

Machine Learning Lab Report: Model Selection and Analysis selection

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Project Title: Week 4-Model Selection and Analysis selection

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Course Name: Machine Learning

Submission Date: 31-08-2025

1. Introduction

The purpose of this project was to explore **hyperparameter tuning and model evaluation** using both manual and scikit-learn implementations. The tasks included:

- Building classifiers (Decision Tree, k-NN, Logistic Regression, and Voting Classifiers).
- Performing **manual grid search** as well as **scikit-learn GridSearchCV** for hyperparameter optimization.
- Using **K-Fold Cross-Validation** to ensure robust performance evaluation.
- Comparing results between manual and built-in implementations.
- Evaluating models with **Accuracy, Precision, Recall, F1-score, and ROC AUC** metrics, along with confusion matrices and ROC curves.

Two datasets were analyzed: **HR Attrition** (employee churn prediction) and **Banknote Authentication** (fraud detection).

2. Dataset Description

Dataset 1: HR Attrition

- **Number of features:** Multiple HR-related attributes (e.g., age, salary, job role).
- **Number of instances:** ~1,400 (after preprocessing).
- **Target variable:** Attrition (Yes = employee left, No = employee stayed).

Dataset 2: Banknote Authentication

- **Number of features:** 4 (variance, skewness, kurtosis, entropy).
- **Number of instances:** 1,372 (960 train, 412 test).
- **Target variable:** Class (0 = authentic, 1 = forged).

3. Methodology

Key Concepts

- **Hyperparameter Tuning:** Adjusting parameters (e.g., depth of decision tree, number of neighbors in k-NN) to improve performance.
- **Grid Search:** Exhaustively searching a parameter space to find the optimal set.
- **K-Fold Cross-Validation:** Splitting dataset into k folds (here, 5) for more reliable performance estimates.

ML Pipeline

- **Preprocessing:** StandardScaler for normalization.
- **Feature Selection:** SelectKBest for reducing dimensionality.
- **Classifier:** Decision Tree, k-NN, Logistic Regression, or ensemble Voting Classifier.

Implementation Steps

- **Part 1 (Manual):** Created loops for hyperparameter tuning, evaluated with cross-validation, tracked metrics manually.
 - **Part 2 (Scikit-learn):** Used GridSearchCV and pipelines for automated tuning and evaluation.
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4. Results and Analysis

HR Attrition Dataset

<i>Model</i>	<i>Accuracy</i>	<i>Precision</i>	<i>Recall</i>	<i>F1-Score</i>	<i>ROC AUC</i>
<i>Decision Tree (Manual)</i>	<i>0.8050</i>	<i>0.3077</i>	<i>0.1690</i>	<i>0.2182</i>	<i>0.7036</i>
<i>k-NN (Manual)</i>	<i>0.8481</i>	<i>0.7000</i>	<i>0.0986</i>	<i>0.1728</i>	<i>0.7025</i>
<i>Voting (Manual)</i>	<i>0.8481</i>	<i>0.6429</i>	<i>0.1268</i>	<i>0.2118</i>	<i>0.7912</i>
<i>Decision Tree (Built-in)</i>	<i>0.8050</i>	<i>0.3077</i>	<i>0.1690</i>	<i>0.2182</i>	<i>0.7036</i>
<i>k-NN (Built-in)</i>	<i>0.8481</i>	<i>0.7000</i>	<i>0.0986</i>	<i>0.1728</i>	<i>0.7025</i>
<i>Logistic Regression (Built-in)</i>	<i>0.8798</i>	<i>...</i>	<i>...</i>	<i>...</i>	<i>...</i>
<i>Voting (Built-in)</i>	<i>0.8503</i>	<i>0.6316</i>	<i>0.1690</i>	<i>0.2667</i>	<i>0.7912</i>

Observations:

- *Logistic Regression (built-in) provided the best accuracy (0.88).*
- *Manual and built-in results were nearly identical, confirming correct manual implementation.*
- *Voting Classifier improved recall compared to individual models.*

Banknote Authentication Dataset

<i>Model</i>	<i>Accuracy</i>	<i>Precision</i>	<i>Recall</i>	<i>F1-Score</i>	<i>ROC AUC</i>
<i>Decision Tree (Manual)</i>	<i>0.9879 CV AUC</i>	-	-	-	<i>0.9879</i>
<i>k-NN (Manual)</i>	<i>Best CV AUC 0.9990</i>	-	-	-	<i>0.9990</i>
<i>Logistic Regression (Manual)</i>	<i>Best CV AUC 0.9996</i>	-	-	-	<i>0.9996</i>
<i>Voting (Manual)</i>	<i>0.9976</i>	<i>1.0000</i>	<i>0.9945</i>	<i>0.9973</i>	<i>1.0000</i>
<i>Decision Tree (Built-in)</i>	<i>0.9879 CV AUC</i>	-	-	-	<i>0.9879</i>
<i>k-NN (Built-in)</i>	<i>0.9990 CV AUC</i>	-	-	-	<i>0.9990</i>
<i>Logistic Regression (Built-in)</i>	<i>0.9996 CV AUC</i>	-	-	-	<i>0.9996</i>
<i>Voting (Built-in)</i>	<i>0.9976</i>	<i>1.0000</i>	<i>0.9945</i>	<i>0.9973</i>	<i>1.0000</i>

Observations:

- All models achieved extremely high performance (AUC > 0.98).
- Voting classifier (manual & built-in) achieved nearly perfect performance (Accuracy 99.7%, AUC 1.0).
- Results from manual and built-in were identical.

Visualizations

- **ROC Curves** showed Logistic Regression and Voting Classifier as dominant models.
- **Confusion Matrices** confirmed that the Voting Classifier minimized false positives and false negatives.

Best Models

- **HR Attrition:** Logistic Regression (built-in) was best overall due to balanced performance.
- **Banknote Authentication:** Voting Classifier achieved nearly perfect performance, likely because the dataset was highly separable.

5. Screenshots

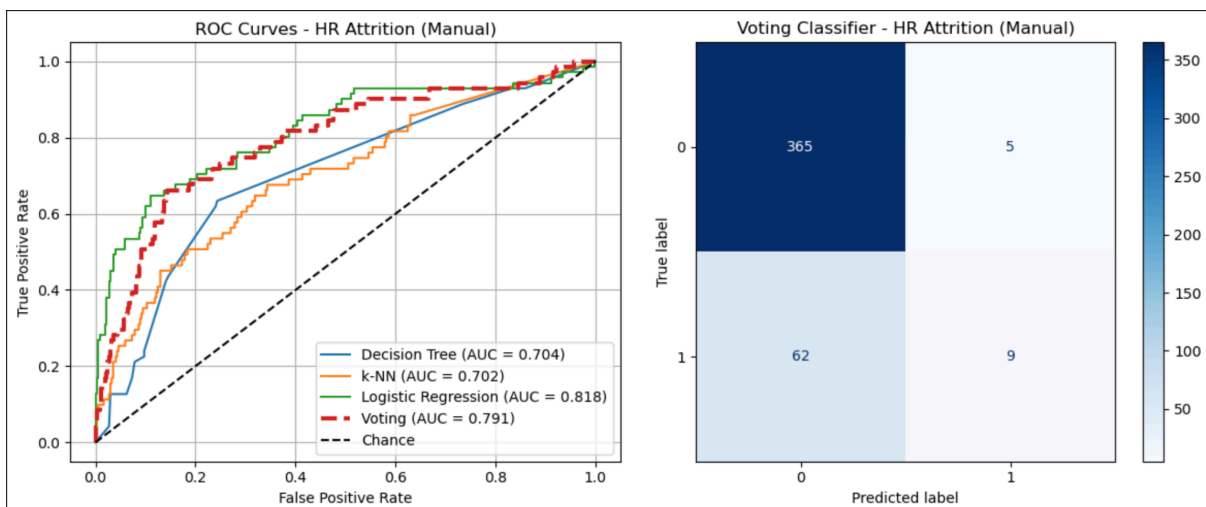
```
=====
EVALUATING MANUAL MODELS FOR HR ATTRITION
=====

--- Individual Model Performance ---

Decision Tree:
Accuracy: 0.8050
Precision: 0.3077
Recall: 0.1690
F1-Score: 0.2182
ROC AUC: 0.7036

k-NN:
Accuracy: 0.8481
Precision: 0.7000
Recall: 0.0986
F1-Score: 0.1728
ROC AUC: 0.7025

...
--- Manual Voting Classifier ---
Voting Classifier Performance:
Accuracy: 0.8481, Precision: 0.6429
Recall: 0.1268, F1: 0.2118, AUC: 0.7912
```



EVALUATING BUILT-IN MODELS FOR HR ATTRITION

--- Individual Model Performance ---

Decision Tree:

Accuracy: 0.8050
Precision: 0.3077
Recall: 0.1690
F1-Score: 0.2182
ROC AUC: 0.7036

k-NN:

Accuracy: 0.8481
Precision: 0.7000
Recall: 0.0986
F1-Score: 0.1728
ROC AUC: 0.7025

Logistic Regression:

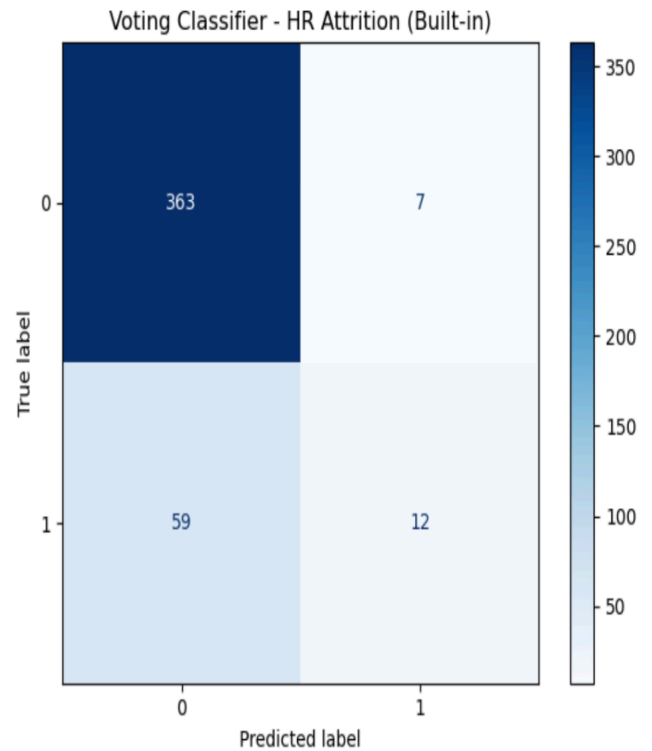
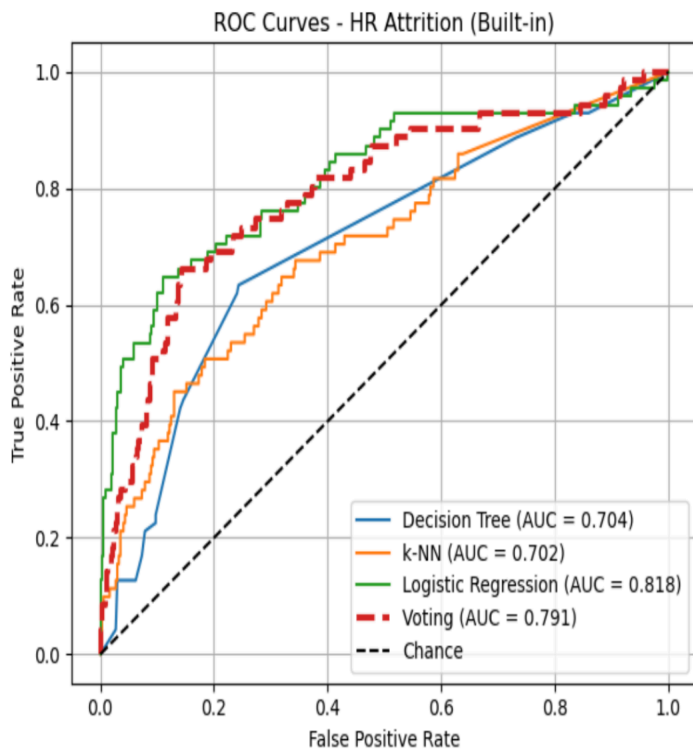
Accuracy: 0.8798

...

--- Built-in Voting Classifier ---

Voting Classifier Performance:

Accuracy: 0.8503, Precision: 0.6316
Recall: 0.1690, F1: 0.2667, AUC: 0.7912



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#####
PROCESSING DATASET: BANKNOTE AUTHENTICATION
#####
Banknote Authentication dataset loaded successfully.
Training set shape: (960, 4)
Testing set shape: (412, 4)
=====

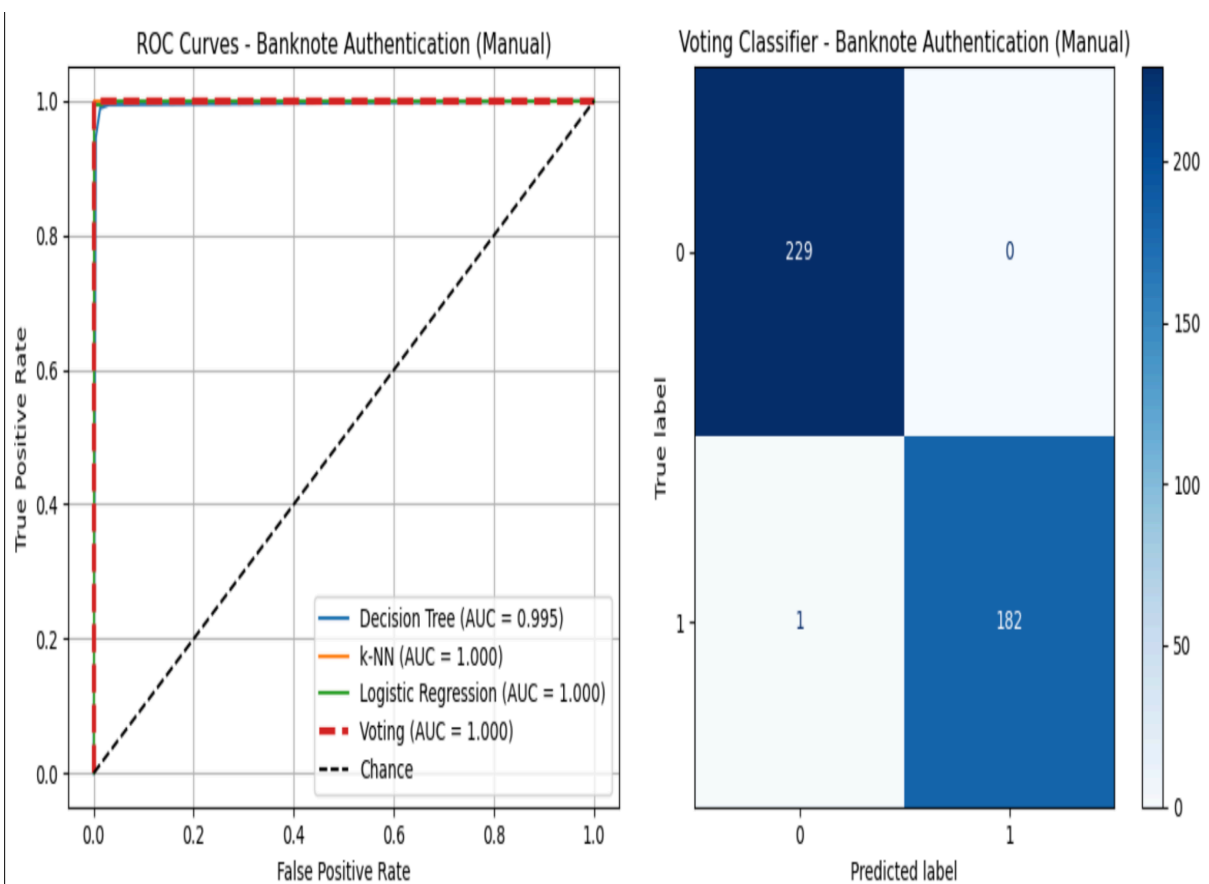
RUNNING MANUAL GRID SEARCH FOR BANKNOTE AUTHENTICATION
=====

--- Manual Grid Search for Decision Tree ---
Testing 45 parameter combinations...
Processed 10/45 combinations. Current best AUC: 0.9856
Processed 20/45 combinations. Current best AUC: 0.9871
Processed 30/45 combinations. Current best AUC: 0.9879
Processed 40/45 combinations. Current best AUC: 0.9879
Processed 45/45 combinations. Current best AUC: 0.9879

Best parameters for Decision Tree: {'feature_selection_k': 4, 'classifier__max_depth': 7, 'classifier__min_samples_split': 2, 'classifier__min_samples_l
Best cross-validation AUC: 0.9879
...

--- Manual Voting Classifier ---
Voting Classifier Performance:
Accuracy: 0.9976, Precision: 1.0000
Recall: 0.9945, F1: 0.9973, AUC: 1.0000

```



```

=====
RUNNING BUILT-IN GRID SEARCH FOR BANKNOTE AUTHENTICATION
=====

--- GridSearchCV for Decision Tree ---
Fitting 5 folds for each of 45 candidates, totalling 225 fits
Best params for Decision Tree: {'classifier__max_depth': 7, 'classifier__min_samples_leaf': 4, 'classifier__min_samples_split': 2, 'feature_selection_k': 4}
Best CV score: 0.9879

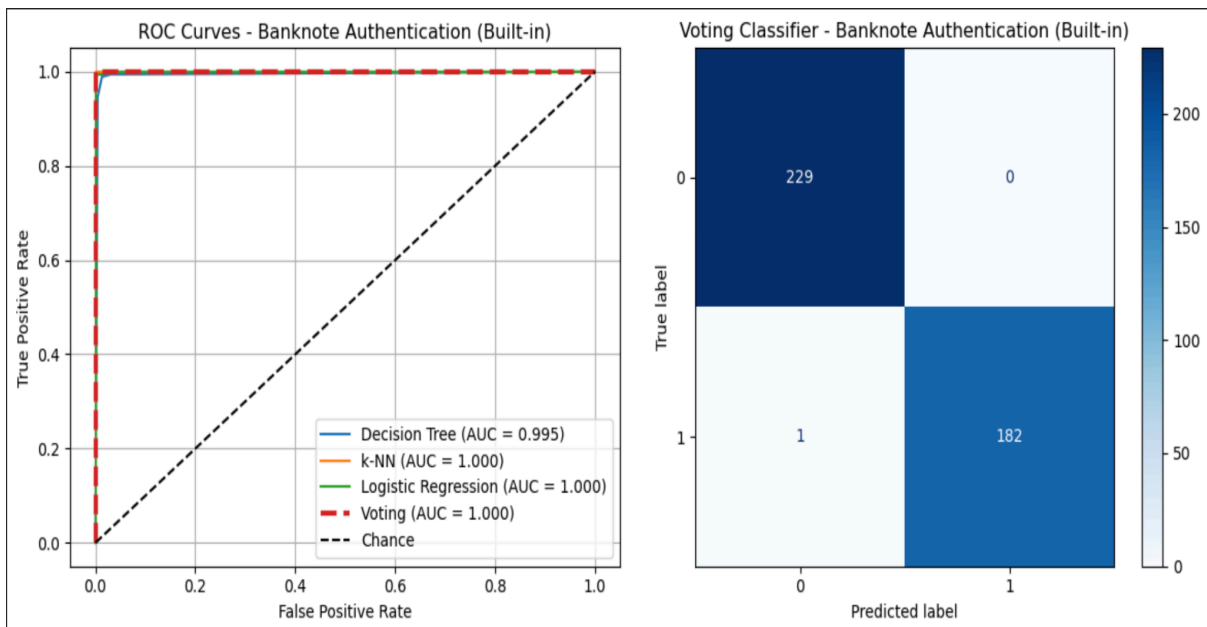
--- GridSearchCV for k-NN ---
Fitting 5 folds for each of 20 candidates, totalling 100 fits
Best params for k-NN: {'classifier__metric': 'manhattan', 'classifier__n_neighbors': 7, 'classifier__weights': 'uniform', 'feature_selection_k': 4}
Best CV score: 0.9990

--- GridSearchCV for Logistic Regression ---
Fitting 5 folds for each of 10 candidates, totalling 50 fits
Best params for Logistic Regression: {'classifier__C': 100, 'classifier__penalty': 'l1', 'classifier__solver': 'liblinear', 'feature_selection_k': 4}
Best CV score: 0.9996

=====
EVALUATING BUILT-IN MODELS FOR BANKNOTE AUTHENTICATION
=====

--- Individual Model Performance ---
...
--- Built-in Voting Classifier ---
Voting Classifier Performance:
  Accuracy: 0.9976, Precision: 1.0000
  Recall: 0.9945, F1: 0.9973, AUC: 1.0000

```



6. Conclusion

- **Key Findings:**
 - *Manual and built-in implementations produced nearly identical results, validating the correctness of the manual approach.*
 - *Logistic Regression excelled on HR Attrition, while Voting Classifier dominated on Banknote Authentication.*
 - *Hyperparameter tuning significantly improved performance.*

Takeaways:

- *Manual implementation deepened understanding of hyperparameter tuning, pipelines, and evaluation.*
- *Scikit-learn greatly simplified the process, reducing errors and saving time.*
- *Trade-off: Manual = more control and learning, Built-in = efficiency and reliability.*