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MLDL - Experiment 3

Aim

Apply a Decision Tree classifier for a binary classification task using the Breast Cancer Wisconsin (Diagnostic) dataset.

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1. Dataset Source

- Dataset: Breast Cancer Wisconsin (Diagnostic)
- Kaggle: https://www.kaggle.com/datasets/uciml/breast-cancer-wisconsin-data

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2. Dataset Description

The Breast Cancer Wisconsin (Diagnostic) dataset consists of features computed from digitized images of fine needle aspirate (FNA) of breast masses, with the goal of classifying tumors as benign or malignant.

Key properties:

- Number of instances: 569
- Number of input features: 30 real-valued features
- Target variable: `diagnosis`
    - `M` – Malignant (cancerous)
    - `B` – Benign (non-cancerous)
- Each feature corresponds to characteristics of cell nuclei such as:
    - `radius_mean`, `texture_mean`, `perimeter_mean`, `area_mean`, `smoothness_mean`, `compactness_mean`, etc.
- Additional columns in Kaggle file:
    - `id`: Sample identifier (not useful for prediction)
    - `diagnosis`: Target label

- 30 numeric feature columns

The dataset is moderately imbalanced, with more benign cases than malignant cases, which reflects realistic clinical screening statistics.

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3. Mathematical Formulation of Decision Tree

A Decision Tree classifier recursively partitions the feature space using if–else rules to create regions that are as pure as possible with respect to the class labels.

At a node S with samples from c classes, let p_i be the proportion of samples in class i.

- Entropy:

$$\boxed{H(S) = -\sum_{i=1}^{c} p_i \log_2(p_i)}$$

- Gini Index (used in CART-based trees):

$$\boxed{Gini(S) = 1 - \sum_{i=1}^{c} p_i^2}$$

For a candidate split that divides node S into child nodes $S_{1,2,\dots,}S_k$, the Information Gain using entropy is:

$$\boxed{IG(S, \text{split}) = H(S) - \sum_{j=1}^{k} \frac{|S_j|}{|S|} H(S_j)}$$

For Gini, we choose the split that minimizes the weighted Gini of the children:

$$\boxed{Gini_{\text{split}} = \sum_{j=1}^{k} \frac{|S_j|}{|S|} Gini(S_j)}$$

The training algorithm:

1. Start with all training samples at the root.
2. For each node, search over features and thresholds to find the split that maximizes information gain (or equivalently minimizes impurity).

3. Recursively apply splitting to child nodes until stopping criteria (max depth, min samples, or pure node) are met.

Prediction for a new sample: traverse from root to a leaf following the feature tests; the predicted label is the majority class of that leaf.

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4. Limitations of Decision Tree

1. Overfitting (High Variance)
   A deep tree can fit noise and outliers in the training data, leading to excellent training accuracy but poor test performance. This is dangerous in medical applications where overfitting may cause misclassification of tumors.
2. Instability / Sensitivity to Data Changes
   Because the algorithm uses a greedy splitting strategy, small changes in the dataset can radically change the learned tree structure, making individual trees unstable.
3. Axis-Aligned Splits
   Decision Trees split along a single feature at a time, which approximates complex boundaries with many rectangular regions. They may require many splits to mimic simple linear or diagonal relationships.
4. Bias with Imbalanced Data
   When one class is more frequent (e.g., benign tumors), the tree may bias predictions toward that class unless class weights or resampling are used.

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5. Methodology / Workflow (Decision Tree)

1. Data Collection
   - Download the Breast Cancer Wisconsin (Diagnostic) dataset as `data.csv` from Kaggle.
2. Data Preprocessing
   - Load the CSV into a Pandas DataFrame.
   - Drop the `id` column as it is not predictive.
   - Encode `diagnosis` into numeric labels using `LabelEncoder` (e.g., `0` for benign, `1` for malignant).
   - Check and confirm there are no missing values (in this dataset there are typically none).
3. Train–Test Split

        - Split the data into training (80%) and testing (20%) sets using `train_test_split` with `stratify=y` and `random_state=42`.
4. Hyperparameter Tuning (Grid Search)
    - Define a `DecisionTreeClassifier`.
    - Use `GridSearchCV` to search over:
        - `criterion`: `['gini', 'entropy']`
        - `max_depth`: `[None, 3, 5, 10, 15, 20]`
        - `min_samples_split`: `[2, 5, 10, 20]`
        - `min_samples_leaf`: `[1, 2, 4, 8]`
    - Use 5-fold cross-validation to select the best hyperparameters.
5. Model Training and Visualization
    - Train the best Decision Tree on the full training data.
    - Visualize only the top 3 levels of the tree for readability, showing which features (e.g., `worst radius`, `worst perimeter`) drive early splits.
6. Model Evaluation
    - Predict on the test set.
    - Compute accuracy, confusion matrix, and classification report (precision, recall, F1-score) for benign and malignant classes.
    - Plot feature importances to understand which features are most influential.
7. Conclusion
    - Comment on accuracy, performance on malignant cases, and interpretability of the tree, and mention that ensemble methods like Random Forest can further improve robustness.

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6. Performance Analysis (Decision Tree)

After running the code below, you will obtain:

- Overall Accuracy: fraction of correctly classified tumors on the test set.
- Class-Specific Metrics:
    - Benign (0): Typically high precision and recall due to majority class.
    - Malignant (1): F1-score is critical; higher recall means fewer cancer cases are missed.
- Confusion Matrix:
    - True Negatives: correctly identified benign tumors.
    - True Positives: correctly identified malignant tumors.

- False Negatives: malignant classified as benign (most critical medical error).
- False Positives: benign classified as malignant.

You can directly record the numeric values printed by the code (accuracy, precision, recall, F1-score, and counts in the confusion matrix) as your performance section.

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7. Hyperparameter Tuning (Decision Tree)

Hyperparameter tuning is used to prevent overfitting and improve generalization:

- `criterion`: decides impurity measure (`gini` or `entropy`).
- `max_depth`: restricts tree depth; smaller values reduce overfitting.
- `min_samples_split`: minimum samples required to split an internal node; larger values avoid very specific splits.
- `min_samples_leaf`: minimum samples required in a leaf; higher values smooth decision boundaries.

`GridSearchCV` builds a model for each combination of these parameters and uses 5-fold cross-validation to estimate performance, finally choosing the best configuration based on mean validation score.

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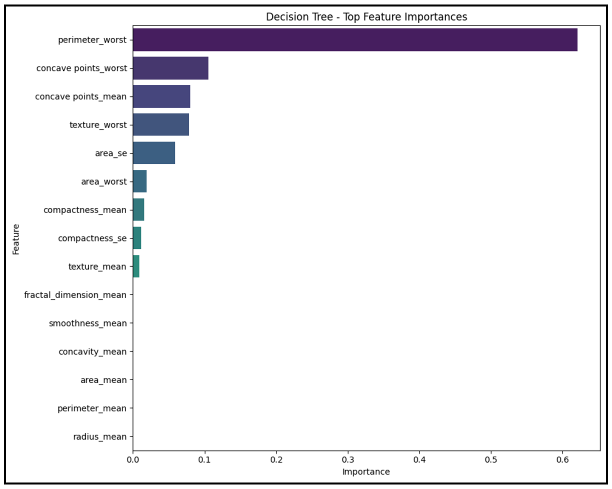
8. Code and Output (Decision Tree)

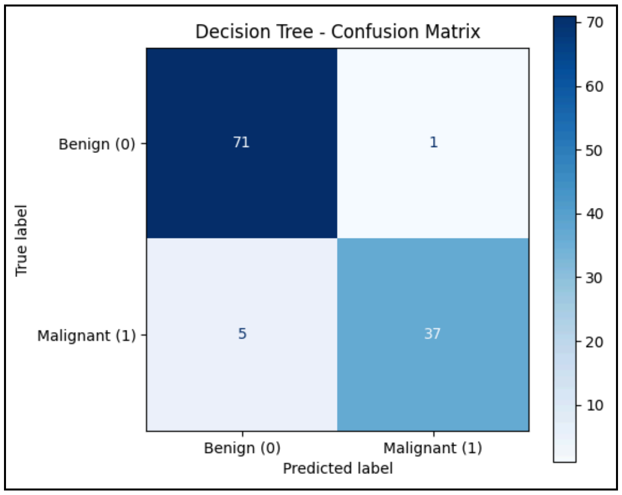
```
import pandas as pd

import numpy as np


from sklearn.model_selection import
train_test_split, GridSearchCV

from sklearn.tree import
DecisionTreeClassifier, plot_tree

from sklearn.preprocessing import
LabelEncoder

from sklearn.metrics import
(accuracy_score,


classification_report,

confusion_matrix,


ConfusionMatrixDisplay)


import matplotlib.pyplot as plt

import seaborn as sns

df = pd.read_csv('data.csv')

print("First 5 rows:")

print(df.head())

print("\nShape:", df.shape)
```

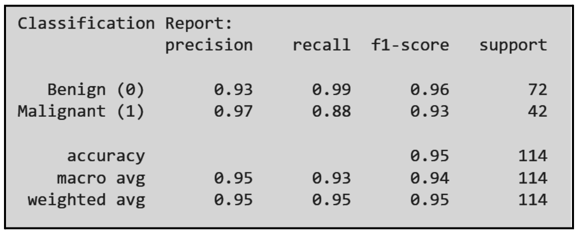
```
if 'id' in df.columns:
    df.drop(columns=['id'],
inplace=True)


le = LabelEncoder()
df['diagnosis'] =
le.fit_transform(df['diagnosis'])


print("\nMissing values per
column:")
print(df.isnull().sum())


X = df.drop('diagnosis', axis=1)
y = df['diagnosis']


X_train, X_test, y_train, y_test =
train_test_split(
    X, y, test_size=0.2,
random_state=42, stratify=y
)


print("\nTrain shape:",
X_train.shape, "Test shape:",
X_test.shape)


dtree_base =
DecisionTreeClassifier(random_state=
42)
dtree_base.fit(X_train, y_train)
y_pred_base =
dtree_base.predict(X_test)
base_acc = accuracy_score(y_test,
y_pred_base)
print(f"\nBaseline Decision Tree
Accuracy: {base_acc:.4f}")


param_grid = {
    'criterion': ['gini',
'entropy'],
    'max_depth': [None, 3, 5, 10,
15, 20],
    'min_samples_split': [2, 5, 10,
20],
    'min_samples_leaf': [1, 2, 4, 8]
}


grid_search = GridSearchCV(

estimator=DecisionTreeClassifier(ran
dom_state=42),
    param_grid=param_grid,
    cv=5,
    n_jobs=-1,
    verbose=1
)


grid_search.fit(X_train, y_train)


print("\nBest Parameters (Decision
Tree):")
print(grid_search.best_params_)
print(f"Best CV Score:
{grid_search.best_score_:.4f}")


best_dt =
grid_search.best_estimator_
```

```
y_pred = best_dt.predict(X_test)


print("\n--- Final Decision Tree
Evaluation ---")

print(f"Accuracy:
{accuracy_score(y_test,
y_pred):.4f}")

print("\nClassification Report:")

print(classification_report(y_test,
y_pred,


target_names=['Benign (0)',
'Malignant (1)']))


cm = confusion_matrix(y_test,
y_pred)

disp =
ConfusionMatrixDisplay(confusion_mat
rix=cm,


display_labels=['Benign (0)',
'Malignant (1)'])


fig, ax = plt.subplots(figsize=(6,
5))

disp.plot(cmap='Blues', ax=ax)

plt.title('Decision Tree - Confusion
Matrix')

plt.tight_layout()

plt.show()
```

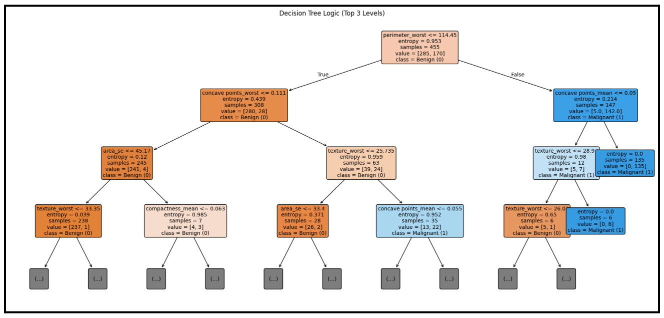
```
plt.figure(figsize=(22, 10))

plot_tree(best_dt,

          max_depth=3,

          feature_names=X.columns,

          class_names=['Benign (0)',
'Malignant (1)'],

          filled=True,

          rounded=True,

          fontsize=10)

plt.title("Decision Tree Logic (Top
3 Levels)")

plt.show()


importances =
best_dt.feature_importances_

feat_imp_df = pd.DataFrame({

    'Feature': X.columns,

    'Importance': importances

}).sort_values(by='Importance',
ascending=False)


plt.figure(figsize=(10, 8))

sns.barplot(x='Importance',
y='Feature',
data=feat_imp_df.head(15),
palette='viridis')

plt.title('Decision Tree - Top
Feature Importances')

plt.tight_layout()

plt.show()
```







```
Classification Report:
              precision    recall  f1-score   support

  Benign (0)       0.93      0.99      0.96        72
Malignant (1)      0.97      0.88      0.93        42

    accuracy                           0.95       114
   macro avg       0.95      0.93      0.94       114
weighted avg       0.95      0.95      0.95       114
```



9. Mathematical Formulation of Random Forest

A Random Forest is an ensemble of Decision Trees constructed using randomness in data sampling and feature selection.

Two main components:

1. Bootstrap Aggregating (Bagging)
    - For each tree, a bootstrap sample is drawn from the training data (sampling with replacement). Each tree sees a slightly different dataset, increasing diversity.
2. Random Feature Selection at Each Split
    - At each node, instead of evaluating splits over all features, the algorithm randomly selects a subset of features and finds the best split only among them. This prevents all trees from focusing on the same strong predictors and reduces correlation between trees.

For classification, given B trees $f_1, f_2, \ldots, f_B$, each tree outputs a class prediction $f_b(x)$.The final prediction $y^\wedge$ is obtained by majority voting:

$$\boxed{\hat{y} = \mathrm{mode}\{f_1(x), f_2(x), \ldots, f_B(x)\}}$$

This ensemble strategy reduces variance compared to a single Decision Tree and typically yields better generalization performance on test data.

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10. Limitations of Random Forest

1. Reduced Interpretability
   A single tree is relatively easy to visualize, but a forest of hundreds of trees behaves like a black box; it is difficult to extract simple decision rules from the overall model.
2. Higher Computational and Memory Cost
   Training and storing many trees is more resource-intensive than training a single Decision Tree, especially when using large numbers of estimators or deep trees.
3. Bias in Impurity-Based Feature Importance
   Features with more potential split points or higher cardinality may be favored in impurity-based importance metrics, even if they are not truly more informative.
4. Limited Extrapolation Ability
   Predictions are averages of seen training outcomes; the model cannot extrapolate beyond the range of values present in the training data.

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11. Methodology / Workflow (Random Forest)

1. Data Collection
   - Use the same `data.csv` file from Kaggle as in Experiment 3A.
2. Data Preprocessing
   - Load the data into a Pandas DataFrame.
   - Drop `id` column.
   - Encode `diagnosis` to numeric (0/1) using `LabelEncoder`.
   - Verify that there are no missing values.
3. Train–Test Split

        - Split into 80% training, 20% testing with `stratify=y` and `random_state=42`.
4. Baseline Model Training
    - Train a default `RandomForestClassifier` with standard hyperparameters.
    - Evaluate baseline accuracy on the test set as a reference.
5. Hyperparameter Tuning (RandomizedSearchCV)
    - Use `RandomizedSearchCV` to sample combinations from:
        - `n_estimators`: number of trees (e.g.,)
        - `max_depth`: tree depth (e.g., [None, 5, 10, 15, 20])
        - `min_samples_split`:
        - `min_samples_leaf`:
        - `bootstrap`: [True, False]
    - Use 3-fold cross-validation to evaluate sampled configurations and select the best model.
6. Optimized Model Training and Prediction
    - Train the best Random Forest on the full training set.
    - Generate predictions on the test set.
7. Model Evaluation
    - Compute accuracy, classification report, and confusion matrix.
    - Compare metrics to the baseline Random Forest and to the Decision Tree experiment.
8. Feature Importance Analysis
    - Extract feature importance scores from the optimized Random Forest.
    - Plot the top features to highlight which tumor characteristics are most predictive.
9. Conclusion
    - Discuss improvements over the baseline and over the Decision Tree model, emphasizing reduced variance and better generalization.

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12. Performance Analysis (Random Forest)

From the code below, you will obtain:

- Baseline Accuracy: default Random Forest performance on the test set.
- Tuned Accuracy: accuracy after hyperparameter tuning (usually higher than both the baseline RF and the Decision Tree).
- Precision, Recall, F1-Score:
    - Benign (0): usually very high precision and recall.

        - Malignant (1): improved recall and F1 compared to the Decision Tree, meaning fewer missed cancer cases.
- Confusion Matrix:
    - Fewer false negatives compared to the Decision Tree, demonstrating the benefit of the ensemble.

You can copy the printed metrics into your lab file to complete this section.

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13. Hyperparameter Tuning (Random Forest)

We tune the following hyperparameters:

- `n_estimators`: more trees usually reduce variance but increase training time.
- `max_depth`: controls tree complexity; shallow trees reduce overfitting.
- `min_samples_split`: minimum number of samples required to split a node.
- `min_samples_leaf`: minimum samples required in each leaf.
- `bootstrap`: whether to use bootstrap samples (bagging) or not.

`RandomizedSearchCV` samples a fixed number of random combinations from the hyperparameter space and uses 3-fold cross-validation to estimate performance more efficiently than exhaustive grid search.

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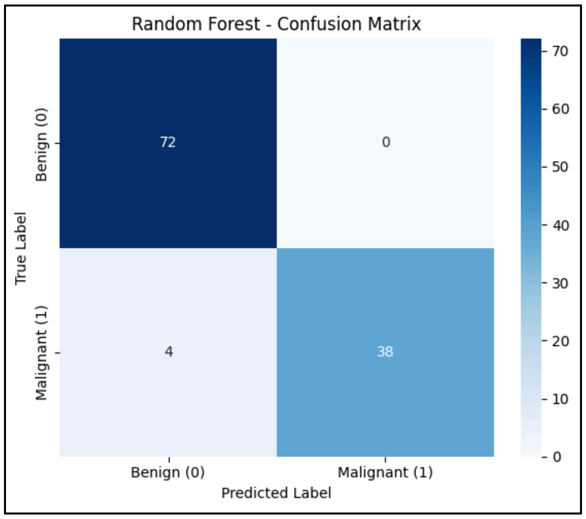
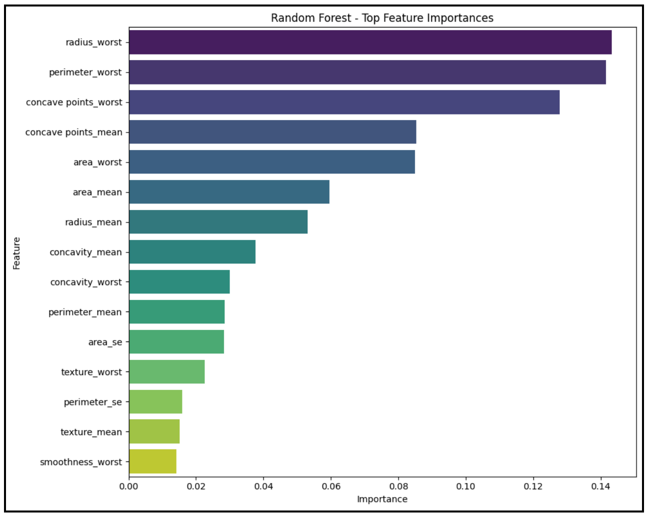
14. Code and Output (Random Forest)

```
import pandas as pd

import numpy as np


from sklearn.model_selection import
train_test_split, RandomizedSearchCV

from sklearn.ensemble import
RandomForestClassifier

from sklearn.preprocessing import
LabelEncoder

from sklearn.metrics import
(accuracy_score,


classification_report,

confusion_matrix)


import matplotlib.pyplot as plt

import seaborn as sns


df = pd.read_csv('data.csv')


print("First 5 rows:")

print(df.head())

print("\nShape:", df.shape)
```

```
if 'id' in df.columns:
    df.drop(columns=['id'],
inplace=True)


le = LabelEncoder()
df['diagnosis'] =
le.fit_transform(df['diagnosis'])


print("\nMissing values per
column:")
print(df.isnull().sum())


X = df.drop('diagnosis', axis=1)
y = df['diagnosis']


X_train, X_test, y_train, y_test =
train_test_split(
    X, y, test_size=0.2,
random_state=42, stratify=y
)


print("\nTrain shape:",
X_train.shape, "Test shape:",
X_test.shape)


rf_base =
RandomForestClassifier(random_state=
42)
rf_base.fit(X_train, y_train)


y_pred_base =
rf_base.predict(X_test)
base_acc = accuracy_score(y_test,
y_pred_base)
print(f"\nBaseline Random Forest
Accuracy: {base_acc:.4f}")


param_dist = {
    'n_estimators': [100, 200, 300],
    'max_depth': [None, 5, 10, 15,
20],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 4],
    'bootstrap': [True, False]
}


print("\nTuning Random Forest (this
may take some time)...")


rf_random = RandomizedSearchCV(

estimator=RandomForestClassifier(ran
dom_state=42),
    param_distributions=param_dist,
    n_iter=15,
    cv=3,
    random_state=42,
    n_jobs=-1,
    verbose=1
)


rf_random.fit(X_train, y_train)


best_rf = rf_random.best_estimator_
```

```
print("\nBest Parameters (Random
Forest):")

print(rf_random.best_params_)


y_pred = best_rf.predict(X_test)


print("\n--- Optimized Random Forest
Evaluation ---")

print(f"Tuned Accuracy:
{accuracy_score(y_test,
y_pred):.4f}")

print("\nClassification Report:")

print(classification_report(y_test,
y_pred,


target_names=['Benign (0)',
'Malignant (1)']))


cm = confusion_matrix(y_test,
y_pred)

plt.figure(figsize=(6, 5))

sns.heatmap(cm, annot=True, fmt='d',
cmap='Blues',

            xticklabels=['Benign
(0)', 'Malignant (1)'],

            yticklabels=['Benign
(0)', 'Malignant (1)'])

plt.title('Random Forest - Confusion
Matrix')

plt.xlabel('Predicted Label')

plt.ylabel('True Label')

plt.tight_layout()

plt.show()


importances =
best_rf.feature_importances_

feat_imp_df = pd.DataFrame({

    'Feature': X.columns,

    'Importance': importances

}).sort_values(by='Importance',
ascending=False)


plt.figure(figsize=(10, 8))

sns.barplot(x='Importance',
y='Feature',
data=feat_imp_df.head(15),
palette='viridis')

plt.title('Random Forest - Top
Feature Importances')

plt.tight_layout()

plt.show(
```





15. Conclusion

The practical showed that both Decision Tree and Random Forest can effectively solve a real-world binary classification problem on the Breast Cancer Wisconsin dataset, after proper preprocessing, train–test splitting, and hyperparameter tuning. The Decision Tree gave an interpretable baseline with clear if–else rules but was more prone to overfitting and instability, especially under class imbalance. The Random Forest, by aggregating many randomized trees, achieved better test performance and more stable precision–recall behavior for the malignant class, illustrating how ensembles improve robustness over single models while sacrificing some interpretability.