0.96	0.98	0.97	50
	1	0.97	0.93	0.95	30
	accuracy			0.96	80
	macro avg	0.96	0.96	0.96	80
	weighted avg	0.96	0.96	0.96	80

	Test Accuracy: 0.9625 Precision: 0.9626 Recall: 0.9625 F1 Score: 0.9624 ROC AUC: 0.9933 PR AUC: 0.9905				
LightGBM		precision	recall	f1-score	support
	0	1.00	1.00	1.00	50
	1	1.00	1.00	1.00	30
	accuracy			1.00	80
	macro avg	1.00	1.00	1.00	80
	weighted avg	1.00	1.00	1.00	80
	Test Accuracy: 1.0000 Precision: 1.0000 Recall: 1.0000 F1 Score: 1.0000 ROC AUC: 1.0000 PR AUC: 1.0000				
Logistic Regression		precision	recall	f1-score	support
	0	1.00	1.00	1.00	50
	1	1.00	1.00	1.00	30
	accuracy			1.00	80
	macro avg	1.00	1.00	1.00	80
	weighted avg	1.00	1.00	1.00	80

	<div>Test Accuracy: 1.0000 Precision: 1.0000 Recall: 1.0000 F1 Score: 1.0000 ROC AUC: 1.0000 PR AUC: 1.0000</div>																														
SVM(RBF)	<table><thead><tr><th></th><th>precision</th><th>recall</th><th>f1-score</th><th>support</th></tr></thead><tbody><tr><td>0</td><td>1.00</td><td>1.00</td><td>1.00</td><td>50</td></tr><tr><td>1</td><td>1.00</td><td>1.00</td><td>1.00</td><td>30</td></tr><tr><td>accuracy</td><td></td><td></td><td>1.00</td><td>80</td></tr><tr><td>macro avg</td><td>1.00</td><td>1.00</td><td>1.00</td><td>80</td></tr><tr><td>weighted avg</td><td>1.00</td><td>1.00</td><td>1.00</td><td>80</td></tr></tbody></table> <div>Test Accuracy: 1.0000 Precision: 1.0000 Recall: 1.0000 F1 Score: 1.0000 ROC AUC: 1.0000 PR AUC: 1.0000</div>		precision	recall	f1-score	support	0	1.00	1.00	1.00	50	1	1.00	1.00	1.00	30	accuracy			1.00	80	macro avg	1.00	1.00	1.00	80	weighted avg	1.00	1.00	1.00	80
	precision	recall	f1-score	support																											
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weighted avg	1.00	1.00	1.00	80																											
Gradient Boosting	<table><thead><tr><th></th><th>precision</th><th>recall</th><th>f1-score</th><th>support</th></tr></thead><tbody><tr><td>0</td><td>0.96</td><td>0.96</td><td>0.96</td><td>50</td></tr><tr><td>1</td><td>0.93</td><td>0.93</td><td>0.93</td><td>30</td></tr><tr><td>accuracy</td><td></td><td></td><td>0.95</td><td>80</td></tr><tr><td>macro avg</td><td>0.95</td><td>0.95</td><td>0.95</td><td>80</td></tr><tr><td>weighted avg</td><td>0.95</td><td>0.95</td><td>0.95</td><td>80</td></tr></tbody></table>		precision	recall	f1-score	support	0	0.96	0.96	0.96	50	1	0.93	0.93	0.93	30	accuracy			0.95	80	macro avg	0.95	0.95	0.95	80	weighted avg	0.95	0.95	0.95	80
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	<div>Test Accuracy: 0.9500 Precision: 0.9500 Recall: 0.9500 F1 Score: 0.9500 ROC AUC: 0.9947 PR AUC: 0.9920</div>																														
CatBoost	<table><thead><tr><th></th><th>precision</th><th>recall</th><th>f1-score</th><th>support</th></tr></thead><tbody><tr><td>0</td><td>1.00</td><td>0.94</td><td>0.97</td><td>50</td></tr><tr><td>1</td><td>0.91</td><td>1.00</td><td>0.95</td><td>30</td></tr><tr><td>accuracy</td><td></td><td></td><td>0.96</td><td>80</td></tr><tr><td>macro avg</td><td>0.95</td><td>0.97</td><td>0.96</td><td>80</td></tr><tr><td>weighted avg</td><td>0.97</td><td>0.96</td><td>0.96</td><td>80</td></tr></tbody></table> <div>Test Accuracy: 0.9625 Precision: 0.9659 Recall: 0.9625 F1 Score: 0.9628 ROC AUC: 0.9973 PR AUC: 0.9958</div>		precision	recall	f1-score	support	0	1.00	0.94	0.97	50	1	0.91	1.00	0.95	30	accuracy			0.96	80	macro avg	0.95	0.97	0.96	80	weighted avg	0.97	0.96	0.96	80
	precision	recall	f1-score	support																											
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Decision Tree	<table><thead><tr><th></th><th>precision</th><th>recall</th><th>f1-score</th><th>support</th></tr></thead><tbody><tr><td>0</td><td>0.95</td><td>0.84</td><td>0.89</td><td>50</td></tr><tr><td>1</td><td>0.78</td><td>0.93</td><td>0.85</td><td>30</td></tr><tr><td>accuracy</td><td></td><td></td><td>0.88</td><td>80</td></tr><tr><td>macro avg</td><td>0.87</td><td>0.89</td><td>0.87</td><td>80</td></tr><tr><td>weighted avg</td><td>0.89</td><td>0.88</td><td>0.88</td><td>80</td></tr></tbody></table>		precision	recall	f1-score	support	0	0.95	0.84	0.89	50	1	0.78	0.93	0.85	30	accuracy			0.88	80	macro avg	0.87	0.89	0.87	80	weighted avg	0.89	0.88	0.88	80
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	Test Accuracy: 0.8750 Precision: 0.8883 Recall: 0.8750 F1 Score: 0.8767 ROC AUC: 0.8867 PR AUC: 0.7509				
KNN	precision		recall	f1-score	support
	0	1.00	1.00	1.00	50
	1	1.00	1.00	1.00	30
	accuracy			1.00	80
	macro avg	1.00	1.00	1.00	80
	weighted avg	1.00	1.00	1.00	80
	Test Accuracy: 1.0000 Precision: 1.0000 Recall: 1.0000 F1 Score: 1.0000 ROC AUC: 1.0000 PR AUC: 1.0000				
Linear Discriminant Analysis	precision		recall	f1-score	support
	0	1.00	1.00	1.00	50
	1	1.00	1.00	1.00	30
	accuracy			1.00	80
	macro avg	1.00	1.00	1.00	80
	weighted avg	1.00	1.00	1.00	80

	Test Accuracy: 1.0000 Precision: 1.0000 Recall: 1.0000 F1 Score: 1.0000 ROC AUC: 1.0000 PR AUC: 1.0000																																		
AdaBoost	<table><thead><tr><th></th><th>precision</th><th>recall</th><th>f1-score</th><th>support</th></tr></thead><tbody><tr><td>0</td><td>0.95</td><td>0.84</td><td>0.89</td><td>50</td></tr><tr><td>1</td><td>0.78</td><td>0.93</td><td>0.85</td><td>30</td></tr><tr><td>accuracy</td><td></td><td></td><td>0.88</td><td>80</td></tr><tr><td>macro avg</td><td>0.87</td><td>0.89</td><td>0.87</td><td>80</td></tr><tr><td>weighted avg</td><td>0.89</td><td>0.88</td><td>0.88</td><td>80</td></tr></tbody></table> Test Accuracy: 0.8750 Precision: 0.8883 Recall: 0.8750 F1 Score: 0.8767 ROC AUC: 0.8867 PR AUC: 0.7509						precision	recall	f1-score	support	0	0.95	0.84	0.89	50	1	0.78	0.93	0.85	30	accuracy			0.88	80	macro avg	0.87	0.89	0.87	80	weighted avg	0.89	0.88	0.88	80
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	Test Accuracy: 1.0000 Precision: 1.0000 Recall: 1.0000 F1 Score: 1.0000 ROC AUC: 1.0000 PR AUC: 1.0000				
Gaussian Naive Bayes	precision		recall	f1-score	support
	0	1.00	0.84	0.91	50
	1	0.79	1.00	0.88	30
	accuracy			0.90	80
	macro avg	0.89	0.92	0.90	80
	weighted avg	0.92	0.90	0.90	80
	Test Accuracy: 0.9000 Precision: 0.9211 Recall: 0.9000 F1 Score: 0.9015 ROC AUC: 1.0000 PR AUC: 1.0000				
Bernoulli Naive Bayes	precision		recall	f1-score	support
	0	1.00	0.96	0.98	50
	1	0.94	1.00	0.97	30
	accuracy			0.97	80
	macro avg	0.97	0.98	0.97	80
	weighted avg	0.98	0.97	0.98	80

	<p>Test Accuracy: 0.9750</p> <p>Precision: 0.9766</p> <p>Recall: 0.9750</p> <p>F1 Score: 0.9751</p> <p>ROC AUC: 1.0000</p> <p>PR AUC: 1.0000</p>
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Final Model Selection Justification (2 Marks):

Final Model	Reasoning
CatBoost	<p>We aimed to identify the model with the lowest risk under each version. For this, we carefully noted the specific hyperparameters that had been tuned for each model so we could recreate and retrain them consistently. After rebuilding the models using those same hyperparameters, we trained them on the original dataset to reproduce the same performance results. Once that was done, we tested these models on a new, valid dataset containing data that wasn't part of the original training set.</p> <p>Among all models tested in Version 1—which included both the original selected features and feature-engineered ones—the CatBoost model performed the best. It was chosen as the top model based on its ability to generalize well (low overfitting) and its high recall, which is especially important in healthcare applications where minimizing false negatives is critical.</p>

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FINAL LEADERBOARD - RANKED BY ACCURACY (VERSION 1)
=====
1 Rank 1: CatBoost          - 1.0000 (100.00%)
2 Rank 2: XGBoost           - 0.9600 (96.00%)
3 Rank 3: Gradient Boosting - 0.9000 (90.00%)
. Rank 4: Random Forest     - 0.8400 (84.00%)
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Leaderboard as DataFrame:

	Rank	Model	Accuracy	Accuracy_Percentage
0	1	CatBoost	1.00	100.0
1	2	XGBoost	0.96	96.0
2	3	Gradient Boosting	0.90	90.0
3	4	Random Forest	0.84	84.0