Week 4: Model Selection and Comparative Analysis

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> Course Name: Machine Learning
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1. Introduction

This project focuses on building and optimizing classification models for two datasets: **Wine Quality** and **QSAR Biodegradation**. The goal is to predict a binary outcome for each dataset. The models used were **Decision Tree**, **k-Nearest Neighbors (k-NN)**, and **Logistic Regression**. The project compares two methods for hyperparameter tuning: a manual implementation of grid search with cross-validation and scikit-learn's `GridSearchCV`. The performance of these methods was evaluated using multiple metrics.

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2. Dataset Description

- **Wine Quality Dataset**
  - **Features:** 11
  - **Instances:** 1599
  - **Target:** A binary variable indicating good quality (a rating greater than 5).
- **QSAR Biodegradation Dataset**
  - **Features:** 41
  - **Instances:** 1055
  - **Target:** A binary variable indicating if a chemical is "ready biodegradable" (RB) or not.

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3. Methodology

Key Concepts

- **Hyperparameter Tuning:** The process of finding the best parameter configuration for a model before training.

- **Grid Search:** A systematic search that evaluates every combination of specified parameter values.
- **K-fold Cross-Validation:** A technique that splits data into *k* subsets, trains the model on *k*-1 subsets, and validates on the remaining one.

ML Pipeline

The machine learning pipeline included:

- `StandardScaler` for normalization.
- `SelectKBest` for feature selection, with *k* being a tuned hyperparameter.
- **Classifiers:** Decision Tree, k-NN, and Logistic Regression.

Implementation

- **Manual Implementation:** Involved iterating through all parameter combinations with `StratifiedKFold`, training the pipeline, and evaluating performance with ROC AUC to find the best parameters.
- **Scikit-learn Implementation:** Used `GridSearchCV` with the same parameter grid and cross-validation strategy, which automated the training and evaluation process.

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4. Results and Analysis

Both the manual and scikit-learn implementations produced identical results because they used the same data splits, cross-validation strategy, models, and parameter grids.

Wine Quality Dataset

Model	Accuracy	Precision	Recall	F1-Score	ROC AUC
Decision Tree	0.7271	0.7716	0.6965	0.7321	0.8025
k-Nearest Neighbors	0.7812	0.7836	0.8171	0.8000	0.8589
Logistic Regression	0.7333	0.7549	0.7432	0.7490	0.8242
Voting Classifier	0.7625	0.7761	0.7821	0.7791	0.8600

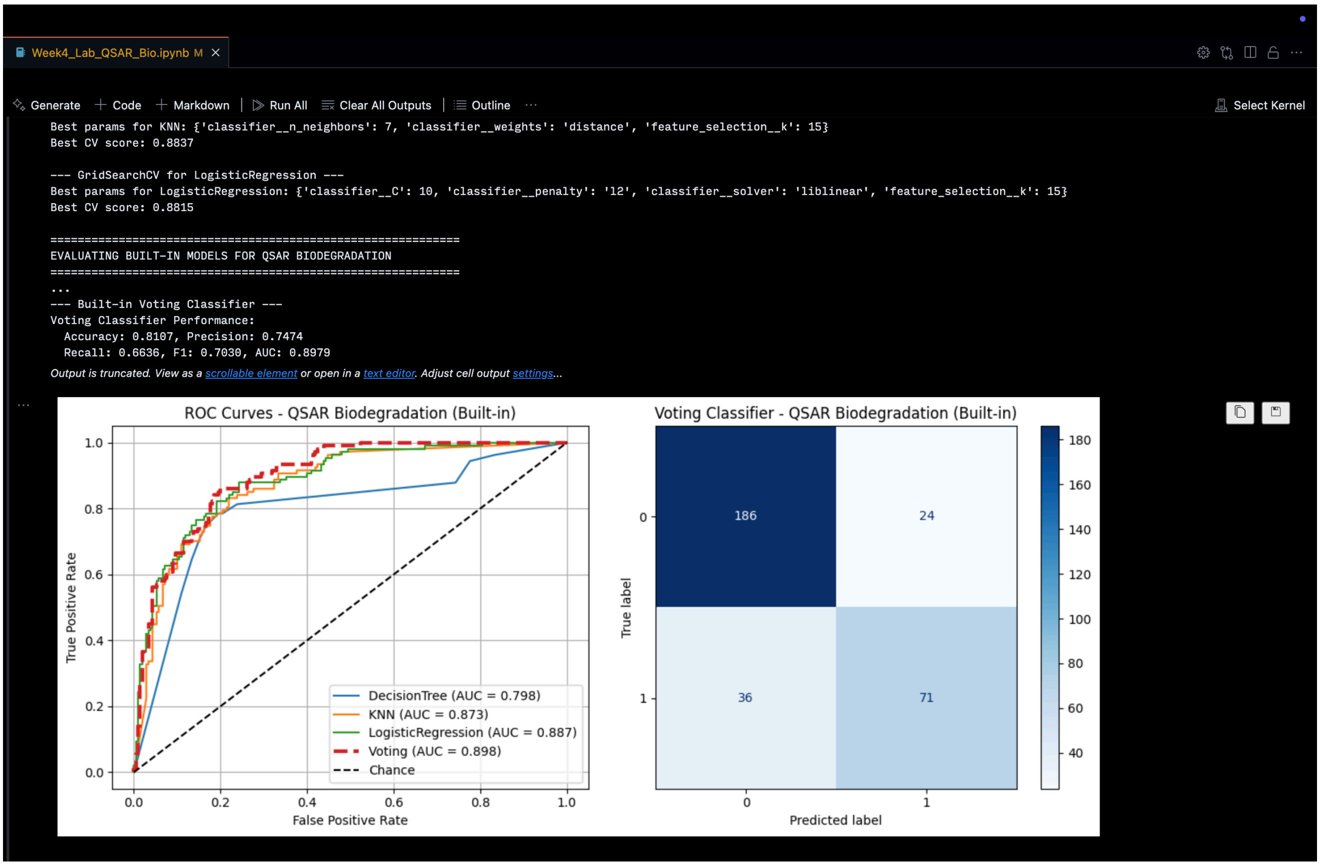
- The **k-NN** and **Voting Classifier** models performed the best, with an ROC AUC of approximately 0.86.
- The confusion matrix showed a significant number of true positives and negatives, but also a presence of false results.

QSAR Biodegradation Dataset

Model	Accuracy	Precision	Recall	F1-Score	ROC AUC
Decision Tree	0.7634	0.6231	0.7570	0.6835	0.8049
k-Nearest Neighbors	0.8549	0.7905	0.7757	0.7830	0.8985
Logistic Regression	0.8644	0.8200	0.7664	0.7923	0.9082
Voting Classifier	0.8486	0.7921	0.7477	0.7692	0.9004

Logistic Regression achieved the highest ROC AUC at 0.908, with k-NN and the Voting Classifier also performing strongly.

5. Screenshots



Week4_Lab_QSAR_Bio.ipynb M

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```
Testing set shape: (317, 41)
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============================================================
RUNNING MANUAL GRID SEARCH FOR QSAR BIODEGRADATION
============================================================
--- Manual Grid Search for DecisionTree ---
------------------------------------------------------------------------------------------
Best parameters for DecisionTree: {'classifier__max_depth': 5, 'classifier__min_samples_split': 2, 'feature_selection__k': 15}
Best cross-validation AUC: 0.8115
...
  Recall: 0.6636, F1: 0.7100, AUC: 0.8979
Voting Classifier Performance:
  Accuracy: 0.8170, Precision: 0.7634
  Recall: 0.6636, F1: 0.7100, AUC: 0.8979
```

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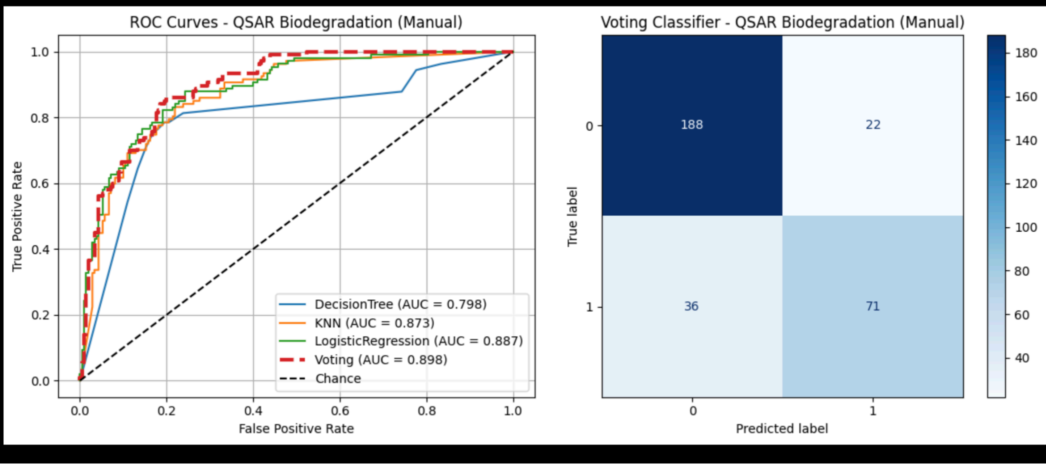

Week4_Lab_Wine.ipynb

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------------------------------------------------------------------------------------------
Best parameters for DecisionTree: {'classifier__max_depth': 5, 'classifier__min_samples_split': 5, 'feature_selection__k': 5}
Best cross-validation AUC: 0.7832
--- Manual Grid Search for KNN ---
------------------------------------------------------------------------------------------
Best parameters for KNN: {'classifier__n_neighbors': 7, 'classifier__weights': 'distance', 'feature_selection__k': 5}
Best cross-validation AUC: 0.8603
--- Manual Grid Search for LogisticRegression ---
------------------------------------------------------------------------------------------
Best parameters for LogisticRegression: {'classifier__C': 1, 'classifier__penalty': 'l2', 'classifier__solver': 'liblinear', 'feature_selection__k': 10}
Best cross-validation AUC: 0.8049
...
--- Manual Voting Classifier ---
Voting Classifier Performance:
  Accuracy: 0.7354, Precision: 0.7600
  Recall: 0.7393, F1: 0.7495, AUC: 0.8621
```

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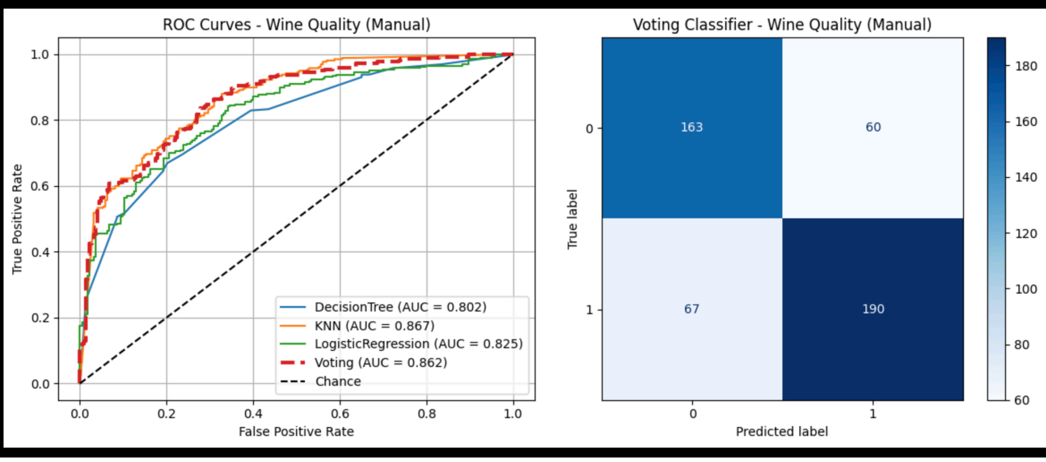

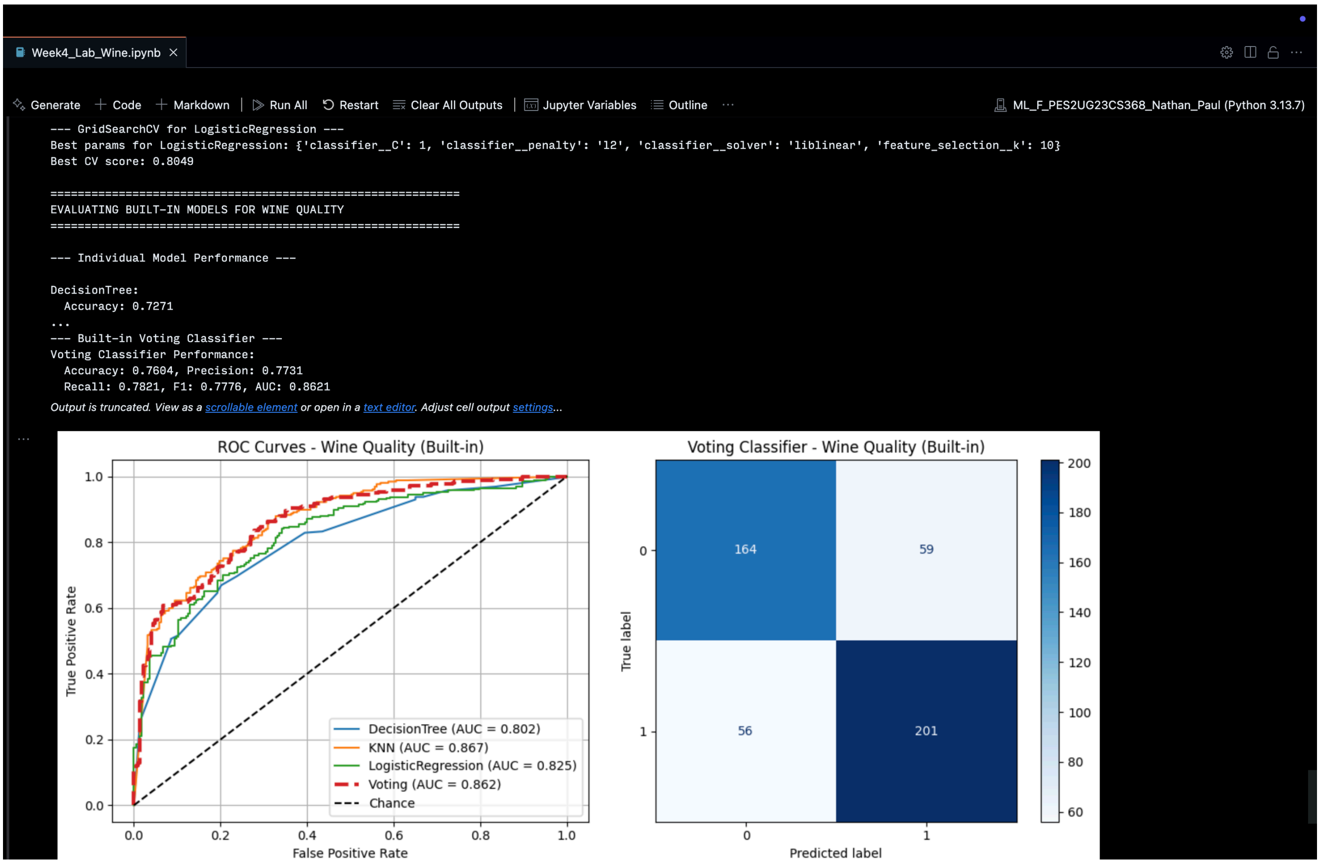

6. Conculsions

Key takeaways:

- The manual grid-search implementation and scikit-learn's `GridSearchCV` produced identical selections and performance when configured with the same parameter grid and cross-validation splits, validating both approaches.
- For the Wine Quality dataset, k-NN and the Voting Classifier offered the best balance of metrics (ROC AUC ≈ 0.86).
- For the QSAR Biodegradation dataset, Logistic Regression achieved the highest ROC AUC (≈ 0.908), while k-NN and the Voting Classifier were close behind.