Project 3: Decision Trees for Classification and Regression

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1. Introduction

Decision trees are tree structures than can be built by machine learning algorithms by training on a data set. A decision tree is a hierarchical structure, consisting of nodes, which can have left or right nodes (children). The root node is the start of the tree and has left and right nodes that would go on to build sub-trees. A node that does not have a left or right child is considered a leaf. Decision trees are built or grown from the training data by deciding which features to build sub-trees on and knowing when to split the data to produce the next node, along with knowing when a leaf node has been encountered. Decision trees can be used in both classification and regression machine learning problems. Decision trees ask "questions" at each node and determine, based on feature observations from the data set, if the left or right node should be taken when traversing the tree. When the leaf node is encountered that will end with the answer for the classification or regression problem.

The problem statement presented in this paper is to understand and implement two major categories of decision tree algorithms. For classification problems the approach explored will be the Iterative Dichotomiser 3 (ID3) algorithm. For regression problems the approach explored will be the Classification and Regression Tree (CART) algorithm. Both ID3 and CART will first be built as standard uni-variate trees, meaning that they will be grown to completion with out intervention. The results of these trees will then be compared with trees that have been edited, for regression problems this will include the process of early stopping, for classification problems this will include the process of reduced error pruning. The uni-variate, early stopping and error pruning trees will be then compared in terms of Classification Error and Mean Square Error for classification and regression problems respectively. *k*-fold cross validation will be the experimental method used in this report.

The hypothesis of this report is that for the both the classification and regression tasks the trees that are error pruned or early stopped will perform better than trees that are grown uni-variate to completion. The hypothesis assumes that trees grown to full completion will exhibit over fitting to the data. Over-fitting is where in a learning system the model has been so tightly fit to the training data, that results on new un-trained data are highly inaccurate. The hypothesis assumes that in allowing the trees to grow to full completion of nodes that additional patterns may be learned in the training data that might not apply to new data feed into the algorithm. The results from experiments ran on the provided data sets will be discussed and presented against the outlined hypothesis.

Section 1 has provided the introduction, problem statement and hypothesis in regards to two major decision tree algorithms that will be explored.. Section 2 will provide an in-depth explanation of the ID3 and CART algorithms, how these algorithms will be modified during the early stopping and error pruning processes and discuss each of the 6 data sets used. Section 3 will present the results obtained by variations of ID3 and CART as uni-variate, early stopping and error pruning implementations on the provided data sets. Section 4 will discuss the results that were obtained and compare them to the hypothesis that was outlined in the introduction. This report will conclude in Section 5 with a discussion of lessons learned and areas of possible future work.

2. Algorithms and Experimental Methods

The ID3 algorithm will be used on classification data sets. The ID3 algorithm is a classification algorithm that follows a greedy heurisitic top down approach by selecting the attribute/feature that provides the maximum information gain at each partition of the data set. The key parameters to understand in the ID3 algorithm are Entropy(I), Expected Entropy, Information Gain and Gain Ratio.

Entropy is a measure of uncertainty there is in a data set. An Entropy of 0 means that the data set is pure, meaning it comprised of only one class. An Entropy of 1 or more indicates that there is lots of uncertainty in the data set meaning there is a high level of mixture of multiple different classes contained in the data set.
Expected Entropy is the Entropy only in feature/attribute f_i in the data set.
Information Gain is the Entropy minus the Expected Entropy. The Information Gain provides a metric of how much uncertainty there would be in the data if we removed feature f_i from the equation. What I mean by removing f_i from the equation is that, from this point on in calculating or making decisions about the data in the data set, we would hold feature f_i fixed. As in we would only look from this point on at observations that had a certain value of f_i when making future calculations about Entropy and Expected Entropy. From a building a tree perspective this is logical as we only want to continue down branches that will tell us the most about the data, so the goal is to maximize the entropy that we would have at the next node of the decision tree.

The issue presented by building a decision tree based on information gain alone, is that is we are always looking for the highest gain when making splits in the data set to build new partitions, this can lead to numerous expensive partitions that would force the algorithm to run longer potentially with no real benefit. Instead of splitting on Information Gain alone, the concept of Gain Ratio is introduced. The gain ratio provides a balance of the highest gain while also adding a penalization factor for the splits that would result in a higher number of partitions being built.

Consider a 2 class classification problem we can define the following equations for Entropy, Expected Entropy, Information Gain and Gain Ratio.

Entropy

$$I(p,n) = -\frac{p}{(p+n)} * log(\frac{p}{p+n}) - \frac{n}{p+n} * log(\frac{n}{p+n}) \tag{1}$$

$I=$ Entropy of Partition

$\pi=$ Current Partition in the Overall Data Set

$p_\pi=$ Number of Class 1 Observations in the Current Partition

$n_\pi=$ Number of Class 2 Observations in the Current Partition

Expected Entropy

$$E_\pi(f_i) = \sum_{j=1}^{m_i}(\frac{p_\pi^j + n_\pi^j}{p_\pi + n_\pi} * I(p_\pi^j, n_\pi^j)) \tag{2}$$

$E_\pi=$ Expected Entropy of Partition

$f_i=$ Feature i of the Data Set

$m_i=$ Size of the Domain of Feature i

$\pi=$ Current Partition in the Overall Data Set

$I=$ Entropy of Partition

$p_\pi^j=$ Number of Class 1 Observations in the Current Partition for the jth item in the Domain of Feature f_i

$n_\pi^j=$ Number of Class 2 Observations in the Current Partition for the jth item in the Domain of Feature f_i

Gain

$$G_\pi(f_i) = I(p_\pi, n_\pi) - E_\pi(f_i) \tag{3}$$

$G_\pi=$ Gain of Partition

$E_\pi=$ Expected Entropy of Partition

$I=$ Entropy of Partition

$p_\pi=$ Number of Class 1 Observations in the Partition

$n_\pi=$ Number of Class 2 Observations in the Partition

Information Value

$$IV_\pi(f_i) = -\sum_{j=1}^{m_i}(\frac{p_\pi^j + n_\pi^j}{p_\pi + n_\pi} * log\frac{p_\pi^j + n_\pi^j}{p_\pi + n_\pi}) \tag{4}$$

$IV_\pi =$ Information Value of Partition

$m_i =$ Size of the Domain of Feature i

$p_\pi =$ Number of Class 1 Observations in the Partition

$n_\pi =$ Number of Class 2 Observations in the Partition

Gain Ratio

$$GR_\pi(f_i) = \frac{G_\pi(f_i)}{IV_\pi(f_i)} \tag{5}$$

$GR_\pi =$ Gain Ratio of Partition

$G_\pi =$ Gain of Partition

$IV_\pi =$ Information Value of Partition

These equations can be expanded to a **k** Class Classification problems as follows: INSERT HERA

These equations will be used in the overall process of building the decision tree in the ID3 algorithm. The following steps outline the algorithm. The algorithm uses recursion to build the tree to completion.

```
Generate Tree
Calculate Entropy on Partition($\pi$)
If Entropy == 0
  Create a leaf with the label of the majority class.
  Return
Split
```

The CART algorithm will be used on regression data sets.

Data Sets

The following data sets were used during the classification and regression tasks for this project.

Breast Cancer

Description:
Task: Classification
Predictor: Diagnosis (Malignant or Benign)
Link:
`https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+%28Original%29`

Car Evaluation

Description:
Task: Classification
Predictor: Car Evaluation (Unacceptable, Acceptable, Good, Very Good)
Link:
`https://archive.ics.uci.edu/ml/datasets/Car+Evaluation`

Congressional Vote

Description: 1984 United Stated Congressional Voting Records
Task: Classification
Predictor: Party (Republican / Democrat)
Link:
`https://archive.ics.uci.edu/ml/datasets/Congressional+Voting+Records`

Albalone

Description: Physical measurements of Albalone
Task: Regression
Predictor: Rings (int)
Link:
`https://archive.ics.uci.edu/ml/datasets/Abalone`

Computer Hardware

Description: Relative CPU performance data.
Task: Regression
Predictor: PRP
Link:
`https://archive.ics.uci.edu/ml/datasets/Computer+Hardware`

Forest Fires

Description: Forest Fire burn area data
Task: Regression
Predictor: Area (float)
Link:
`https://archive.ics.uci.edu/ml/datasets/Forest+Fires`

3. Results

Tables 1-3 display the results from Classification Tasks: the Breast Cancer, Car Evaluation and Congressional Vote data sets while running a full uni-variate tree and reduced error pruning. The number of nodes to prune was determined using the tuning process that was discussed earlier. These tables show the results from the train set and the test set during each fold of the k-fold validation process. The results of each iteration of the tuning process were omitted from this report for brevity. The error used is Classification error and can be described as the Number of Times the Prediction was Wrong / Total Number of Comparisons. This error was averaged across the 5 folds to provide the Average Classification Error against each data set.

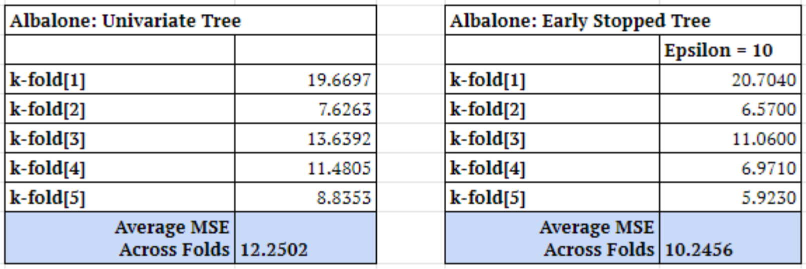
Tables 4-6 display the results from the Regression Tasks: the Albalone, Computer Hardware and Forest Fire data setswhile running a full uni-variate tree and early stopping. The value ϵ used in the early stopping was determined using the tuning process for regression that was discussed earlier. These tables show the result from the train set and the test set during each fold of the k-fold validation process.The results of the tuning process were omitted from this report for brevity.The error used is Mean Square Error. INSERT DECRIPTION OF MSE!!!!!!!

Table 1: Car Evaluation: ID3 - Experimental Results

Table 2: Breast Cancer: ID3 - Experimental Results

Table 3: Congressional Vote: ID3 - Experimental Results

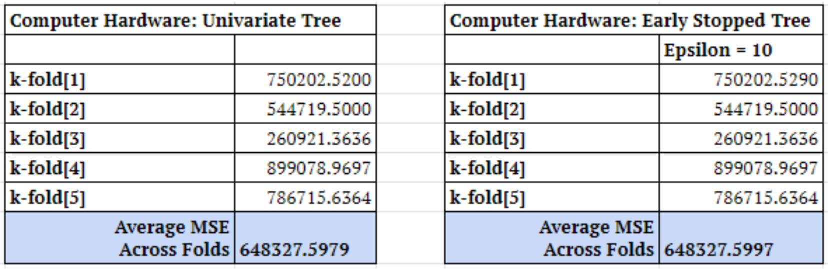
Table 4: Albalone: CART - Experimental Results



Albalone: Univariate Tree	
k-fold[1]	19.6697
k-fold[2]	7.6263
k-fold[3]	13.6392
k-fold[4]	11.4805
k-fold[5]	8.8353
Average MSE Across Folds	12.2502

Albalone: Early Stopped Tree	
	Epsilon = 10
k-fold[1]	20.7040
k-fold[2]	6.5700
k-fold[3]	11.0600
k-fold[4]	6.9710
k-fold[5]	5.9230
Average MSE Across Folds	10.2456

Table 5: Computer Hardware: CART - Experimental Results



Computer Hardware: Univariate Tree	
k-fold[1]	750202.5200
k-fold[2]	544719.5000
k-fold[3]	260921.3636
k-fold[4]	899078.9697
k-fold[5]	786715.6364
Average MSE Across Folds	648327.5979

Computer Hardware: Early Stopped Tree	
	Epsilon = 10
k-fold[1]	750202.5290
k-fold[2]	544719.5000
k-fold[3]	260921.3636
k-fold[4]	899078.9697
k-fold[5]	786715.6364
Average MSE Across Folds	648327.5997

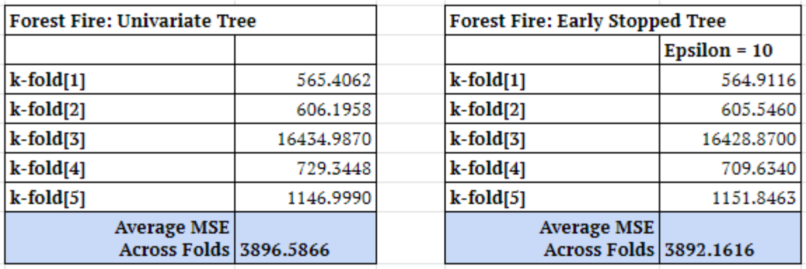
4. Discussion

The hypothesis that was presented at the start of this report for the both the classification and regression tasks the trees that are error pruned or early stopped will perform better than trees that are grown uni-variate to completion.

Looking at the classification data sets

Looking at the Regression data sets, the values of ϵ that were evaluated were 0, 0.01, 0.1, 1, 10. During the tuning process it was determined that 10 was the optimal value to use for ϵ and it was observed that there was not large difference between the results obtained for ϵ values such as 0, 0.01, 0.1, 1. One reason for this might that due to range of possible values for the prediction value in the regression data sets, a large ϵ makes a larger impact as it allows for the account of outliers in the data. The Albalone data set was the only one that had measurable improvement, with an Average MSE dropping from 12.5 to 10.2 between the uni-variate tree and the early stopped tree. The Forest Fire and Computer Hardware data sets, did not see measurable improvements between the uni-variate tree and the early stopped tree. The Albalone data set did not include multiple features that needed to be one hot encoded, Sex was the only attributes and it only provided 3 options to one hot encode. The Forest Fire and Computer Hardware data sets on the other hand had multiple attributes that were one hot encoded, and each of those attributes had multiple options that were derived because of this one hot encoding. It is possible that one hot encoding this data was the wrong approach, and alternative methods should have been used, such as dropping those attributes completely. Since one hot encoding offers only 0 or 1 for the options the splits that will be generated when performing the regression might be highly

Table 6: Forest Fires: CART - Experimental Results



Forest Fire: Univariate Tree	
k-fold[1]	565.4062
k-fold[2]	606.1958
k-fold[3]	16434.9870
k-fold[4]	729.3448
k-fold[5]	1146.9990
Average MSE Across Folds	3896.5866

Forest Fire: Early Stopped Tree	
	Epsilon = 10
k-fold[1]	564.9116
k-fold[2]	605.5460
k-fold[3]	16428.8700
k-fold[4]	709.6340
k-fold[5]	1151.8463
Average MSE Across Folds	3892.1616

skewed towards on particular branch as the data is classified through the regression tree.

5. Conclusion

6. References

1. Alpaydin, E. (2004). Introduction to machine learning (Oip). Mit Press.