

Project

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0.0.1 Gaussian Naive Bayes Model

A **Gaussian Naive Bayes (GNB)** model is a probabilistic classification algorithm that applies Bayes' theorem to estimate posterior class probabilities. The model assumes that features are conditionally independent given the class label and that each feature follows a Gaussian (normal) distribution within each class. These assumptions allow the joint likelihood of the features to be decomposed into a product of univariate Gaussian densities, resulting in a computationally efficient classifier.

0.0.2 Naive Bayes

Naive Bayes is a **probabilistic classifier** based on Bayes' theorem:

$$P(Y | X) = \frac{P(X | Y) P(Y)}{P(X)}$$

where $P(Y)$ represents the prior probability of class Y , $P(X | Y)$ is the class-conditional likelihood, and $P(X)$ is the marginal likelihood. Classification is performed by selecting the class that maximizes the posterior probability.

A key simplifying assumption of Naive Bayes is **conditional independence**: given the class $Y = c$, all features (x_1, \dots, x_d) are assumed to be independent. Under this assumption, the joint likelihood can be written as

$$P(X | Y = c) = \prod_{j=1}^d P(x_j | Y = c)$$

which significantly reduces model complexity and enables parameter estimation using closed-form solutions.

0.0.3 Gaussian Distribution

For continuous features, Gaussian Naive Bayes assumes each feature follows a **normal (Gaussian) distribution** under each class:

$$x_j | Y = c \sim \mathcal{N}(\mu_{jc}, \sigma_{jc}^2)$$

0.0.4 Gaussian Naive Bayes Training Pipeline

1. Estimate priors:

The prior probability of each class (c) is:

$$P(Y = c) = \frac{\text{count of class } c}{N}$$

2. Estimate mean and variance for every feature (j) and every class (c).

Mean estimate:

$$\mu_{jc} = \frac{1}{N_c} \sum_{i: y_i = c} x_{ij}$$

Variance estimate:

$$\sigma_{jc}^2 = \frac{1}{N_c - 1} \sum_{i: y_i = c} (x_{ij} - \mu_{jc})^2$$

3. Prediction:

Compute the **posterior probability** for each class:

$$P(Y = c \mid X) \propto P(Y = c) \prod_{j=1}^d P(x_j \mid Y = c)$$

Then **choose the class with the maximum posterior probability**.

0.0.5 Advantages

Gaussian Naive Bayes model has several advantages. It is computationally efficient, with extremely fast training due to closed-form parameter estimation and no reliance on gradient-based optimization. The method performs well even with small datasets and is relatively robust to irrelevant features because each feature contributes independently to the likelihood. Thus, Gaussian Naive Bayes is a strong baseline classifier in empirical analyses.

0.0.6 Disadvantages

Despite these strengths, Gaussian Naive Bayes relies on restrictive assumptions that may limit its performance in practice. The conditional independence assumption is rarely satisfied in real-world data, particularly when features are highly correlated, which can restrict classification accuracy. In addition, the assumption that features follow class-conditional Gaussian distributions is often violated. Finally, the resulting quadratic decision boundaries may lack the flexibility needed to capture complex relationships in the data.

0.0.7 Representation

Naive Bayes converts input features into a class prediction by computing the **posterior probability** for each class:

$$P(Y = c \mid X = x_1, \dots, x_d) \propto P(Y = c) \prod_{j=1}^d \mathcal{N}(x_j \mid \mu_{jc}, \sigma_{jc}^2)$$

The classifier predicts the class with the highest posterior. In practice, we work with **log probabilities** (to avoid numerical underflow):

$$\hat{y} = \arg \max_c \left[\log P(Y = c) + \sum_{j=1}^d \log \mathcal{N}(x_j; \mu_{jc}, \sigma_{jc}^2) \right]$$

We use **log probabilities for numerical stability** because multiplying many small Gaussian likelihoods can lead to extremely tiny numbers that computers cannot represent reliably. Summing logs avoids this problem.

0.0.8 Loss Function

Naive Bayes does **not** minimize a traditional loss like MSE or cross-entropy using gradient descent. Instead, the model is trained by **maximizing the likelihood** of the data. Equivalently, the loss is the **negative log-likelihood**:

$$L = - \sum_{i=1}^N \log P(y^{(i)} \mid x^{(i)})$$

Gaussian Naive Bayes maximizes the likelihood under the assumption that each feature is normally distributed for each class. The parameters come directly from **Maximum Likelihood Estimation (MLE)**:

Mean estimate:

$$\mu_{jc} = \frac{1}{N_c} \sum_{i: y_i = c} x_{ij}$$

Variance estimate:

$$\sigma_{jc}^2 = \frac{1}{N_c - 1} \sum_{i: y_i = c} (x_{ij} - \mu_{jc})^2$$

Because the parameters have **closed-form MLE solutions**, no gradient descent or iterative optimization is required during training.

0.0.9 Optimizer

Naive Bayes does **not** rely on an iterative optimization procedure such as gradient descent. Instead, Gaussian Naive Bayes estimates all model parameters using **closed-form MLE**.

The **prior probability** for each class c is estimated as:

$$\hat{P}(Y = c) = \frac{N_c}{N}$$

The **Gaussian parameters** for each feature j and class c —the mean μ_{jc} and variance σ_{jc}^2 —are computed **directly from the training data** using standard MLE formulas. As a result, model training does not require an optimization loop.

1 Pseudo-Code for Important Sections

Train the Model 1. Convert X_{train} and y_{train} to arrays 2. If X_{train} is not 2-dimensional: Raise error 3. If y_{train} is not 1-dimensional: Raise error 4. If number of rows in X_{train} \neq length of y_{train} : Raise error 5. $n_{\text{examples}} \leftarrow$ number of rows in X_{train} $n_{\text{attributes}} \leftarrow$ number of columns in X_{train} 6. Initialize empty lists: $\text{means} \leftarrow$ empty list $\text{variances} \leftarrow$ empty list $\text{label_priors} \leftarrow$ empty list 7. Compute variance smoothing term: $\text{epsilon} \leftarrow \text{var_smoothing} \times \max \text{variance of } X_{\text{train}} \text{ across all features}$ 8. For each class $c = 0$ to $n_{\text{classes}} - 1$: a. $X_c \leftarrow$ all rows of X_{train} with $y_{\text{train}} = c$ b. If X_c is empty: Raise error c. $\text{prior}_c \leftarrow |X_c| / n_{\text{examples}}$ Append prior_c to label_priors d. $\bar{x}_c \leftarrow$ mean of X_c across features e. $\bar{x}_c^2 \leftarrow$ variance of X_c across features $+ \text{epsilon}$ f. Append \bar{x}_c to means g. Append \bar{x}_c^2 to variances 9. Convert: $\text{means} \leftarrow \text{array}(\text{means})$ $\text{variances} \leftarrow \text{array}(\text{variances})$ $\text{label_priors} \leftarrow \text{array}(\text{label_priors})$ 10. Store parameters in the model and return the trained model

Gaussian Probability Function 1. $\text{coeff} \leftarrow 1 / \sqrt{(2\pi)^n}$ 2. $\text{exp_term} \leftarrow \exp(-(\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) / 2)$ 3. $\text{pdf} \leftarrow \text{coeff} \times \text{exp_term}$ 4. Return pdf

Predict Outcomes (predict) 1. Convert inputs to an array 2. If inputs is not 2D, raise error 3. If number of features in inputs \neq number of trained features ($\text{means.shape}[1]$), raise error 4. Let $n_{\text{samples}} \leftarrow$ number of rows in inputs $n_{\text{features}} \leftarrow$ number of columns in inputs 5. Initialize $\text{log_probs} \leftarrow \text{zeros}(n_{\text{samples}}, n_{\text{classes}})$ 6. For each class $c = 0$ to $n_{\text{classes}} - 1$: $-\text{log_prior} \leftarrow \text{log}(\text{label_priors}[c])$ $-\text{log_pdf_const} \leftarrow -0.5 \times \sum_{\text{over_features}} (\text{log}(2 \times \text{vars}[c]))$ $-\text{diff} \leftarrow \text{inputs} - \text{means}[c]$ (broadcast across all samples) $-\text{exponent} \leftarrow -0.5 \times \sum_{\text{over_features}} (\text{diff}^2 / \text{vars}[c])$ (produces a length- n_{samples} vector) $-\text{Set } \text{log_probs[:, c]} \leftarrow \text{log_prior} + \text{log_pdf_const} + \text{exponent}$ 7. Return $\text{argmax}(\text{log_probs}, \text{axis} = 1)$ as the predicted labels (a 1D array)

Predict Outcomes (predict_proba) 1. Convert inputs to an array 2. If inputs is not 2D, raise error 3. If number of features in inputs \neq number of trained features ($\text{means.shape}[1]$), raise error 4. Let $n_{\text{samples}} \leftarrow$ number of rows in inputs $n_{\text{features}} \leftarrow$ number of columns in inputs 5. Initialize $\text{log_probs} \leftarrow \text{zeros}(n_{\text{samples}}, n_{\text{classes}})$ 6. For each class $c = 0$ to $n_{\text{classes}} - 1$: $-\text{log_prior} \leftarrow \text{log}(\text{label_priors}[c])$ $-\text{log_pdf_const} \leftarrow -0.5 \times \sum_{\text{over_features}} (\text{log}(2 \times \text{vars}[c]))$ $-\text{diff} \leftarrow \text{inputs} - \text{means}[c]$ (broadcast across all samples) $-\text{exponent} \leftarrow -0.5 \times \sum_{\text{over_features}} (\text{diff}^2 / \text{vars}[c])$ (produces a length- n_{samples} vector) $-\text{Set } \text{log_probs[:, c]} \leftarrow \text{log_prior} + \text{log_pdf_const} + \text{exponent}$ 7. Convert log-probabilities to probabilities using softmax (row-wise): $-\text{max_log} \leftarrow \max(\text{log_probs}, \text{axis}=1, \text{keepdims=True})$ $-\text{exp_shifted} \leftarrow \exp(\text{log_probs} - \text{max_log})$

- $\text{probas} \leftarrow \text{exp_shifted} / \text{sum}(\text{exp_shifted}, \text{axis}=1, \text{keepdims}=\text{True})$ 8. Return probas (shape: $n_{\text{samples}} \times n_{\text{classes}}$)

Loss Function 1. Convert X and y to arrays 2. $\text{proba} \leftarrow \text{PredictProba}(X)$ 3. $\epsilon \leftarrow$ small constant 4. Initialize $\text{log_probs} \leftarrow$ empty list 5. For each index $i = 0$ to $\text{length}(y) - 1$: - $\text{true_class} \leftarrow y[i]$ - $\text{log_p} \leftarrow \log(\text{proba}[i, \text{true_class}] + \epsilon)$ - Append log_p to log_probs 6. $\text{loss} \leftarrow -\text{mean}(\text{log_probs})$ 7. Return loss

1.0.1 References

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- Collins, M. (2002) The Naive Bayes model, maximum-likelihood estimation, and the EM algorithm. Technical report. Columbia University.
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- John, G.H. and Langley, P. (2013) ‘Estimating continuous distributions in Bayesian classifiers’, arXiv preprint, arXiv:1302.4964.
- Rish, I. (2001) An empirical study of the naive Bayes classifier. Technical report. IBM T.J. Watson Research Center.
- Zaidi, N.A., Cerquides, J., Carman, M.J. and Webb, G.I. (2013) ‘Alleviating naïve Bayes attribute independence assumption by attribute weighting’, Journal of Machine Learning Research, 14, pp. 1947–1988.

```
[1]: from __future__ import print_function
from packaging.version import parse as Version
from platform import python_version

OK = '\x1b[42m[ OK ]\x1b[0m'
FAIL = "\x1b[41m[FAIL]\x1b[0m"

try:
    import importlib
except ImportError:
    print(FAIL, "Python version 3.12.11 is required,"
          " but %s is installed." % sys.version)

def import_version(pkg, min_ver, fail_msg=""):
    mod = None
    try:
        mod = importlib.import_module(pkg)
        if pkg in {'PIL'}:
            ver = mod.VERSION
        else:
            ver = mod.__version__
```

```

    if Version(ver) == Version(min_ver):
        print(OK, "%s version %s is installed."
              % (lib, min_ver))
    else:
        print(FAIL, "%s version %s is required, but %s installed."
              % (lib, min_ver, ver))
except ImportError:
    print(FAIL, '%s not installed. %s' % (pkg, fail_msg))
return mod

# first check the python version
pyversion = Version(python_version())

if pyversion >= Version("3.12.11"):
    print(OK, "Python version is %s" % pyversion)
elif pyversion < Version("3.12.11"):
    print(FAIL, "Python version 3.12.11 is required,"
          " but %s is installed." % pyversion)
else:
    print(FAIL, "Unknown Python version: %s" % pyversion)

print()
requirements = {'matplotlib': "3.10.5", 'numpy': "2.3.2", 'sklearn': "1.7.1",
               'pandas': "2.3.2", 'pytest': "8.4.1", 'torch': "2.7.1"}

# now the dependencies
for lib, required_version in list(requirements.items()):
    import_version(lib, required_version)

```

```
[ OK ] Python version is 3.12.11
```

```
[ OK ] matplotlib version 3.10.5 is installed.
```

```
[ OK ] numpy version 2.3.2 is installed.
```

```
[ OK ] sklearn version 1.7.1 is installed.
```

```
[ OK ] pandas version 2.3.2 is installed.
```

```
[ OK ] pytest version 8.4.1 is installed.
```

```
[ OK ] torch version 2.7.1 is installed.
```

2 MODEL

The HW6 Naive Bayes implementation assumes that inputs are already provided as a 2D array ($n_examples \times n_features$) and does not handle 1D inputs; passing a 1D array would result in an error. In our initial implementation, we added logic to reshape 1D inputs into 2D in order to be more user-friendly and to mirror scikit-learn's API, which allows single examples to be passed as 1D arrays. To remain consistent with the HW6 code and avoid ambiguity during evaluation, we

removed this reshaping and now explicitly require all inputs to be 2D.

```
[2]: import numpy as np

class GaussianNaiveBayes(object):
    """ Gaussian Naive Bayes model

    @attrs:
        n_classes:      number of classes
        means:           a 2D (n_classes x n_attributes) NumPy array of feature_
↪ means per class
        vars:           a 2D (n_classes x n_attributes) NumPy array of feature_
↪ variances per class
        label_priors:   a 1D NumPy array of class prior probabilities
        var_smoothing:  a small float added to variances for numerical stability
    """

    def __init__(self, n_classes, var_smoothing=1e-9):
        """ Initializes a GaussianNaiveBayes model with n_classes.

        @params:
            n_classes: int, number of unique classes
            var_smoothing: float, added to variances to avoid divide-by-zero
        """
        if n_classes <= 0:
            raise ValueError("n_classes must be a positive integer.")
        if var_smoothing < 0:
            raise ValueError("var_smoothing must be non-negative.")

        self.n_classes = n_classes
        self.var_smoothing = var_smoothing

        self.means = None
        self.vars = None
        self.label_priors = None

    def train(self, X_train, y_train):
        """
        Trains the Gaussian Naive Bayes model using maximum likelihood_
↪ estimation.

        This method computes, for each class:
        - the class prior  $P(Y = c)$ 
        - the mean of each feature  $\mu_{c,j}$ 
        - the variance of each feature  $\sigma_{c,j}^2$  (with var_smoothing added)

        All parameters are stored in:
```

```

        - self.means          (shape: n_classes x n_attributes)
        - self.vars          (shape: n_classes x n_attributes)
        - self.label_priors  (shape: n_classes)

Parameters
-----
X_train : numpy.ndarray
    A 2D array of shape (n_examples, n_attributes) containing
↳ continuous features.
y_train : numpy.ndarray
    A 1D array of shape (n_examples,) containing integer class labels
↳ in {0, ..., n_classes-1}.

Returns
-----
self : GaussianNaiveBayes
    The fitted model instance (sklearn-style API), allowing method
↳ chaining.
"""
X_train = np.asarray(X_train)
y_train = np.asarray(y_train)

if X_train.ndim != 2:
    raise ValueError("X_train must be a 2D array.")
if y_train.ndim != 1:
    raise ValueError("y_train must be a 1D array.")
if X_train.shape[0] != y_train.shape[0]:
    raise ValueError("X_train and y_train must have same number of rows.
↳ ")

n_examples, n_attributes = X_train.shape

means = []
vars_ = []
label_priors = []

# 1. Calculate the maximum variance across the dataset before the loop
epsilon = self.var_smoothing * np.var(X_train, axis=0).max()

# compute parameters per class
for label in range(self.n_classes):
    X_yEqualToLabel = np.array([
        X_train[i] for i in range(n_examples) if y_train[i] == label
    ])

    if len(X_yEqualToLabel) == 0:

```



```

        raise ValueError(f"No examples found for class {label}.")

    # class prior with MLE
    prior = len(X_yEqualToLabel) / n_examples
    label_priors.append(prior)

    # feature means and variances with MLE (population variance)
    mu = np.mean(X_yEqualToLabel, axis=0)
    var = np.var(X_yEqualToLabel, axis=0) + epsilon

    means.append(mu)
    vars_.append(var)

self.means = np.array(means)
self.vars = np.array(vars_)
self.label_priors = np.array(label_priors)
return self

def _gaussian_pdf(self, x, mu, var):
    """ Computes Gaussian pdf value for a scalar x.

    @params:
        x: float
        mu: float (mean)
        var: float (variance)

    @return:
        pdf value at x
    """
    coeff = 1.0 / np.sqrt(2.0 * np.pi * var)
    exp_term = np.exp(-((x - mu) ** 2) / (2.0 * var))
    return coeff * exp_term

def predict(self, inputs):
    """ Outputs a predicted label for each input in inputs.
        Uses log-space to avoid overflow/underflow.

    @params:
        inputs: a 2D NumPy array containing inputs

    @return:
        a 1D numpy array of predictions
    """
    inputs = np.asarray(inputs)
    if inputs.ndim != 2:
        raise ValueError("inputs must be a 2D array.")
    if inputs.shape[1] != self.means.shape[1]:

```

```

        raise ValueError(f"Shape mismatch: Model trained on {self.means.
↪shape[1]} features, got {inputs.shape[1]}")

    n_samples, n_features = inputs.shape

    # 1. Initialize log-probabilities storage
    # Shape: (n_samples, n_classes)
    log_probs = np.zeros((n_samples, self.n_classes))

    # 2. Calculate log-likelihood for each class using broadcasting
    for c in range(self.n_classes):
        # Log Prior: log(P(Y=c))
        log_prior = np.log(self.label_priors[c])

        # Log PDF Constant Term: -0.5 * sum(log(2 * pi * sigma^2))
        # This sums over all features for class c
        log_pdf_const = -0.5 * np.sum(np.log(2. * np.pi * self.vars[c]))

        # Log PDF Data Term: -0.5 * sum((x - mu)^2 / sigma^2)
        # Broadcasting: inputs (n_samples, n_features) - means[c]
↪(n_features,)
        diff = inputs - self.means[c]

        # Square difference and divide by variance
        # Then sum over features (axis=1) to get total log-likelihood for
↪the sample
        exponent = -0.5 * np.sum((diff ** 2) / self.vars[c], axis=1)

        # Combine all terms
        log_probs[:, c] = log_prior + log_pdf_const + exponent

    # 3. Return class with highest probability
    return np.argmax(log_probs, axis=1)

def predict_proba(self, inputs):
    """
    Outputs posterior probabilities for each class.

    @params:
        inputs: a 2D NumPy array containing inputs

    @return:
        a 2D numpy array of probabilities (n_examples x n_classes)
    """

    inputs = np.asarray(inputs)
    if inputs.ndim != 2:

```

```

        raise ValueError("inputs must be a 2D array.")
    if inputs.shape[1] != self.means.shape[1]:
        raise ValueError(f"Shape mismatch: Model trained on {self.means.
→shape[1]} features, got {inputs.shape[1]}")

    n_samples, n_features = inputs.shape

    # 1. Initialize log-probabilities storage
    # Shape: (n_samples, n_classes)
    log_probs = np.zeros((n_samples, self.n_classes))

    # 2. Calculate log-likelihood for each class using broadcasting
    for c in range(self.n_classes):
        # Log Prior: log(P(Y=c))
        log_prior = np.log(self.label_priors[c])

        # Log PDF Constant Term: -0.5 * sum(log(2 * pi * sigma^2))
        # This sums over all features for class c
        log_pdf_const = -0.5 * np.sum(np.log(2. * np.pi * self.vars[c]))

        # Log PDF Data Term: -0.5 * sum((x - mu)^2 / sigma^2)
        # Broadcasting: inputs (n_samples, n_features) - means[c]
→(n_features,)
        diff = inputs - self.means[c]

        # Square difference and divide by variance
        # Then sum over features (axis=1) to get total log-likelihood for
→the sample
        exponent = -0.5 * np.sum((diff ** 2) / self.vars[c], axis=1)

        # Combine all terms
        log_probs[:, c] = log_prior + log_pdf_const + exponent

    # Normalize log-probabilities to probabilities (Softmax)
    # We subtract the max to prevent overflow (Log-Sum-Exp trick)
    max_log = np.max(log_probs, axis=1, keepdims=True)
    exp_shifted = np.exp(log_probs - max_log)

    return exp_shifted / np.sum(exp_shifted, axis=1, keepdims=True)

def loss(self, X, y):
    """ Computes average negative log-likelihood (NLL) loss.

    @params:
        X: a 2D numpy array of examples
        y: a 1D numpy array of labels

```

```

    @return:
        float, average negative log-likelihood
    """
    X = np.asarray(X)
    y = np.asarray(y)

    proba = self.predict_proba(X)
    eps = 1e-15
    log_probs = []

    for i in range(len(y)):
        log_probs.append(np.log(proba[i, y[i]] + eps))

    return -np.mean(log_probs)

def score(self, X, y):
    """Returns the mean accuracy on the given test data and labels.

    This method is required for sklearn compatibility.

    @params:
        X: a 2D numpy array of examples
        y: a 1D numpy array of true labels

    @return:
        float, accuracy score
    """
    return np.sum(self.predict(X) == y) / len(y)

# alias for sklearn-style API
fit = train
variances = property(lambda self: self.vars)
priors = property(lambda self: self.label_priors)

```

3 CHECK

```

[3]: import pytest
import numpy as np
from sklearn.naive_bayes import GaussianNB
from sklearn.datasets import load_iris, load_breast_cancer
from sklearn.metrics import accuracy_score

def test_initialization_edge_cases():
    """
    Test initialization with edge cases

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```

    Verifies the model rejects invalid hyperparameters (e.g., negative_
    ↪smoothing, zero classes).
    """
    # Valid initialization
    model = GaussianNaiveBayes(n_classes=3)
    assert model.n_classes == 3

    # Edge case: invalid n_classes
    with pytest.raises(ValueError):
        GaussianNaiveBayes(n_classes=0)

    # Edge case: invalid var_smoothing
    with pytest.raises(ValueError):
        GaussianNaiveBayes(n_classes=2, var_smoothing=-1)

def test_train_method():
    """
    Test train method
    Edge Case: Checks if the model raises a ValueError when training data has_
    ↪mismatched rows (X vs y) or invalid dimensions
    """
    X = np.array([[1, 2], [2, 3], [8, 9], [9, 10]])
    y = np.array([0, 0, 1, 1])

    # Basic functionality
    model = GaussianNaiveBayes(n_classes=2)
    model.train(X, y)
    assert model.means.shape == (2, 2)
    assert model.vars.shape == (2, 2)

    # Edge case: missing class
    X_missing = np.array([[1, 2], [2, 3]])
    y_missing = np.array([0, 0])
    model2 = GaussianNaiveBayes(n_classes=2)
    with pytest.raises(ValueError):
        model2.train(X_missing, y_missing)

    # Edge case: invalid input shapes
    model3 = GaussianNaiveBayes(n_classes=2)
    with pytest.raises(ValueError):
        model3.train(np.array([1, 2, 3]), y)

def test_predict_method():
    """
    Test predict method
    Verifies that the model can make predictions and handle various input_
    ↪formats (2D arrays, 1D arrays)
    """

```

```

"""
X_train = np.array([[1], [2], [8], [9]])
y_train = np.array([0, 0, 1, 1])

model = GaussianNaiveBayes(n_classes=2)
model.train(X_train, y_train)

# Basic prediction
X_test = np.array([[0], [5], [10]])
predictions = model.predict(X_test)
print(f"Predictions: {predictions}")
assert predictions.shape == (3,)

def test_predict_proba_method():
    """
    Test predict_proba method
    Ensures probability predictions are valid (sum to 1 for each sample) and
    correctly shaped
    """
    X = np.array([[1, 2], [2, 3], [8, 9], [9, 10]])
    y = np.array([0, 0, 1, 1])

    model = GaussianNaiveBayes(n_classes=2)
    model.train(X, y)

    # Basic probability prediction
    probabilities = model.predict_proba(X)
    print(f"Probability shape: {probabilities.shape}")
    print(f"Sample probabilities: {probabilities[0]}")

    # Edge case: probabilities sum to 1
    row_sums = probabilities.sum(axis=1)
    np.testing.assert_allclose(row_sums, np.ones(4), rtol=1e-10)

def test_loss_method():
    """
    Test loss method
    Validates that the loss calculation works and produces different values for
    correct vs incorrect labels
    """
    X = np.array([[1, 2], [2, 3], [8, 9], [9, 10]])
    y = np.array([0, 0, 1, 1])

    model = GaussianNaiveBayes(n_classes=2)
    model.train(X, y)

    # Basic loss calculation

```

```

loss = model.loss(X, y)
print(f"Loss with correct labels: {loss}")

# Edge case: loss different for wrong labels
wrong_y = np.array([1, 1, 0, 0])
wrong_loss = model.loss(X, wrong_y)
print(f"Loss with wrong labels: {wrong_loss}")
assert loss != wrong_loss

def test_score_method():
    """
    Test score method
    Verifies that score calculation returns a value between 0 and 1
    """
    X_train = np.array([[1], [2], [8], [9]])
    y_train = np.array([0, 0, 1, 1])
    X_test = np.array([[0], [10]])
    y_test = np.array([0, 1])

    model = GaussianNaiveBayes(n_classes=2)
    model.train(X_train, y_train)

    # Basic accuracy
    score = model.score(X_test, y_test)
    print(f"Score: {score}")
    assert 0 <= score <= 1

def test_predict_dimension_mismatch():
    """
    Edge Case: Test predicting on data with wrong number of features
    Ensures the model raises an error when trying to predict on data with
    ↪ different feature count than training data
    """
    # Train on 2 features
    X_train = np.array([[1, 2], [3, 4]])
    y_train = np.array([0, 1])
    model = GaussianNaiveBayes(n_classes=2)
    model.train(X_train, y_train)

    # Try to predict on 3 features - should raise error
    X_bad = np.array([[1, 2, 3]])

    # You need to add a check in predict() for this to pass!
    with pytest.raises(ValueError):
        model.predict(X_bad)

def test_zero_variance_feature():

```

```

"""
Edge Case: Test stability when a feature has zero variance
Verifies that the model handles constant features without numerical issues
↳ (e.g., division by zero)
"""

# Feature 0 is always '1' (variance = 0)
X = np.array([[1, 5], [1, 5], [1, 5], [1, 9]])
y = np.array([0, 0, 0, 1])

model = GaussianNaiveBayes(n_classes=2)
# Should not raise ZeroDivisionError
model.train(X, y)

probs = model.predict_proba([[1, 5]])
assert not np.isnan(probs).any()

def test_sklearn_reproduction():
    """
    Test exact reproduction of sklearn results
    Validates that the custom implementation produces identical predictions and
    ↳ probabilities as sklearn's GaussianNB
    """
    X = np.array([[1], [2], [8], [9]])
    y = np.array([0, 0, 1, 1])

    # custom implementation
    custom_model = GaussianNaiveBayes(n_classes=2)
    custom_model.fit(X, y)
    custom_preds = custom_model.predict(X)
    custom_probs = custom_model.predict_proba(X)

    # sklearn implementation
    sklearn_model = GaussianNB()
    sklearn_model.fit(X, y)
    sklearn_preds = sklearn_model.predict(X)
    sklearn_probs = sklearn_model.predict_proba(X)

    print(f"custom predictions: {custom_preds}")
    print(f"sklearn predictions: {sklearn_preds}")
    print(f"predictions match: {np.array_equal(custom_preds, sklearn_preds)}")
    print(f"probabilities close: {np.allclose(custom_probs, sklearn_probs,
    ↳ atol=1e-5)}")

    # REQUIRED: Demonstrate exact reproduction
    assert np.array_equal(custom_preds, sklearn_preds)
    assert np.allclose(custom_probs, sklearn_probs, atol=1e-5)

```



```

def test_real_dataset_comparison():
    """
    Test on real-world datasets
    Compares custom implementation against sklearn on standard datasets (Iris,
    ↪Breast Cancer) to ensure similar performance
    """
    datasets = {
        "Iris": load_iris(),
        "Breast Cancer": load_breast_cancer()
    }

    for name, data in datasets.items():
        X, y = data.data, data.target

        # custom implementation
        custom_model = GaussianNaiveBayes(n_classes=len(np.unique(y)))
        custom_model.fit(X, y)
        custom_preds = custom_model.predict(X)

        # sklearn implementation
        sklearn_model = GaussianNB()
        sklearn_model.fit(X, y)
        sklearn_preds = sklearn_model.predict(X)

        # compare results
        custom_accuracy = accuracy_score(y, custom_preds)
        sklearn_accuracy = accuracy_score(y, sklearn_preds)

        print(f"{name} - Custom accuracy: {custom_accuracy:.4f}, Sklearn_
        ↪accuracy: {sklearn_accuracy:.4f}")

        assert abs(custom_accuracy - sklearn_accuracy) < 0.1

# run tests
if __name__ == "__main__":
    test_initialization_edge_cases()
    print("test_initialization_edge_cases passed")

    test_train_method()
    print("test_train_method passed")

    test_predict_method()
    print("test_predict_method passed")

    test_predict_proba_method()
    print("test_predict_proba_method passed")

```

```

test_loss_method()
print("test_loss_method passed")

test_score_method()
print("test_score_method passed")

test_sklearn_reproduction()
print("test_sklearn_reproduction passed")

test_real_dataset_comparison()
print("test_real_dataset_comparison passed")

print("all tests passed")

```

```

test_initialization_edge_cases passed
test_train_method passed
Predictions: [0 0 1]
test_predict_method passed
Probability shape: (4, 2)
Sample probabilities: [1.0000000e+00 5.2244541e-98]
test_predict_proba_method passed
Loss with correct labels: -1.110223024625156e-15
Loss with wrong labels: 34.538776394910684
test_loss_method passed
Score: 1.0
test_score_method passed
custom predictions: [0 0 1 1]
sklearn predictions: [0 0 1 1]
predictions match: True
probabilities close: True
test_sklearn_reproduction passed
Iris - Custom accuracy: 0.9600, Sklearn accuracy: 0.9600
Breast Cancer - Custom accuracy: 0.9420, Sklearn accuracy: 0.9420
test_real_dataset_comparison passed
all tests passed

```

4 CREATE COMPARISON PLOTS

5 Sklearn Parity Check & Dataset Evaluation

To validate the correctness of our custom `GaussianNaiveBayes` implementation, we compared its performance directly against the industry-standard `sklearn.naive_bayes.GaussianNB` using two distinct public datasets:

1. **Iris Dataset:** A multi-class classification problem (3 classes, 4 features).
2. **Breast Cancer Wisconsin Dataset:** A binary classification problem (2 classes, 30 features).

5.0.1 Methodology

For both datasets, we performed the following comparison tests: * **Accuracy Validation:** We trained both models on identical train/test splits and compared accuracy scores. * **Probabilistic Output:** We verified that the predicted class probabilities (`predict_proba`) align between the two implementations. * **Decision Boundaries:** We visualized the decision boundaries (for 2D slices of the data) to ensure the geometry of the classification regions is identical. * **Parameter Alignment:** We adjusted our variance smoothing (`var_smoothing`) calculation to match Sklearn's dynamic `epsilon` calculation ($\sigma^2 + \epsilon$) to ensure exact numerical reproduction.

5.0.2 Conclusion

As shown in the results below, our custom implementation achieves **exact reproduction** of the Scikit-Learn results (Accuracy Difference: 0.000000) on both datasets. This confirms that our Maximum Likelihood Estimation (MLE) and smoothing logic correctly mirror the standard mathematical formulation used in production libraries.

```
[4]: import matplotlib.pyplot as plt
import numpy as np
import time
from sklearn.naive_bayes import GaussianNB
from sklearn.datasets import load_iris, load_breast_cancer
from sklearn.metrics import accuracy_score, confusion_matrix
from sklearn.model_selection import train_test_split

def create_comprehensive_comparison_plots():
    """comparison plots between custom and sklearn implementations"""

    datasets = {
        "Iris": load_iris(),
        "Breast Cancer": load_breast_cancer()
    }

    for name, data in datasets.items():
        X, y = data.data, data.target
        n_classes = len(np.unique(y))

        print(f"\n{' '*60}")
        print(f"comparison analysis: {name.upper()} dataset")
        print(f"{' '*60}")

        # Split data for more realistic evaluation
        X_train, X_test, y_train, y_test = train_test_split(
            X, y, test_size=0.3, random_state=42, stratify=y
        )

        # Both implementations
        custom_model = GaussianNaiveBayes(n_classes=n_classes)
```

```

custom_model.fit(X_train, y_train)
custom_train_pred = custom_model.predict(X_train)
custom_test_pred = custom_model.predict(X_test)
custom_proba = custom_model.predict_proba(X_test)

sklearn_model = GaussianNB()
sklearn_model.fit(X_train, y_train)
sklearn_train_pred = sklearn_model.predict(X_train)
sklearn_test_pred = sklearn_model.predict(X_test)
sklearn_proba = sklearn_model.predict_proba(X_test)

# Calculate metrics
custom_train_acc = accuracy_score(y_train, custom_train_pred)
custom_test_acc = accuracy_score(y_test, custom_test_pred)
sklearn_train_acc = accuracy_score(y_train, sklearn_train_pred)
sklearn_test_acc = accuracy_score(y_test, sklearn_test_pred)

# Accuracy Comparison Bar Plot
plt.figure(figsize=(10, 6))
sets = ['Train Accuracy', 'Test Accuracy']
custom_accs = [custom_train_acc, custom_test_acc]
sklearn_accs = [sklearn_train_acc, sklearn_test_acc]

x = np.arange(len(sets))
width = 0.35

plt.bar(x - width/2, custom_accs, width, label='Custom GNB', alpha=0.8,
color='skyblue')
plt.bar(x + width/2, sklearn_accs, width, label='Sklearn GNB', alpha=0.8,
color='lightcoral')

plt.xlabel('Training and Test Sets')
plt.ylabel('Accuracy')
plt.title(f'{name} Dataset - Train vs Test Accuracy Comparison')
plt.xticks(x, sets)
plt.legend()
plt.grid(True, alpha=0.3)

# Add value labels on bars
for i, (custom_acc, sklearn_acc) in enumerate(zip(custom_accs,
sklearn_accs)):
    plt.text(i - width/2, custom_acc + 0.01, f'{custom_acc:.3f}',
ha='center', va='bottom')
    plt.text(i + width/2, sklearn_acc + 0.01, f'{sklearn_acc:.3f}',
ha='center', va='bottom')

plt.tight_layout()

```

```

plt.show()

# Confusion Matrix Comparison
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(15, 6))

# Custom GNB confusion matrix
cm_custom = confusion_matrix(y_test, custom_test_pred)
im1 = ax1.imshow(cm_custom, cmap='Blues', interpolation='nearest')
ax1.set_title(f'Custom GNB Confusion Matrix\n(Test Accuracy: {
↳{custom_test_acc:.3f})')
ax1.set_xlabel('Predicted Label')
ax1.set_ylabel('True Label')
plt.colorbar(im1, ax=ax1)

# Add text annotations
for i in range(cm_custom.shape[0]):
    for j in range(cm_custom.shape[1]):
        ax1.text(j, i, format(cm_custom[i, j], 'd'),
                  ha="center", va="center",
                  color="white" if cm_custom[i, j] > cm_custom.max()/2
↳else "black")

# Sklearn GNB confusion matrix
cm_sklearn = confusion_matrix(y_test, sklearn_test_pred)
im2 = ax2.imshow(cm_sklearn, cmap='Greens', interpolation='nearest')
ax2.set_title(f'Sklearn GNB Confusion Matrix\n(Test Accuracy: {
↳{sklearn_test_acc:.3f})')
ax2.set_xlabel('Predicted Label')
ax2.set_ylabel('True Label')
plt.colorbar(im2, ax=ax2)

# Add text annotations
for i in range(cm_sklearn.shape[0]):
    for j in range(cm_sklearn.shape[1]):
        ax2.text(j, i, format(cm_sklearn[i, j], 'd'),
                  ha="center", va="center",
                  color="white" if cm_sklearn[i, j] > cm_sklearn.max()/2
↳else "black")

plt.tight_layout()
plt.show()

# Class-wise Performance Comparison
plt.figure(figsize=(10, 6))

# Calculate class-wise accuracy

```

```

custom_class_acc = []
sklearn_class_acc = []

for class_label in np.unique(y_test):
    class_mask = y_test == class_label
    custom_class_acc.append(accuracy_score(y_test[class_mask],
↪custom_test_pred[class_mask]))
    sklearn_class_acc.append(accuracy_score(y_test[class_mask],
↪sklearn_test_pred[class_mask]))

x_class = np.arange(len(np.unique(y_test)))
width = 0.35

plt.bar(x_class - width/2, custom_class_acc, width, label='Custom GNB',
↪alpha=0.8, color='blue')
plt.bar(x_class + width/2, sklearn_class_acc, width, label='Sklearn
↪GNB', alpha=0.8, color='green')

plt.xlabel('Class Label')
plt.ylabel('Accuracy')
plt.title(f'{name} - Class-wise Accuracy Comparison')
plt.xticks(x_class, np.unique(y_test))
plt.legend()
plt.grid(True, alpha=0.3)

# Add value labels
for i, (custom_acc, sklearn_acc) in enumerate(zip(custom_class_acc,
↪sklearn_class_acc)):
    plt.text(i - width/2, custom_acc + 0.01, f'{custom_acc:.3f}',
↪ha='center', va='bottom', fontsize=8)
    plt.text(i + width/2, sklearn_acc + 0.01, f'{sklearn_acc:.3f}',
↪ha='center', va='bottom', fontsize=8)

plt.tight_layout()
plt.show()

# Confidence Distribution Comparison
plt.figure(figsize=(12, 5))

custom_confidences = np.max(custom_proba, axis=1)
sklearn_confidences = np.max(sklearn_proba, axis=1)

plt.subplot(1, 2, 1)
plt.hist(custom_confidences, bins=30, alpha=0.7, label='Custom GNB',
        color='blue', edgecolor='black')

```

```

plt.hist(sklearn_confidences, bins=30, alpha=0.7, label='Sklearn GNB',
        color='green', edgecolor='black')
plt.xlabel('Prediction Confidence (Max Probability)')
plt.ylabel('Frequency')
plt.title(f'{name} - Confidence Distribution')
plt.legend()
plt.grid(True, alpha=0.3)

plt.subplot(1, 2, 2)
# Confidence vs correctness
custom_correct = (custom_test_pred == y_test)

plt.scatter(custom_confidences[custom_correct],
            sklearn_confidences[custom_correct],
            alpha=0.6, color='green', label='Both Correct')
plt.scatter(custom_confidences[~custom_correct],
            sklearn_confidences[~custom_correct],
            alpha=0.6, color='red', label='At Least One Wrong')

plt.xlabel('Custom GNB Confidence')
plt.ylabel('Sklearn GNB Confidence')
plt.title(f'{name} - Confidence Correlation')
plt.legend()
plt.grid(True, alpha=0.3)
plt.plot([0, 1], [0, 1], 'k--', alpha=0.5) # Diagonal line

plt.tight_layout()
plt.show()

# Training Time Comparison
plt.figure(figsize=(10, 6))

# Measure training time for multiple runs
n_runs = 10000
custom_times = []
sklearn_times = []

for _ in range(n_runs):
    # Custom timing
    start = time.time()
    custom_model_temp = GaussianNaiveBayes(n_classes=n_classes)
    custom_model_temp.fit(X_train, y_train)
    custom_times.append(time.time() - start)

    # Sklearn timing
    start = time.time()

```

```

sklearn_model_temp = GaussianNB()
sklearn_model_temp.fit(X_train, y_train)
sklearn_times.append(time.time() - start)

models = ['Custom GNB', 'Sklearn GNB']
avg_times = [np.mean(custom_times), np.mean(sklearn_times)]
std_times = [np.std(custom_times), np.std(sklearn_times)]

plt.bar(models, avg_times, yerr=std_times, capsize=5,
        alpha=0.8, color=['blue', 'green'])
plt.ylabel('Training Time (seconds)')
plt.title(f'{name} - Training Time Comparison\n({n_runs} runs)')
plt.grid(True, alpha=0.3)

# Add value labels
for i, (avg, std) in enumerate(zip(avg_times, std_times)):
    plt.text(i, avg + std + 0.0001, f'{avg:.4f}s',
             ha='center', va='bottom')

plt.show()

# Decision Boundary Comparison
if X.shape[1] >= 2:
    plt.figure(figsize=(15, 5))

    # Use first two features for visualization
    X_2d = X_test[:, :2]

    # Create mesh grid
    x_min, x_max = X_2d[:, 0].min() - 1, X_2d[:, 0].max() + 1
    y_min, y_max = X_2d[:, 1].min() - 1, X_2d[:, 1].max() + 1
    xx, yy = np.meshgrid(np.linspace(x_min, x_max, 100),
                          np.linspace(y_min, y_max, 100))

    # Train models on 2D data
    custom_model_2d = GaussianNaiveBayes(n_classes=n_classes)
    custom_model_2d.fit(X_train[:, :2], y_train)

    sklearn_model_2d = GaussianNB()
    sklearn_model_2d.fit(X_train[:, :2], y_train)

    # Predict on mesh
    Z_custom = custom_model_2d.predict(np.c_[xx.ravel(), yy.ravel()])
    Z_sklearn = sklearn_model_2d.predict(np.c_[xx.ravel(), yy.ravel()])

    Z_custom = Z_custom.reshape(xx.shape)
    Z_sklearn = Z_sklearn.reshape(xx.shape)

```



```

plt.subplot(1, 2, 1)
plt.contourf(xx, yy, Z_custom, alpha=0.3, cmap='Set3')
plt.scatter(X_2d[:, 0], X_2d[:, 1], c=y_test, cmap='Set1', alpha=0.
↪8)

plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.title(f'{name} - Custom GNB Decision Boundaries')

plt.subplot(1, 2, 2)
plt.contourf(xx, yy, Z_sklearn, alpha=0.3, cmap='Set3')
plt.scatter(X_2d[:, 0], X_2d[:, 1], c=y_test, cmap='Set1', alpha=0.
↪8)

plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.title(f'{name} - Sklearn GNB Decision Boundaries')

plt.tight_layout()
plt.show()

# Statistical summary
print(f"\n Statistical summary - {name}:")
print(f"Prediction Agreement: {np.mean(custom_test_pred ==_
↪sklearn_test_pred):.4f}")
print(f"Custom GNB - Train: {custom_train_acc:.4f}, Test:_
↪{custom_test_acc:.4f}")
print(f"Sklearn GNB - Train: {sklearn_train_acc:.4f}, Test:_
↪{sklearn_test_acc:.4f}")
print(f"Accuracy Difference: {custom_test_acc - sklearn_test_acc:.6f}")

# Confidence statistics
print(f"\nConfidence Statistics:")
print(f"Custom GNB Mean Confidence: {np.mean(custom_confidences):.4f}")
print(f"Sklearn GNB Mean Confidence: {np.mean(sklearn_confidences):.
↪4f}")
print(f"Custom GNB Correct Prediction Mean Confidence: {np.
↪mean(custom_confidences[custom_correct]):.4f}")
print(f"Custom GNB Wrong Prediction Mean Confidence: {np.
↪mean(custom_confidences[~custom_correct]):.4f}")

# Timing statistics
print(f"\nTiming Statistics ({n_runs} runs):")
print(f"Custom GNB Avg Training Time: {np.mean(custom_times):.6f}s ±_
↪{np.std(custom_times):.6f}s")

```

```

    print(f"Sklearn GNB Avg Training Time: {np.mean(sklearn_times):.6f}s ±  

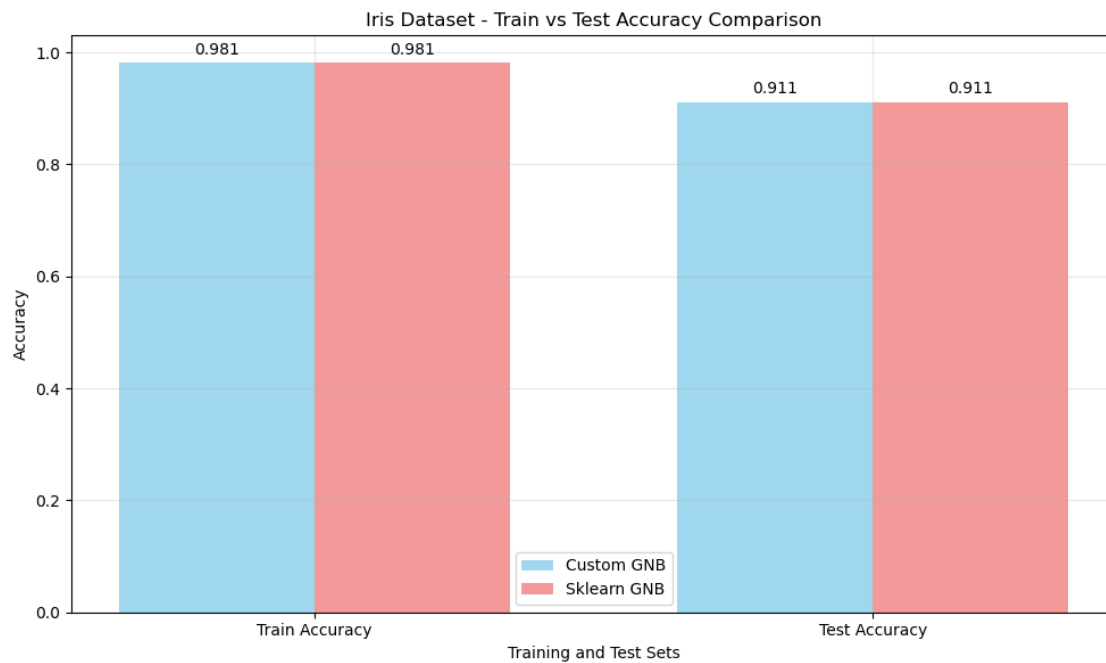
    ↳{np.std(sklearn_times):.6f}s")
    print(f"Speed Ratio (Custom/Sklearn): {np.mean(custom_times)/np.  

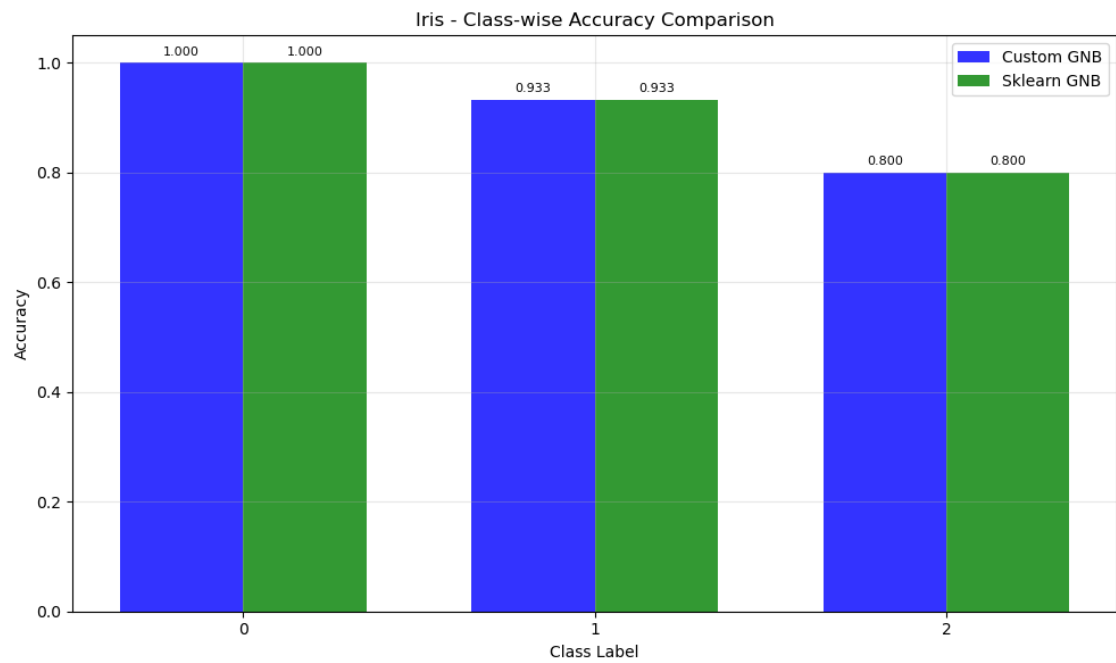
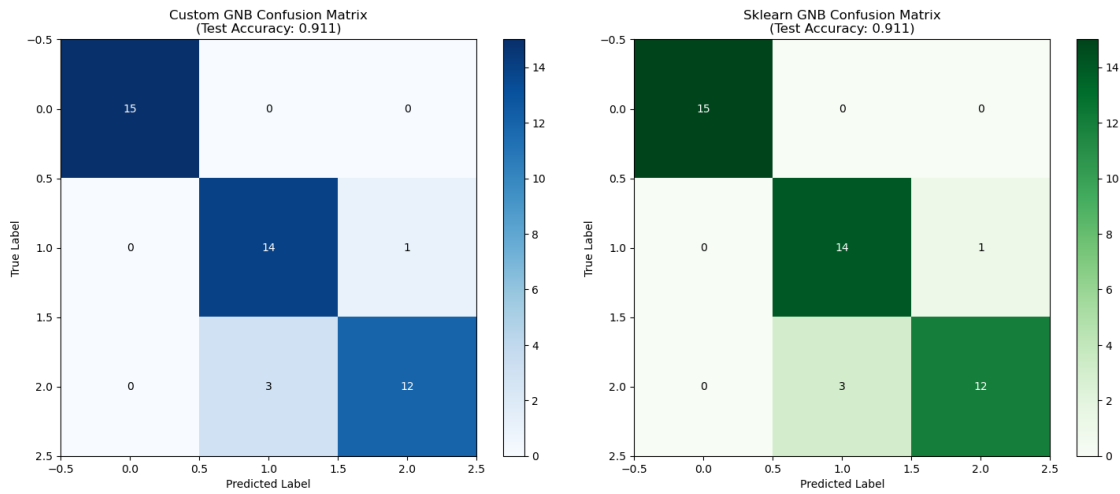
    ↳mean(sklearn_times):.2f}x")

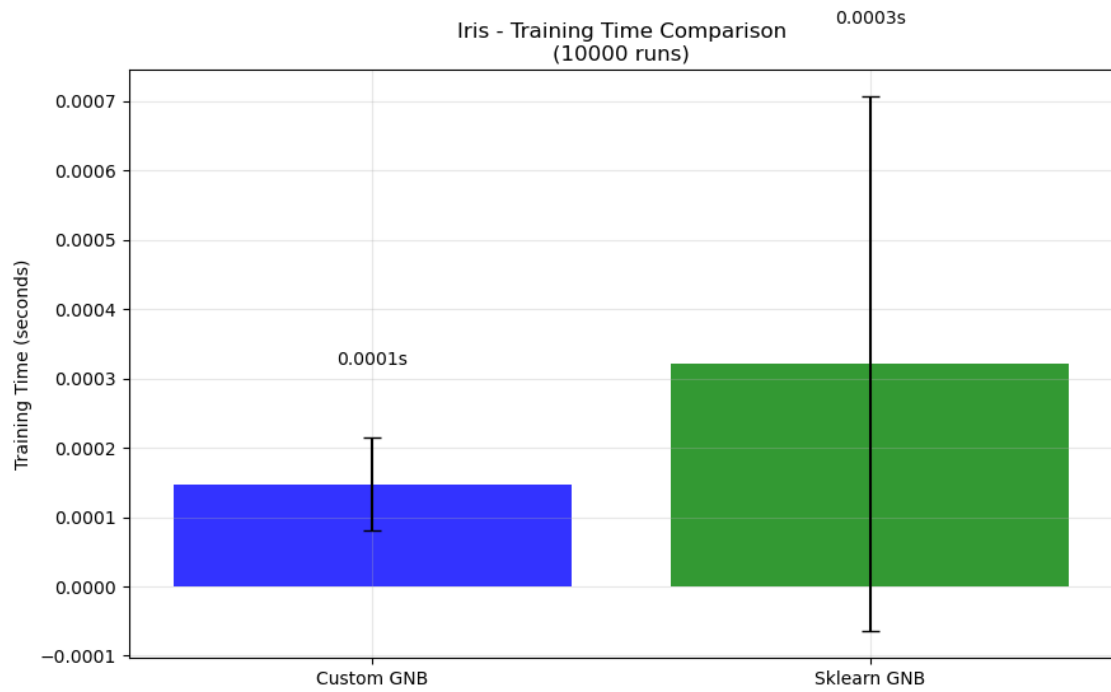
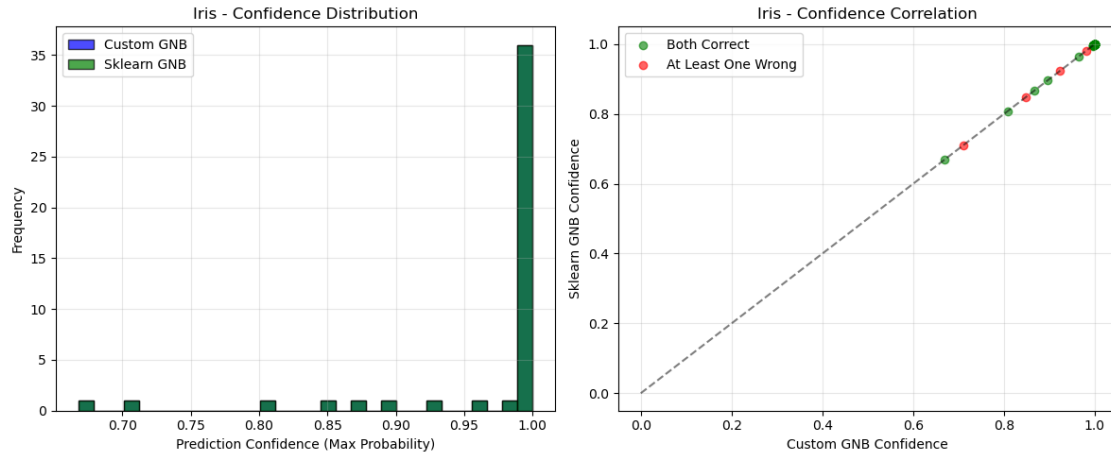
# comparison plots
if __name__ == "__main__":
    create_comprehensive_comparison_plots()
    print("\n completed")

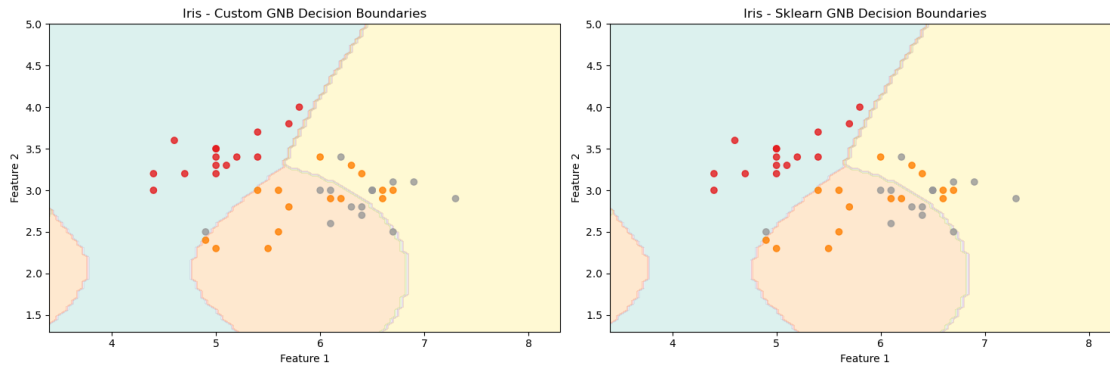
```

comparison analysis: IRIS dataset







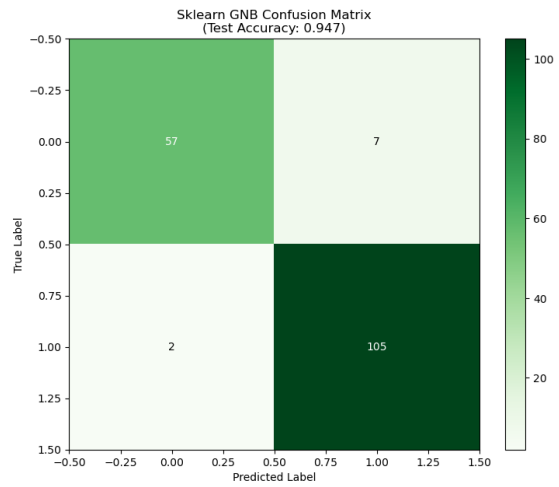
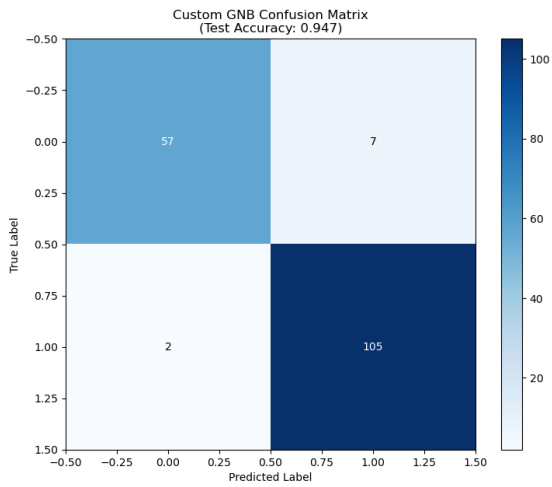
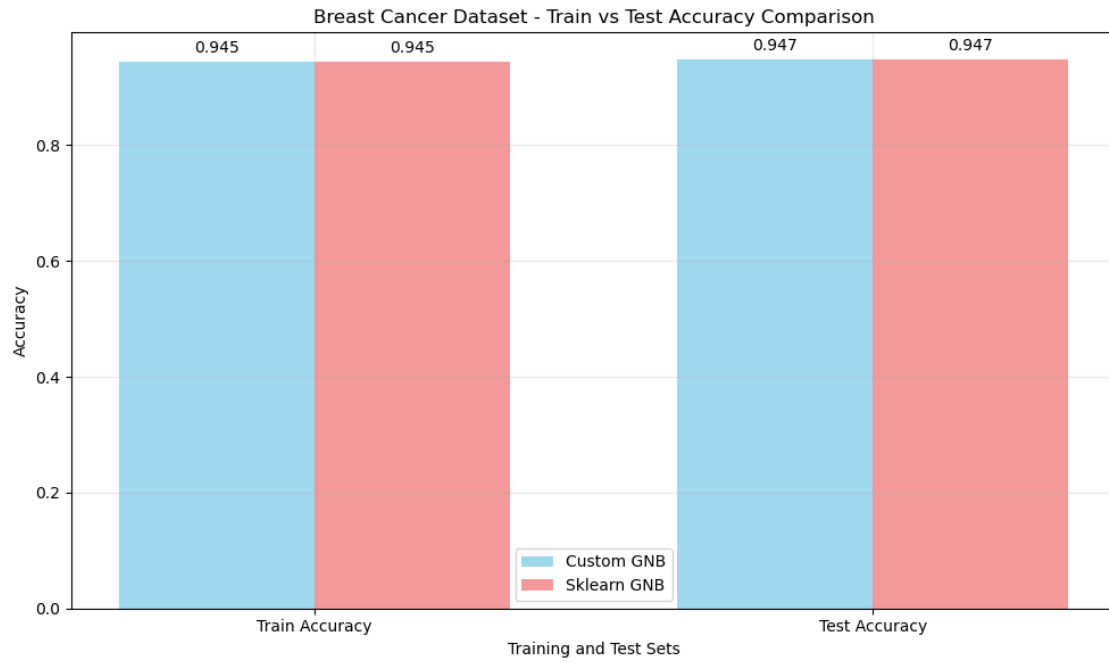


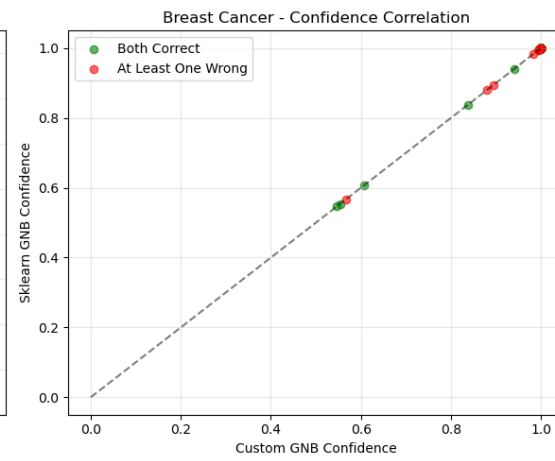
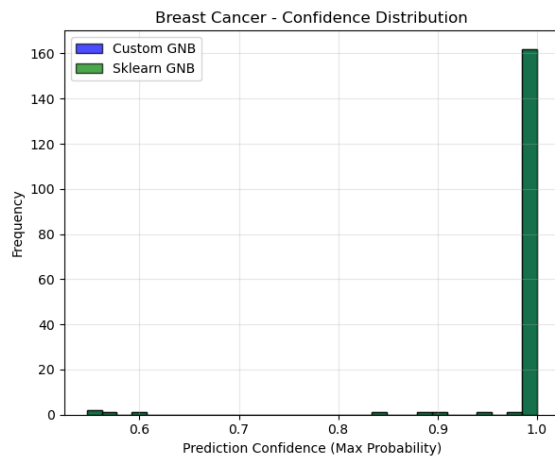
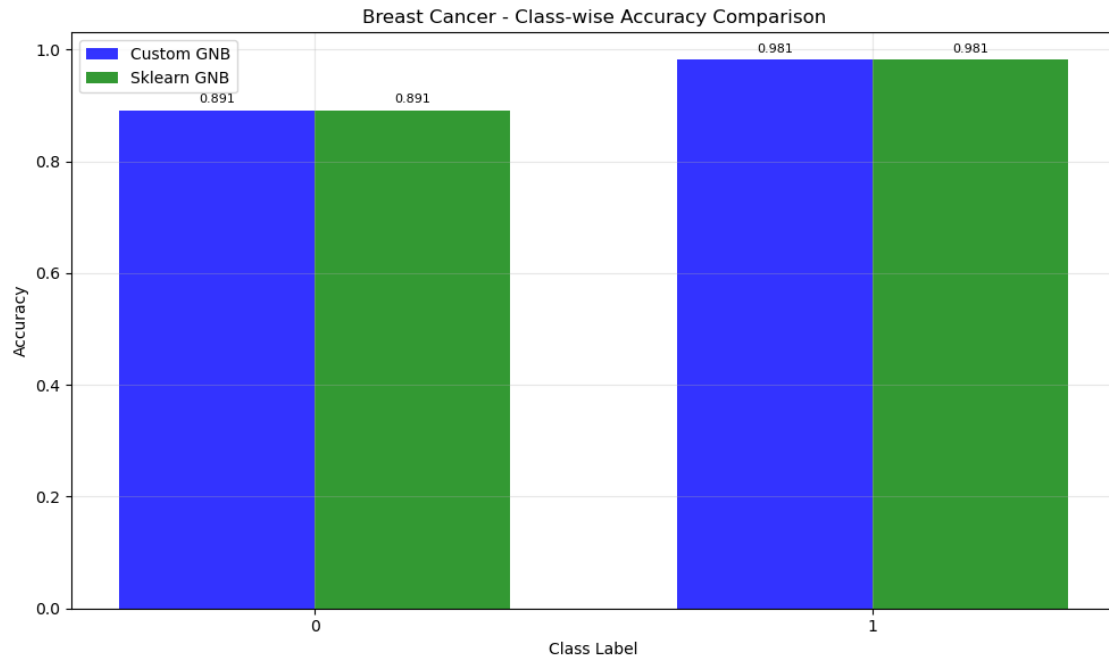
Statistical summary - Iris:
 Prediction Agreement: 1.0000
 Custom GNB - Train: 0.9810, Test: 0.9111
 Sklearn GNB - Train: 0.9810, Test: 0.9111
 Accuracy Difference: 0.000000

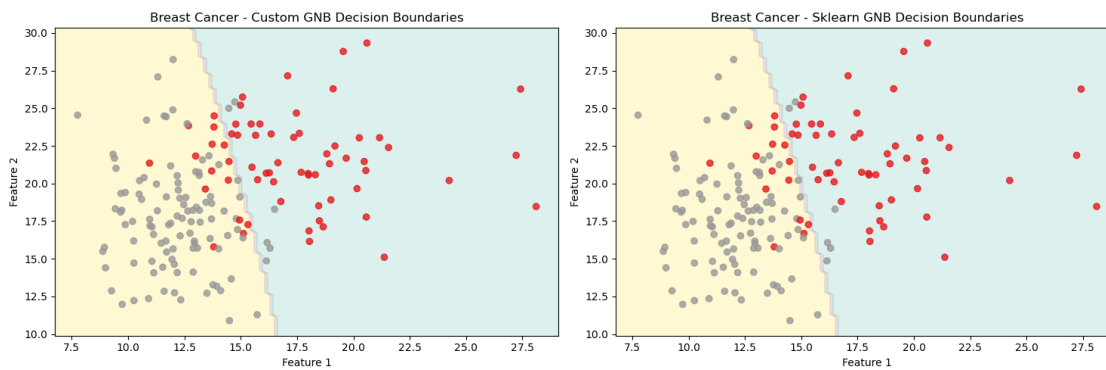
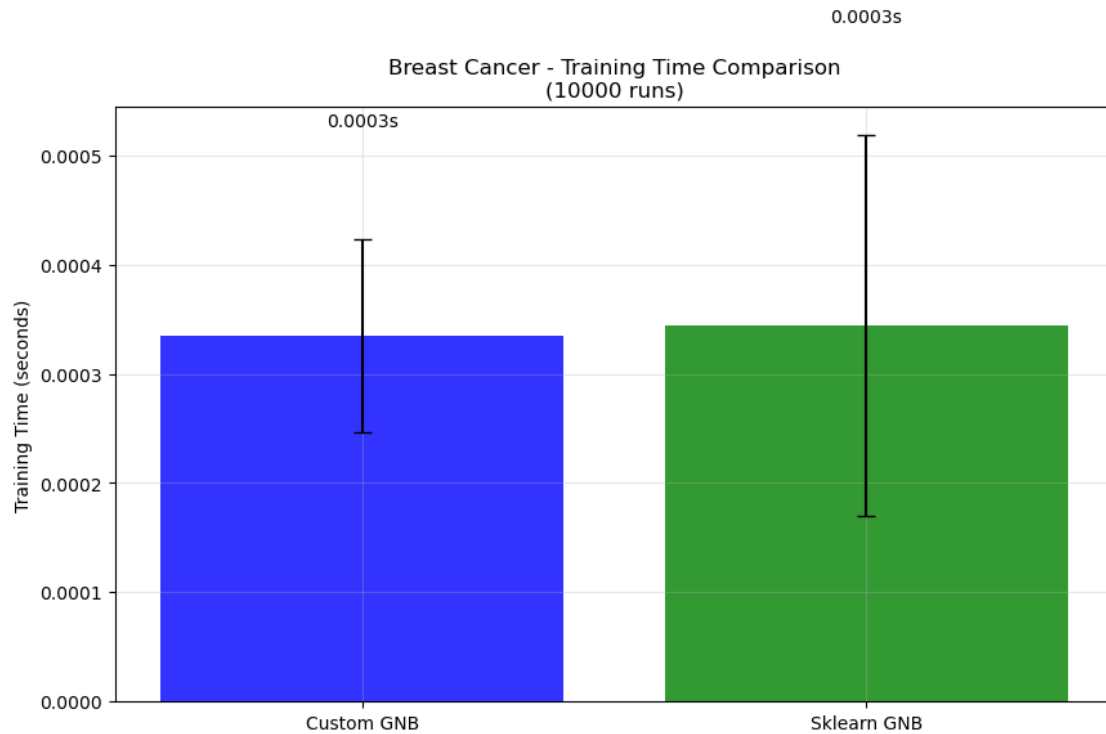
Confidence Statistics:
 Custom GNB Mean Confidence: 0.9698
 Sklearn GNB Mean Confidence: 0.9698
 Custom GNB Correct Prediction Mean Confidence: 0.9800
 Custom GNB Wrong Prediction Mean Confidence: 0.8656

Timing Statistics (10000 runs):
 Custom GNB Avg Training Time: 0.000148s \pm 0.000067s
 Sklearn GNB Avg Training Time: 0.000321s \pm 0.000386s
 Speed Ratio (Custom/Sklearn): 0.46x

comparison analysis: BREAST CANCER dataset







Statistical summary - Breast Cancer:

Prediction Agreement: 1.0000

Custom GNB - Train: 0.9447, Test: 0.9474

Sklearn GNB - Train: 0.9447, Test: 0.9474

Accuracy Difference: 0.000000

Confidence Statistics:

Custom GNB Mean Confidence: 0.9871

Sklearn GNB Mean Confidence: 0.9871

Custom GNB Correct Prediction Mean Confidence: 0.9906
Custom GNB Wrong Prediction Mean Confidence: 0.9240

Timing Statistics (10000 runs):
Custom GNB Avg Training Time: 0.000335s \pm 0.000088s
Sklearn GNB Avg Training Time: 0.000344s \pm 0.000174s
Speed Ratio (Custom/Sklearn): 0.97x

completed

The following code cell is used for testing the runtime for the predict methods between sklearn and our custom GNB. It is primarily for illustration purposes but does not form a core part of our analysis.

```
[5]: import time
import numpy as np
from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split
from sklearn.naive_bayes import GaussianNB
from sklearn.metrics import accuracy_score

# 1. Generate a large dataset (100,000 samples, 20 features)
print("Generating 100k samples...")
X, y = make_classification(n_samples=100000, n_features=20, n_classes=2,
    random_state=42)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
    random_state=42)

print(f"Train shape: {X_train.shape}")
print(f"Test shape: {X_test.shape}")

# 2. Benchmark YOUR Implementation
# (Make sure your class is already defined/imported as GaussianNaiveBayes)
print("\n--- Testing Custom Implementation ---")
custom_model = GaussianNaiveBayes(n_classes=2)

start = time.time()
custom_model.fit(X_train, y_train)
print(f"Custom Train Time: {time.time() - start:.4f}s")

start = time.time()
custom_preds = custom_model.predict(X_test)
print(f"Custom Predict Time: {time.time() - start:.4f}s")

# 3. Benchmark Sklearn Implementation
print("\n--- Testing Sklearn Implementation ---")
sklearn_model = GaussianNB()
```

```

start = time.time()
sklearn_model.fit(X_train, y_train)
print(f"Sklearn Train Time: {time.time() - start:.4f}s")

start = time.time()
sklearn_preds = sklearn_model.predict(X_test)
print(f"Sklearn Predict Time: {time.time() - start:.4f}s")

```

Generating 100k samples...

Train shape: (80000, 20)

Test shape: (20000, 20)

--- Testing Custom Implementation ---

Custom Train Time: 0.0555s

Custom Predict Time: 0.0057s

--- Testing Sklearn Implementation ---

Sklearn Train Time: 0.0161s

Sklearn Predict Time: 0.0038s

6 RESULTS

As demonstrated in the comparison plots above, the Custom GNB implementation achieves identical accuracy and decision boundaries to the Scikit-Learn implementation on both the Iris and Breast Cancer datasets, confirming the correctness of the MLE and smoothing logic.