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# Using K-Fold Cross Validation on Decision Tree and Logistic Regression Models to Classify Iris Species

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Abstract— Determining if a logistic regression model or a decision tree model is more effective in classifying Iris species is an example of a case where performing k-fold cross validation may be appropriate. After evaluating each model individually as a classifer for the iris dataset, the performance of each models was then examined via cross validation. It was found that the logistic regression model consistently performed with a higher accuracy score. The effects varying k values also had effects on the projected accuracy of the two models. Being able to validate developing models is very important for model implementation and application. Examining the behavior of the cross validation method will aid future model development and applications.

## I. INTRODUCTION

Being able to evaluate the effectiveness of a prediction model is just as important as the development. One method that is conventionally used to determine the skill of a model is cross validation. This method involves breaking the dataset up evenly into a number of random sample groups, or folds, and systematically training a model of all groups but one of the groups and testing the model of the remaining group until all groups have been used as a separate testing set. The accuracy scores for each model are then used to evaluate the effectiveness of the model for that dataset. Cross validation is commonly used to determine the optimal model for a dataset because it is fairly easy to implement and understand [1].

Cross validation is a method that can be used to determine which classification model is a better predictor of the Iris dataset: the decision tree classification model or the logistic regression classification model. These models were evaluated separately in previous investigations where modifications of these methods were examined to optimize accuracy. The model with parameters that yielded the greatest accuracy for this dataset was selected for this investigation. Specifically, the decision tree model using entropy as a purity measure will be compared to a logistic regression model without any penalties [2], [3]. As in previous reports, these models will be predicting the class of each iris flower based on the following features: sepal length, sepal width, petal length, and petal width.

The Python sklearn library is used to perform cross validation in section II to conclude the optimal model between decision tree and logistic regression for the Iris dataset. The results are outlined in section III. The importance of this investigation is in section IV.

## II. METHODOLOGY

This investigation entails using SKLearns's cross\_validate function from the model\_selection  $\rightarrow$  module to compare the accuracy between a decision tree model and logistic regression model. Several Python packages were utilized including sklearn, pandas, and numpy. Specifically from sklearn, we use the following modules: linear\_model, preprocessing, model\_selection  $\rightarrow$ , metrics, and tree.

First, the Iris dataset was loaded as an sklearn.utils  $\rightarrow$  .Bunch object called iris\_data via the load\_iris  $\rightarrow$  () function. This object is similar to a Python dictionary. To make the data easier to read, it was transformed into the df\_iris dataframe, where the data parameter was set as the data attribute of the dataset and the columns parameter as the feature\_names attribute. A new column called "class" was added to this dataframe which contains the target variable of the Iris dataset; this is the class of the Iris plant - setosa, versicolor, or virginica. Since the target attribute contains an array with values from 0-2, the .replace function was used to map these numerical values to their corresponding classifications: setosa for 0, versicolor for 1, and virginica for 2.

After loading in and setting up the Iris dataset, cross validation was performed on both a decision tree and logistic regression model, which were built using the same sklearn functions as in our previous studies [2], [3]. The criterion parameter of the decision tree model was set to entropy and the penalty parameter in the logistic regression model was set to None.

The type of cross validation used is called k-fold cross validation. This kind of cross validation involves splitting the data into k groups or folds, using k-1 folds as training data, and using the remaining fold as test data. Some sort of measurement or calculation is done (in this case we chose to use accuracy) to validate the model. These steps are repeated until every fold has become test data and the mean accuracy value is computed. Figure 1 visualizes this concept with k=5 folds.



Fig. 1. Example of k-fold Cross Validation with k=5 folds [4]

In the cross validation process for both the decision tree and logistic regression models, the cv parameter was set to None meaning it uses the default of k=5 folds, and the scoring parameter was set to accuracy since that was the strategy chosen to determine the effectiveness of the models. The mean and standard deviation of the cross validation of both models was determined.

To validate the <code>cross\_validate</code> function from sklearn, we also created our own cross validation function called <code>perform\_manual\_cross\_validation</code> that goes through the same algorithm of splitting the Iris data into folds, using one fold as the test data, and iterating through until all the folds have been used as test data. We ran this function on the same decision tree and linear regression models; the accuracy each iteration was printed and the mean and standard deviation of those accuracies were compared to when the <code>cross\_validate</code> function was used.

Returning to using the cross\_validate function we changed the cv parameter, setting it to the values of 3, 7, and 10 to see how the accuracy of the cross validated decision tree and linear regression models would change. We were especially interested in seeing how setting k=10 would affect accuracy because k=5 and k=10 are the more common fold values.

# III. RESULTS

The mean and standard deviation accuracy values from performing 5-fold cross validation on our logistic regression and decision tree models are shown in Table I.

| Measure            | Logistic Regression | Decision Tree |
|--------------------|---------------------|---------------|
| Mean               | 0.973333            | 0.960000      |
| Standard Deviation | 0.036515            | 0.036515      |
|                    | TABLE I             |               |

5-FOLD CROSS VALIDATION STATISTICS FOR LOGISTIC REGRESSION AND DECISION TREE MODELS

It can be seen that the logistic regression model is slightly more accurate than the decision tree model, at 0.973 compared to 0.960. This lines up with our previous study; when the results of that linear regression model were briefly compared to that of the decision tree model, the logistic regression model was more accurate. Here, we used a more robust method of evaluating effectiveness of the models and found the same conclusion to be true.

The results of our own k-fold cross validation function perform\_manual\_cross\_validation produced similar results, seen in Table II.

| Measure            | Logistic Regression | Decision Tree |
|--------------------|---------------------|---------------|
| Mean               | 0.953333            | 0.933333      |
| Standard Deviation | 0.038006            | 0.0.062361    |
|                    | TARLE II            |               |

5-FOLD MANUAL CROSS VALIDATION STATISTICS FOR LOGISTIC REGRESSION AND DECISION TREE MODELS

Although the values are not exactly the same as when the <code>cross\_validate</code> function was used, it still confirms that the logistic regression model is slightly more accurate than the decision tree model. The higher standard deviation values may be attributed to the way the data is being split into the folds; it is just splitting the Iris dataset into fifths without implementing a random order.

The results of performing k-fold cross validation using sklearn and changing the number of folds are shown below. The additional k values of 3, 7, 10, 15, and 50 are used.

| k         | Measure       | Logistic Regression | Decision Tree |  |  |
|-----------|---------------|---------------------|---------------|--|--|
| 3         | Mean          | 0.973333            | 0.96          |  |  |
|           | Standard Dev. | 0.023094            | 0.02          |  |  |
| 5         | Mean          | 0.973333            | 0.96          |  |  |
|           | Standard Dev. | 0.036515            | 0.036515      |  |  |
| 7         | Mean          | 0.959802            | 0.939703      |  |  |
|           | Standard Dev. | 0.074425            | 0.065443      |  |  |
| 10        | Mean          | 0.98                | 0.953333      |  |  |
|           | Standard Dev. | 0.044997            | 0.044997      |  |  |
| 15        | Mean          | 0.980000            | 0.960000      |  |  |
|           | Standard Dev. | 0.041404            | 0.063246      |  |  |
| 50        | Mean          | 0.980000            | 0.946667      |  |  |
|           | Standard Dev. | 0.104545            | 0.123443      |  |  |
| TABLE III |               |                     |               |  |  |

CROSS VALIDATION STATISTICS FOR LOGISTIC REGRESSION AND DECISION TREE MODELS (K=3, 5, 7, 10, 15, 50)

For all k-values, the logistic tree models consistently has greater accuracy than the decision tree model. Between k=3 and k=5, the accuracy of both the models did not change. When k=7, the accuracy of both models decreased. This could be because the folds do not have the same amount of data, as 150 data points do not divide evenly between 7 groups, also causing more variance within the accuracy of the folds. When k=50, the accuracy for the decision tree decreases which indicates underfitting of the data, the number of data points in each fold must be too low to effectively train a decision tree model. The standard deviation also greatly increased for both models when k=50. When k=10 and 15, the accuracy of both models increases slightly compared to k=3 and k=5. Compared to k=50, the models (evaluated where k=10, 15) have much lower standard deviations. The methods with k=10 and 15 have the highest accuracies and relatively low standard deviations which indicates that 10-15 folds is the optimal number of folds to validate this dataset.

Evaluating the method at k=10 through 15, we concluded that k=14 would be the optimal k value for this validation procedure as it produced high accuracy and low variance indicating it was unbiased and balanced.

 Measure Mean
 Logistic Regression
 Decision Tree

 Standard Dev.
 0.980519
 0.953896

 Standard Dev.
 0.038710
 0.047901

 TABLE IV
 K=14 CROSS VALIDATION STATISTICS

## IV. DISCUSSION

Through this investigation, we were able to confirm that the logistic regression model was more effective as a predictive model for the Iris dataset as compared with a decision tree model. Here, we used a more robust method of evaluating effectiveness of the models and found the same results. K-fold cross validation allows for a relatively quick confirmation of which model in question is more accurate as compared to other models.

K=10 is commonly used and may be found to work better for other datasets. The accuracy of both testing and training data could be observed to determine if overfitting or underfitting is occurring. In general, lower k values can lead to overfitting and high variance whereas higher k values can lead to underfitting and higher bias [5]. This is why evaluating multiple k values is so important. For this study, we were able to determine a balance.

In the future, the Iris dataset could be split into test and train partitions, more similar to what was done in previous studies. Then, k-fold cross validation would only be performed on the training data and the results of that would finally be applied to the testing data. Additionally, rather than using k folds where each group consists of randomly selected samples, expanding this investigation to encompass stratified sampling and portioning could be beneficial and decrease standard deviation of the accuracy scores.

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