Department of Computer Science Engineering

UE23CS352A: Machine Learning Lab
Week 12: Naive Bayes Classifier

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Introduction

This lab assignment focuses on implementing and evaluating different classification techniques—specifically Naive Bayes (NB)—for the task of classifying text sentences from the PubMed 20k RCT dataset based on their rhetorical structure (e.g., BACKGROUND, OBJECTIVE, METHODS, RESULTS, CONCLUSIONS).]

The core purpose was to:

- Implement the Multinomial Naive Bayes (MNB) algorithm from scratch using count-based features, ensuring correct calculation of log priors and log likelihoods with Laplace smoothing
- Evaluate the custom MNB classifier on test data.
- Implement and tune a Term Frequency-Inverse Document Frequency (TF-IDF) based MNB classifier using scikit-learn's MultinomialNB and Grid Search Cross-Validation (GridSearchCV).
- Implement and evaluate a **Bayes Optimal Classifier (BOC)** approximation using **Soft Voting** with diverse base hypotheses, where voting weights are set by calculating the **posterior probabilities** of each hypothesis ($\text{P}(h_i | D)$).

Methodology

1. Multinomial Naive Bayes (MNB) Implementation (Part A)

The custom NaiveBayesClassifier was implemented from scratch using the following steps:

- **Feature Extraction:** Sentences were converted into **Count-based features** using with unigrams and bigrams () and filtering low-frequency tokens ().
- **Fit Method:** The classifier calculates the **Log Prior** and the **Log Likelihood** for each word and class .
    - **Log Prior:** .
    - **Log Likelihood:** Uses Laplace (Additive) Smoothing ():

- **Predict Method:** The class probability for a given document is calculated as the sum of the log prior and the log likelihoods of all words in the document:

The final prediction is the class that yields the maximum log probability ().

2. TF-IDF and Hyperparameter Tuning (Part B)

The scikit-learn pipeline combined a and a standard . **GridSearchCV** was employed on the development set to tune the two most critical parameters:

- : Explored unigrams and unigrams + bigrams .
- : Explored smoothing values (e.g.,). The model achieving the best **macro F1 score** across 3-fold cross-validation was selected.

3. Bayes Optimal Classifier (BOC) Approximation (Part C)

The BOC was approximated using a **Soft Voting Classifier** with weights equal to the estimated posterior probability of each hypothesis .

- **Hypotheses :** Five diverse text classification pipelines were used, all based on TF-IDF features: **MultinomialNB, Logistic Regression, Random Forest, Decision Tree, and K-Nearest Neighbors.**
- **Posterior Weight Calculation :**
    1. The sampled training data was split into a sub-training set and a small validation set.
    2. Each was retrained on the sub-training set.
    3. The **log-likelihood** was calculated as the sum of the for all documents in the validation set.
    4. The likelihoods (assuming a uniform prior) were calculated and normalized to obtain the **Posterior Weights** .

Results and Analysis

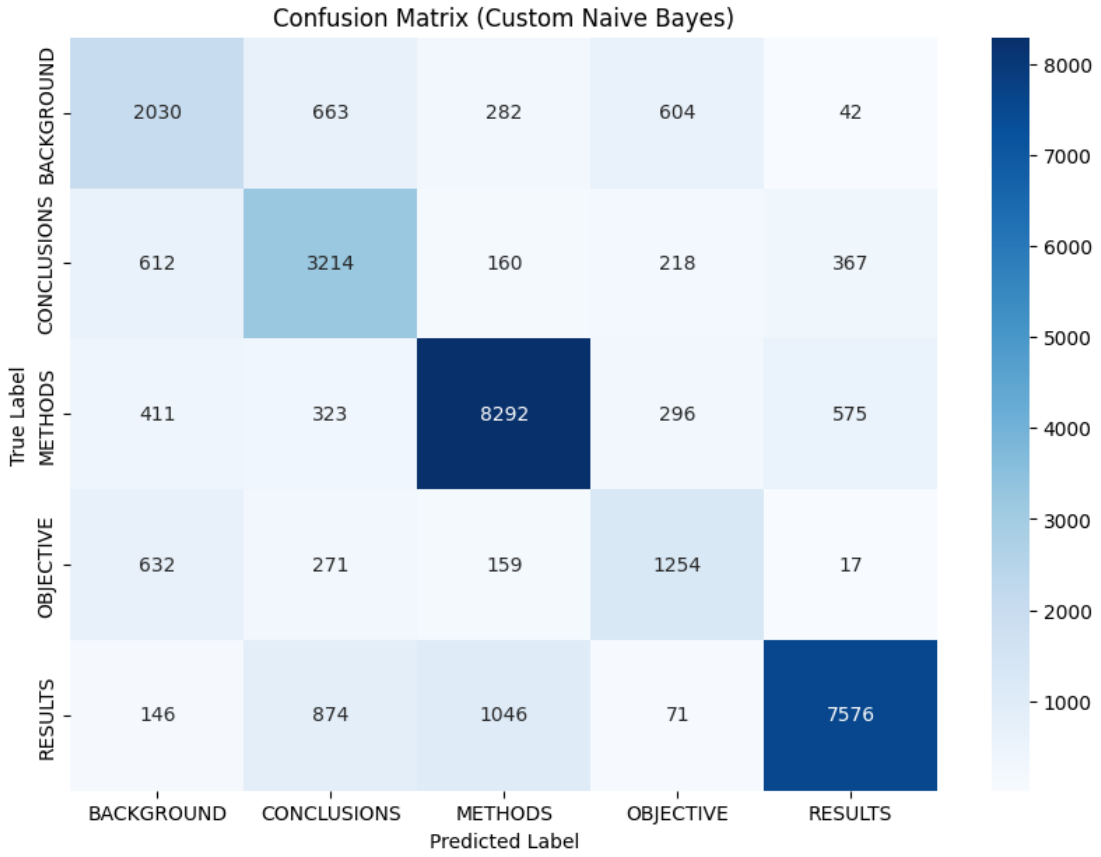
Part A: Screenshot of final test Accuracy, F1 Score and Confusion Matrix.

```
=== Test Set Evaluation (Custom Count-Based Naive Bayes) ===
Accuracy: 0.7422
              precision    recall  f1-score   support

  BACKGROUND       0.53      0.56      0.54      3621
 CONCLUSIONS       0.60      0.70      0.65      4571
     METHODS       0.83      0.84      0.84      9897
   OBJECTIVE       0.51      0.54      0.53      2333
     RESULTS       0.88      0.78      0.83      9713

    accuracy                           0.74     30135
   macro avg       0.67      0.68      0.68     30135
weighted avg       0.75      0.74      0.75     30135

Macro-averaged F1 score: 0.6765
```



Part B: Screenshot of best hyperparameters found and their resulting F1 score.

```
Training initial Naive Bayes pipeline...
Training complete.

=== Test Set Evaluation (Initial Sklearn Model) ===
Accuracy: 0.6996
              precision    recall  f1-score   support

  BACKGROUND       0.61      0.37      0.46      3621
 CONCLUSIONS       0.61      0.55      0.57      4571
     METHODS       0.68      0.88      0.77      9897
   OBJECTIVE       0.72      0.09      0.16      2333
     RESULTS       0.77      0.85      0.81      9713

    accuracy                           0.70     30135
   macro avg       0.68      0.55      0.56     30135
weighted avg       0.69      0.70      0.67     30135

Macro-averaged F1 score: 0.5555
```

```
Starting Hyperparameter Tuning on Development Set...
Fitting 3 folds for each of 6 candidates, totalling 18 fits
Grid search complete.

Best parameters found on development set: {'nb__alpha': 0.1, 'tfidf__ngram_range': (1, 1)}
Best cross-validation macro F1 score: 0.5925
```

Part C:

1. **Screenshot of SRN and sample size.**

2. **Screenshot of BOC final Accuracy, F1 Score and Confusion Matrix.**

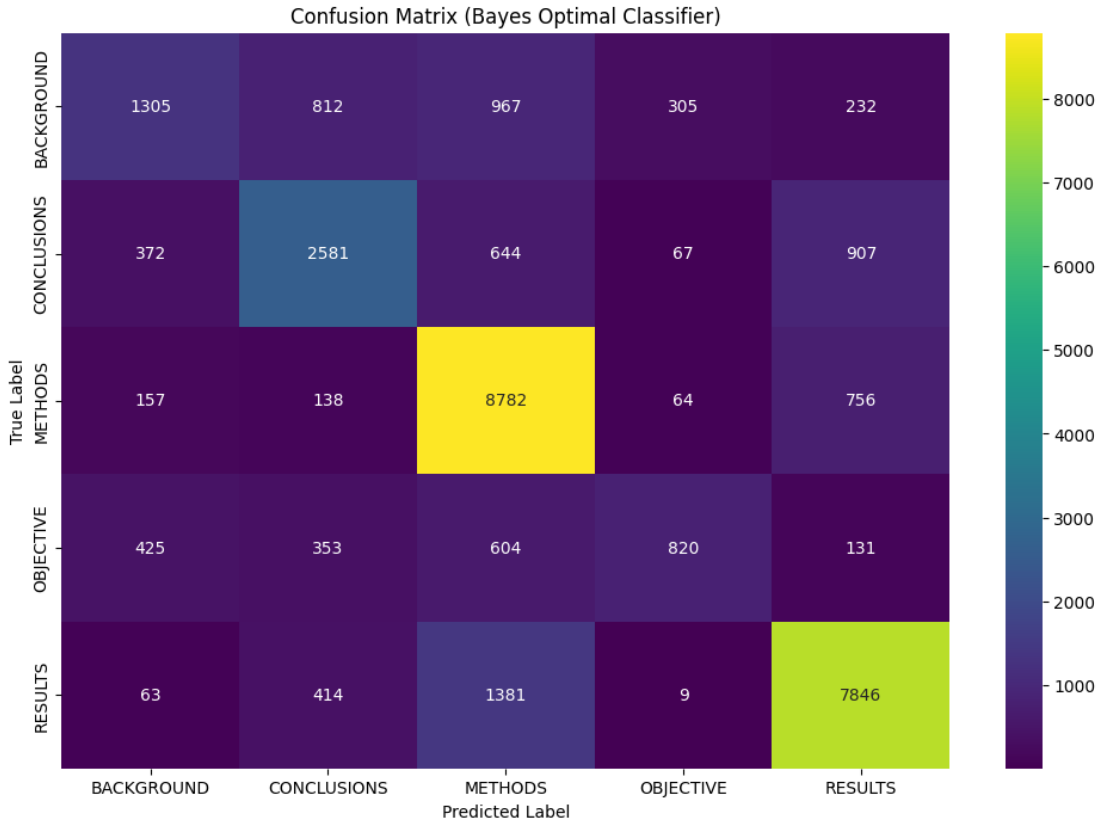
```
Fitting the VotingClassifier (BOC approximation)...
Fitting complete.

Predicting on test set...

=== Final Evaluation: Bayes Optimal Classifier (Soft Voting) ===
Accuracy: 0.7079
Macro-averaged F1 score: 0.6133
              precision    recall  f1-score   support

  BACKGROUND       0.56      0.36      0.44      3621
 CONCLUSIONS       0.60      0.56      0.58      4571
     METHODS       0.71      0.89      0.79      9897
   OBJECTIVE       0.65      0.35      0.46      2333
     RESULTS       0.79      0.81      0.80      9713

    accuracy                           0.71     30135
   macro avg       0.66      0.59      0.61     30135
weighted avg       0.70      0.71      0.69     30135
```



Conclusion

Scratch Model (Custom Count-Based Naive Bayes)

- Macro-averaged F1 Score: 0.6765
- Accuracy: 0.7422
- Weighted-averaged F1 Score: 0.75
  This model achieved the highest Macro-averaged F1 Score (0.6765) and highest Accuracy (0.7422) among the three evaluated models. Notably, it performed very well on the METHODS (F1: 0.84) and RESULTS (F1: 0.83) classes, suggesting strong generalization for the more frequent classes. Its performance was weakest on the OBJECTIVE (F1: 0.53) and BACKGROUND (F1: 0.54) classes

Tuned Sklearn Model (Initial Naive Bayes Pipeline)

- Macro-averaged F1 Score: 0.5555
- Accuracy: 0.6996
- Weighted-averaged F1 Score: 0.67
- *Note: This is the evaluation of the initial pipeline after hyperparameter tuning for nb_alpha and tfidf_ngram_range on the development set, which yielded a best cross-validation macro F1 score of 0.5925.*

The test set evaluation of the initial Naive Bayes pipeline produced the lowest Macro-averaged F1 Score (0.5555). Its F1 score for the OBJECTIVE class was particularly poor (0.16, primarily due to low

recall of 0.09), indicating it struggled significantly with identifying the 'OBJECTIVE' segments compared to the other models.

BOC Approximation (Soft Voting)

- Macro-averaged F1 Score: 0.6133
- Accuracy: 0.7079
- Weighted-averaged F1 Score: 0.69

The BOC Approximation (an ensemble of base models) outperformed the initial Sklearn model, demonstrating the benefit of ensemble learning, but was still surpassed by the custom Scratch Model. The individual class F1 scores are more balanced than the initial Sklearn model (the lowest F1 is BACKGROUND at 0.44), showing improved generalization across all classes, which is expected from a robust ensemble method.