ML Assignment 1 — Naive Bayes & Decision Tree on UCI Iris

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This notebook builds and evaluates multiple classifiers on two UCI datasets using **scikit-learn**:

- Naive Bayes: **GaussianNB**, **MultinomialNB**, **BernoulliNB**
- **DecisionTreeClassifier** (both *gini* and *entropy*)

It reports **Accuracy, Precision, Recall, F1-score** and **Confusion Matrix**, then saves **decision tree images** (with impurity shown) for both criteria.

> Tip: Run all cells top-to-bottom. Outputs (images, CSV) are written to the `outputs/` folder.

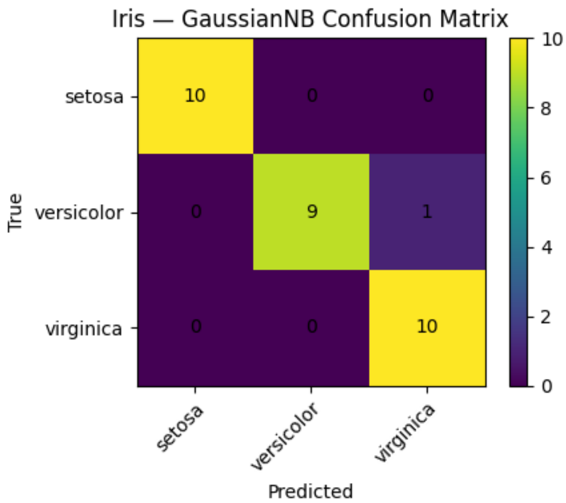
```
import os, itertools, joblib
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn import datasets
from sklearn.model_selection import train_test_split, GridSearchCV, StratifiedKFold
from sklearn.preprocessing import StandardScaler, MinMaxScaler
from sklearn.pipeline import Pipeline
from sklearn.naive_bayes import GaussianNB, MultinomialNB, BernoulliNB
from sklearn.tree import DecisionTreeClassifier, plot_tree
from sklearn.metrics import accuracy_score, precision_recall_fscore_support, confusion_matrix, classification_report


RANDOM_STATE = 42
np.random.seed(RANDOM_STATE)


OUT_DIR = "outputs"
os.makedirs(OUT_DIR, exist_ok=True)

def ensure_dir(path):
    if not os.path.exists(path):
        os.makedirs(path, exist_ok=True)



def plot_confusion(cm, classes, title, save_path=None):
    fig, ax = plt.subplots(figsize=(5,4))
    im = ax.imshow(cm, interpolation='nearest')
    ax.figure.colorbar(im, ax=ax)
    ax.set(xticks=np.arange(cm.shape[1]), yticks=np.arange(cm.shape[0]),
           xticklabels=classes, yticklabels=classes, title=title, ylabel='True', xlabel='Predicted')
    plt.setp(ax.get_xticklabels(), rotation=45, ha="right", rotation_mode="anchor")
    thresh = cm.max() / 2.
    for i in range(cm.shape[0]):
        for j in range(cm.shape[1]):
            ax.text(j, i, format(cm[i, j], 'd'),
                    ha="center", va="center")
    fig.tight_layout()
    if save_path:
        plt.savefig(save_path, dpi=300, bbox_inches='tight')
    plt.show()
    plt.close(fig)

def compute_metrics(y_true, y_pred, average='weighted'):
    acc = accuracy_score(y_true, y_pred)
    prec, rec, f1, _ = precision_recall_fscore_support(y_true, y_pred, average=average, zero_division=0)
    return acc, prec, rec, f1



iris = datasets.load_iris()
#bc = datasets.load_breast_cancer()

datasets_map = {
    "Iris": (iris.data, iris.target, iris.feature_names, iris.target_names),
    #"BreastCancer": (bc.data, bc.target, bc.feature_names, bc.target_names),
}
```

```
splits = {}
for name, (X, y, feat_names, class_names) in datasets_map.items():
    X_train, X_test, y_train, y_test = train_test_split(
        X, y, test_size=0.2, stratify=y, random_state=RANDOM_STATE
    )
    splits[name] = {
        "X_train": X_train, "X_test": X_test,
        "y_train": y_train, "y_test": y_test,
        "feature_names": feat_names, "class_names": class_names
    }
print("Datasets prepared:", list(splits.keys()))
```

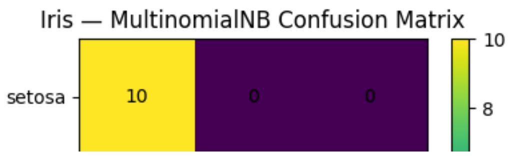
```
Datasets prepared: ['Iris']
```

```
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=RANDOM_STATE)

def run_nb_models(dataset_name, split, outdir):
    results = []

    gnb_pipe = Pipeline([('scaler', StandardScaler()), ('clf', GaussianNB())])
    gnb_grid = {'clf__var_smoothing': [1e-9, 1e-8, 1e-7, 1e-6]}


    mnb_pipe = Pipeline([('scaler', MinMaxScaler()), ('clf', MultinomialNB())])
    mnb_grid = {'clf__alpha': [0.1, 0.5, 1.0, 1.5], 'clf__fit_prior': [True, False]}


    bnb_pipe = Pipeline([('scaler', MinMaxScaler()), ('clf', BernoulliNB())])
    bnb_grid = {'clf__alpha': [0.1, 0.5, 1.0], 'clf__binarize': [0.1, 0.2, 0.3, 0.4, 0.5]}

    configs = [
        ("GaussianNB", gnb_pipe, gnb_grid),
        ("MultinomialNB", mnb_pipe, mnb_grid),
        ("BernoulliNB", bnb_pipe, bnb_grid),
    ]

    X_train, X_test = split["X_train"], split["X_test"]
    y_train, y_test = split["y_train"], split["y_test"]
    class_names = split["class_names"]

    for name, pipe, grid in configs:
        print(f"\n[{dataset_name}] Tuning {name} ...")
        gs = GridSearchCV(pipe, grid, cv=cv, n_jobs=-1, scoring='accuracy', refit=True)
        gs.fit(X_train, y_train)
        y_pred = gs.predict(X_test)
        acc, prec, rec, f1 = compute_metrics(y_test, y_pred)
        print(f"Best params: {gs.best_params_}")
        print(f"Test Accuracy: {acc:.4f} | Precision: {prec:.4f} | Recall: {rec:.4f} | F1: {f1:.4f}")
        print(classification_report(y_test, y_pred, target_names=class_names, zero_division=0))
        cm = confusion_matrix(y_test, y_pred)
        ensure_dir(outdir)
        cm_path = os.path.join(outdir, f"{dataset_name}_{name}_confusion.png")
        plot_confusion(cm, class_names, f"{dataset_name} — {name} Confusion Matrix", save_path=cm_path)
        results.append({
            "dataset": dataset_name, "model": name, "best_params": gs.best_params_,
            "accuracy": acc, "precision": prec, "recall": rec, "f1": f1
        })
    return pd.DataFrame(results)

all_nb_results = []

for dname, split in splits.items():
    outdir = os.path.join(OUT_DIR, dname, "NB")
    df = run_nb_models(dname, split, outdir)
    all_nb_results.append(df)

nb_results = pd.concat(all_nb_results, ignore_index=True)
nb_csv_path = os.path.join(OUT_DIR, "naive_bayes_results.csv")
nb_results.to_csv(nb_csv_path, index=False)
print("\nSaved NB summary to:", nb_csv_path)
nb_results
```

```
[Iris] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9667 | Precision: 0.9697 | Recall: 0.9667 | F1: 0.9666
              precision    recall  f1-score   support

      setosa       1.00      1.00      1.00        10
  versicolor       1.00      0.90      0.95        10
   virginica       0.91      1.00      0.95        10

    accuracy                           0.97        30
   macro avg       0.97      0.97      0.97        30
weighted avg       0.97      0.97      0.97        30
```



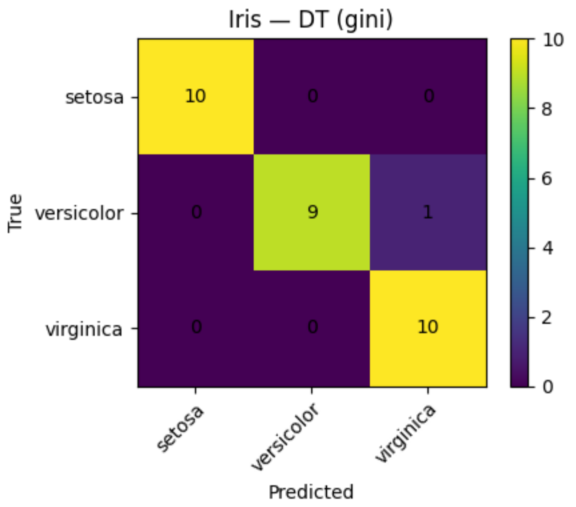

```
[Iris] Tuning MultinomialNB ...
Best params: {'clf__alpha': 0.1, 'clf__fit_prior': True}
Test Accuracy: 0.8333 | Precision: 0.8350 | Recall: 0.8333 | F1: 0.8329
              precision    recall  f1-score   support

      setosa       1.00      1.00      1.00        10
  versicolor       0.78      0.70      0.74        10
   virginica       0.73      0.80      0.76        10

    accuracy                           0.83        30
   macro avg       0.84      0.83      0.83        30
weighted avg       0.84      0.83      0.83        30
```

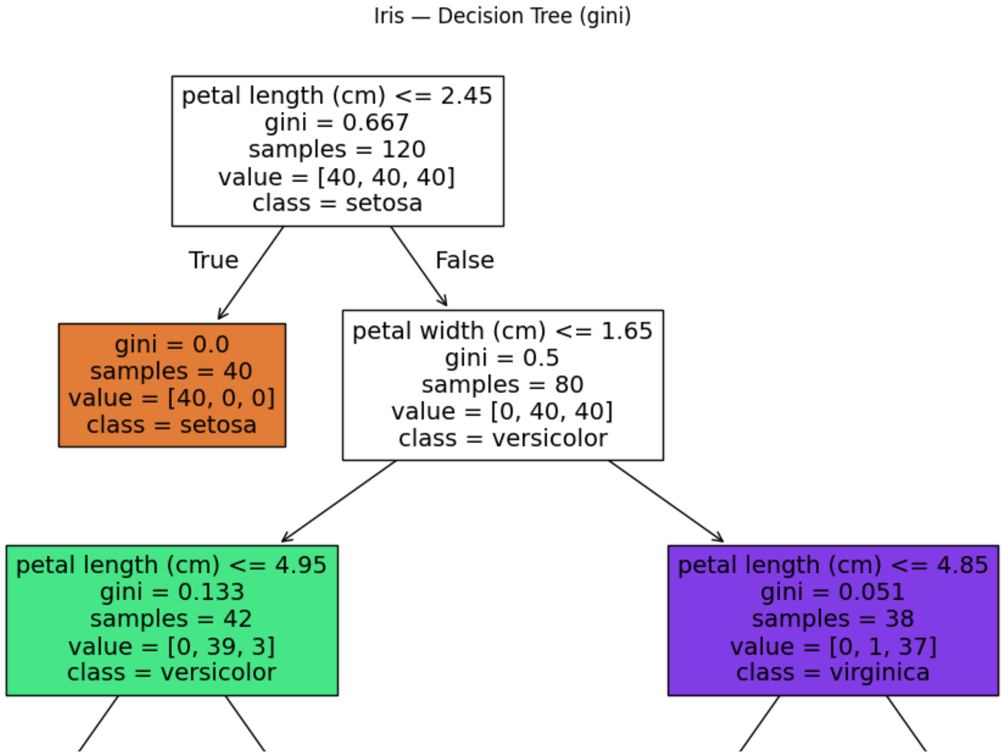



```
def fit_dt_for_criterion(dataset_name, split, criterion, base_outdir):
    X_train, X_test = split["X_train"], split["X_test"]
    y_train, y_test = split["y_train"], split["y_test"]
    feat_names = split["feature_names"]
    class_names = split["class_names"]

    pipe = Pipeline([('clf', DecisionTreeClassifier(random_state=RANDOM_STATE))])
    grid = {
        'clf__criterion': [criterion],
        'clf__max_depth': [None, 3, 4, 5, 6, 8, 10],
        'clf__min_samples_split': [2, 4, 6, 8, 10],
        'clf__min_samples_leaf': [1, 2, 3, 4],
        'clf__class_weight': [None, 'balanced'],
        'clf__splitter': ['best', 'random']
    }
    gs = GridSearchCV(pipe, grid, cv=StratifiedKFold(n_splits=5, shuffle=True, random_state=RANDOM_STATE),
                      n_jobs=-1, scoring='accuracy', refit=True)
    gs.fit(X_train, y_train)
    best_clf = gs.best_estimator_['clf']
    y_pred = gs.predict(X_test)
    acc, prec, rec, f1 = compute_metrics(y_test, y_pred)
    print(f"[{dataset_name}] DecisionTree ({criterion}) best params:", gs.best_params_)
    print(f"Test Accuracy: {acc:.4f} | Precision: {prec:.4f} | Recall: {rec:.4f} | F1: {f1:.4f}")


    cm = confusion_matrix(y_test, y_pred)
    outdir = os.path.join(base_outdir, criterion.capitalize())
```

```
        ensure_dir(outdir)
        cm_path = os.path.join(outdir, f"{dataset_name}_DT_{criterion}_confusion.png")
        plot_confusion(cm, class_names, f"{dataset_name} — DT ({criterion})", save_path=cm_path)


        fig, ax = plt.subplots(figsize=(14, 10))
        plot_tree(best_clf, feature_names=feat_names, class_names=class_names, filled=True, impurity=True)
        ax.set_title(f"{dataset_name} — Decision Tree ({criterion})")
        tree_img_path = os.path.join(outdir, f"{dataset_name}_DT_{criterion}_tree.png")
        plt.savefig(tree_img_path, dpi=300, bbox_inches='tight')
        plt.show()
        plt.close(fig)

        return {
            "dataset": dataset_name, "model": f"DecisionTree-{criterion}",
            "best_params": gs.best_params_, "accuracy": acc, "precision": prec, "recall": rec, "f1": f1,
            "tree_image": tree_img_path
        }

    dt_rows = []
    for dname, split in splits.items():
        base_out = os.path.join(OUT_DIR, dname, "DecisionTree")
        ensure_dir(base_out)
        for crit in ["gini", "entropy"]:
            row = fit_dt_for_criterion(dname, split, crit, base_out)
            dt_rows.append(row)

    dt_results = pd.DataFrame(dt_rows)
    dt_csv_path = os.path.join(OUT_DIR, "decision_tree_results.csv")
    dt_results.to_csv(dt_csv_path, index=False)
    print("\nSaved Decision Tree summary to:", dt_csv_path)
    dt_results
```

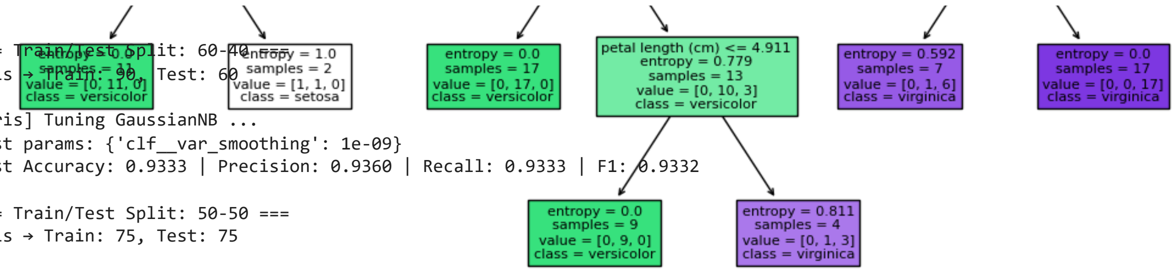
```
[Iris] DecisionTree (gini) best params: {'clf__class_weight': None, 'clf__criterion': 'gini', 'clf__max_depth': None, 'clf__min_samp
Test Accuracy: 0.9667 | Precision: 0.9697 | Recall: 0.9667 | F1: 0.9666
```






```python
split_ratios = [0.4, 0.5, 0.7, 0.2] # Corresponds to test sizes for 60-40, 50-50, 30-70, 80-20 splits

nb_split_results = []

for ratio in split_ratios:
    print(f"\n=== Train/Test Split: {int((1-ratio)*100)}-{int(ratio*100)} ===")
    for name, (X, y, feat_names, class_names) in datasets_map.items():
        X_train, X_test, y_train, y_test = train_test_split(
            X, y, test_size=ratio, stratify=y, random_state=RANDOM_STATE
        )
        print(f"{name} → Train: {len(X_train)}, Test: {len(X_test)}")

        # Run GaussianNB
        gnb_pipe = Pipeline([('scaler', StandardScaler()), ('clf', GaussianNB())])
        gnb_grid = {'clf__var_smoothing': [1e-9, 1e-8, 1e-7, 1e-6]}
        cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=RANDOM_STATE)

        print(f"\n[{name}] Tuning GaussianNB ...")
        gs = GridSearchCV(gnb_pipe, gnb_grid, cv=cv, n_jobs=-1, scoring='accuracy', refit=True)
        gs.fit(X_train, y_train)
        y_pred = gs.predict(X_test)
        acc, prec, rec, f1 = compute_metrics(y_test, y_pred)
        print(f"Best params: {gs.best_params_}")
        print(f"Test Accuracy: {acc:.4f} | Precision: {prec:.4f} | Recall: {rec:.4f} | F1: {f1:.4f}")

        nb_split_results.append({
            "dataset": name, "model": "GaussianNB", "best_params": gs.best_params_,
```

```
            "accuracy": acc, "precision": prec, "recall": rec, "f1": f1,
            "split_ratio": f"{int((1-ratio)*100)}-{int(ratio*100)}"
        })

nb_split_results_df = pd.DataFrame(nb_split_results)


def plot_nb_comparison_chart(df, metric, title):
    plt.figure(figsize=(10, 6))
    for dataset in df['dataset'].unique():
        dataset_data = df[df['dataset'] == dataset]
        plt.plot(dataset_data['split_ratio'], dataset_data[metric], marker='o', label=dataset)

    plt.title(title)
    plt.xlabel('Train-Test Split Ratio')
    plt.ylabel(metric)
    plt.legend()
    plt.grid(True)
    plt.show()

plot_nb_comparison_chart(nb_split_results_df, 'accuracy', 'GaussianNB Accuracy Comparison by Split Ratio'
plot_nb_comparison_chart(nb_split_results_df, 'f1', 'GaussianNB F1-score Comparison by Split Ratio')


nb_split_csv_path = os.path.join(OUT_DIR, "gaussiannb_split_results.csv")
nb_split_results_df.to_csv(nb_split_csv_path, index=False)
print("\nSaved GaussianNB split results to:", nb_split_csv_path)
display(nb_split_results_df)
```




```
=== Train/Test Split: 60-40 ===
Iris → Train: 90, Test: 60

[Iris] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9333 | Precision: 0.9360 | Recall: 0.9333 | F1: 0.9332

=== Train/Test Split: 50-50 ===
Iris → Train: 75, Test: 75

[Iris] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9467 | Precision: 0.9485 | Recall: 0.9467 | F1: 0.9466

Saved Decision Tree summary to: outputs/decision_tree_results.csv
=== Train/Test Split: 30-70 ===
Iris → Train: 45, Test: 105

[Iris] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9524 | Precision: 0.9526 | Recall: 0.9524 | F1: 0.9524

=== Train/Test Split: 80-20 ===
Iris → Train: 120, Test: 30

[Iris] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9667 | Precision: 0.9697 | Recall: 0.9667 | F1: 0.9666
```

	dataset	model	best_params	accuracy	precision	recall	f1	tree_image
0	Iris	DecisionTree-gini	{'clf__class_weight': None, 'clf__criterion': ...	0.966667	0.969697	0.966667	0.966583	outputs/Iris DecisionTree/Gini/Iris_DT_gini_tr...
1	Iris	DecisionTree-entropy	{'clf__class_weight': None, 'clf__criterion': ...	0.933333	0.933333	0.933333	0.933333	outputs/Iris/I ecisionTree/Entropy/Iris_DT_entr...