ML Assignment 1 — Naive Bayes & Decision Tree on Breast Cancer

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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.

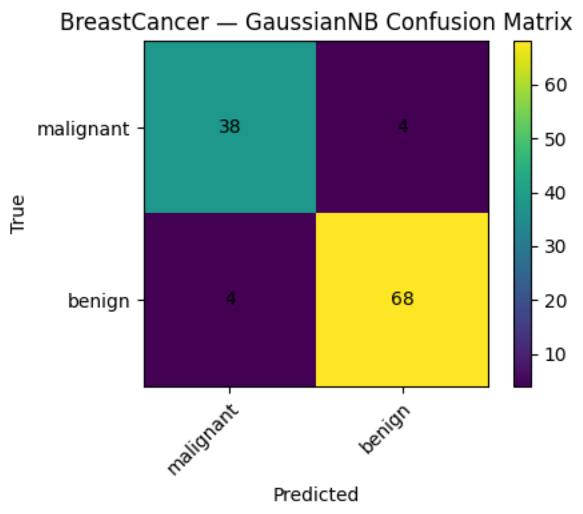
```python
import os, itertools, joblib
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

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),
}
```

```
# Train/test split for each dataset (stratified)
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()))
```

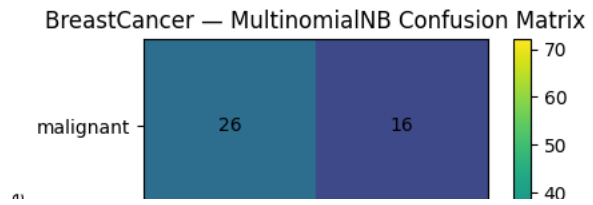
```
Datasets prepared: ['BreastCancer']
```

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

def run_nb_models(dataset_name, split, outdir):
    results = []
    # 1) GaussianNB (works fine on real-valued features)
    gnb_pipe = Pipeline([('scaler', StandardScaler()), ('clf', GaussianNB())])
    gnb_grid = {'clf__var_smoothing': [1e-9, 1e-8, 1e-7, 1e-6]}

    # 2) MultinomialNB (expects non-negative features) -> MinMax scale
    mnb_pipe = Pipeline([('scaler', MinMaxScaler()), ('clf', MultinomialNB())])
    mnb_grid = {'clf__alpha': [0.1, 0.5, 1.0, 1.5], 'clf__fit_prior': [True, False]}

    # 3) BernoulliNB (best with binary features) -> scale then use clf's binarize
    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
```

```
[BreastCancer] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9298 | Precision: 0.9298 | Recall: 0.9298 | F1: 0.9298
              precision    recall  f1-score   support

   malignant       0.90      0.90      0.90        42
      benign       0.94      0.94      0.94        72

    accuracy                           0.93       114
   macro avg       0.92      0.92      0.92       114
weighted avg       0.93      0.93      0.93       114
```



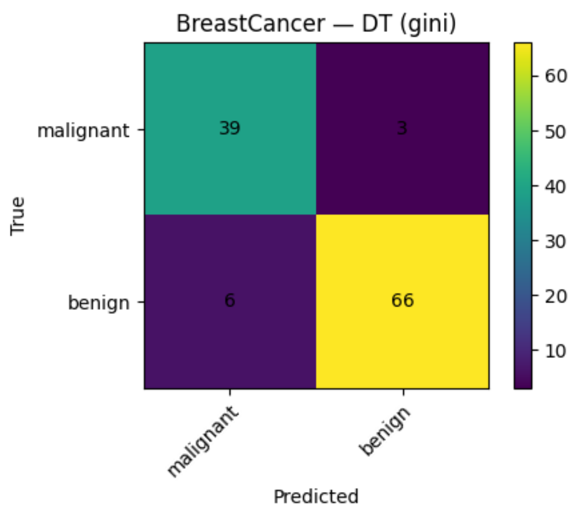
```
[BreastCancer] Tuning MultinomialNB ...
Best params: {'clf__alpha': 0.1, 'clf__fit_prior': True}
Test Accuracy: 0.8596 | Precision: 0.8852 | Recall: 0.8596 | F1: 0.8502
              precision    recall  f1-score   support

   malignant       1.00      0.62      0.76        42
      benign       0.82      1.00      0.90        72

    accuracy                           0.86       114
   macro avg       0.91      0.81      0.83       114
weighted avg       0.89      0.86      0.85       114
```

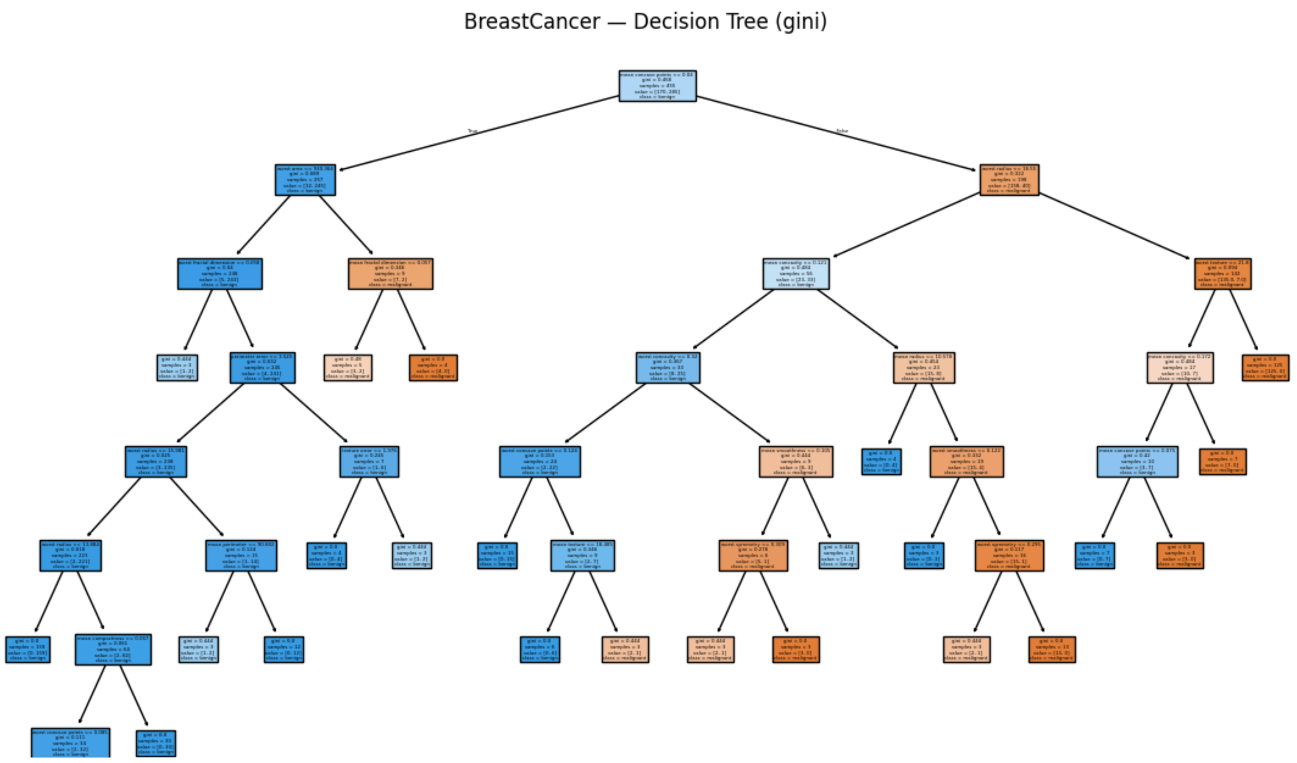


```
def fit_dt_for_criterion(dataset_name, split, criterion, base_outdir):
    X_train, X_test = split["X_train"], split["X_test"]
    y_train, y_test = split["y_train"], split["y_test"]
    feat_names = split["feature_names"]
    class_names = split["class_names"]

    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())
```

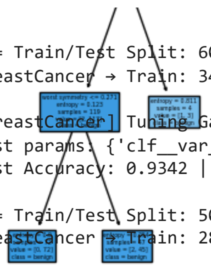
```
        ensure_dir(outdir)
        cm_path = os.path.join(outdir, f"{dataset_name}_DT_{criterion}_confusion.png")
        plot_confusion(cm, class_names, f"{dataset_name} — DT ({criterion})", save_path=cm_path)


        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
```

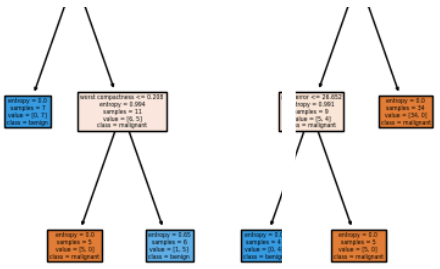
```
[BreastCancer] DecisionTree (gini) best params: {'clf__class_weight': None, 'clf__criterion': 'gini', 'clf__max_depth': None, 'clf_
Test Accuracy: 0.9211 | Precision: 0.9234 | Recall: 0.9211 | F1: 0.9216
```





```
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 ===
BreastCancer → Train: 341, Test: 228

[BreastCancer] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9342 | Precision: 0.9343 | Recall: 0.9342 | F1: 0.9338

=== Train/Test Split: 50-50 ===
BreastCancer → Train: 284, Test: 285

[BreastCancer] Tuning GaussianNB ...
Best params: {'clf__var_smoothing': 1e-09}
Test Accuracy: 0.9368 | Precision: 0.9374 | Recall: 0.9368 | F1: 0.9363

Saved Decision Tree summary to: outputs/decision_tree_results.csv
=== Train/Test Split: 30-70 ===
BreastCancer → Train: 170, Test: 399

[BreastCancer] Tuning GaussianNB ...
```

	dataset	model	best_params	accuracy	precision	recall	f1	tree_image
0	BreastCancer	DecisionTree	{'clf__class_weight': None,	0.921053	0.923417	0.921053	0.921574	outputs/BreastCancer/DecisionTree/Gini/BreastC...