CSCI 446 Artificial Intelligence Project 3 Design Report

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November 4, 2016

1 Introduction

Introduce Machine Learning Algorithm (MLA)!!!! Explain classification problem!!!

2 Datasets

2.1 Dataset Representation

We will define a *datum* to be a vector consisting of the class as the zeroth element and the associated attributes as the rest of the elements. Classes and attributes will be represented by an integer. Continuous data will be binned before it is inserted into each datum. The resolution of the bins will be a variable that will have to be tuned. Each dataset will be represented as a vector of datums.

2.2 Data Imputation

Imputation is the process of approximating missing values in the datasets. To our knowledge there is only one dataset that has real missing values: the Wisconsin Breast Cancer Database. The 1984 United States Congressional Voting Records Database appears to have missing values, but these can actually be interpreted as a stance on a particular issue. Since the breast cancer database has a small proportion of missing values, it is appropriate to simply eliminate datums with missing values. The authors assert that trying to train a MLA with imputed values would only create unnecessary bias in the network.

However, it is a common real-world problem to attempt to classify an unknown, incomplete datum, therefore we will perform imputation on the validation datasets. To approximate the missing values we will first try a hot-deck imputation, where missing attribute values of a given datum are constructed by selecting a random member of that datum's class and copying the value of the attribute. If the hot-deck is unsuccessful, we will attempt to fill in the missing values using a regression model developed in *Mathematica*.

2.3 Cross-validation

To partition the full datasets into test and training datasets, we will use 10-fold cross validation. This method partitions the data into ten *folds* and uses one fold for testing data and the remaining nine folds for the training dataset. This process is repeated nine more times until every fold has been used as a test dataset. We selected this method because it will allow the convergence measurement described in Section 5.3 to be applied over a larger range, which allows us to measure the rate of convergence for each MLA more accurately.

3 Machine Learning Algorithms

3.1 k-Nearest Neighbors

3.2 Naive Bayes

3.2.1 Description

Naive Bayes uses the principle of Bayesian learning to solve the classification problem. This algorithm is said to be naive because it considers the attributes to be conditionally independent when performing classifications. Under this scheme, the probability distribution of each class C is given the set of attributes $x_1, ..., x_n$ is written by [Russel and Norvig, 2010] as

$$\mathbf{P}(C|x_1, ..., x_n) = \alpha \mathbf{P}(C) \prod_i \mathbf{P}(x_i|C) \tag{1}$$

where, using the maximum likelihood hypothesis, $\mathbf{P}(C)$ prior probability of the class C in the training dataset, $\mathbf{P}(x_i|C)$ is the likelihood of attribute x_i given C, and α is a normalization constant. To find $\mathbf{P}(C)$ the we simply say it is equal to the proportion of C observed in the training dataset. Likewise we can calculate the likelihood using

$$P(a|b) = \frac{P(a \wedge b)}{P(b)}$$

where the probabilities are calculated using the number of occurrences in the training dataset. So, using equation 1 we can calculate the probability of a particular set of attributes being classified as class C. Then, we simply select the class with the largest probability for our prediction. In this way, naive Bayes can make predictions using only the probability ratios constructed from the training dataset. The probability distribution in the naive Bayes algorithm can be viewed as a Bayesian network, shown in Figure 1 where each attribute is only connected to the class, and there are no relationships between attributes.

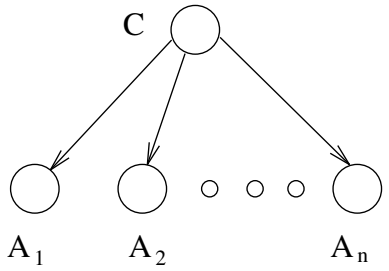

Figure 1: *An example of a Bayesian network for naive Bayes. The root C is the class, the leaves $A_1, ..., A_n$ are the attributes [Friedman et al., 1997]*

3.2.2 Design Implications

This algorithm should be very straightforward to implement. During the training phase, we simply loop through the dataset and tally how many times each class takes on every value of each attribute. During the testing phase, the algorithm uses the equations described in Section 3.2.1 to select the most probable class.

3.3 TAN

3.3.1 Description

Tree-Augmented Naive Bayes (TAN) is an extension to the naive Bayes algorithm described in Section 3.2. First described by [Friedman et al., 1997] TAN relaxes the assumption that the attributes are conditionally

independent and allows each attribute to depend on only one other attribute. It accomplishes this by constructing a fully-connected, undirected graph out of the attributes in the Bayesian network for the naive Bayes algorithm (Figure 1). TAN then assigns a weight to each connection in the graph using the *mutual information function*, given by

$$I_P(\mathbf{X};\mathbf{Y}) = \sum_{\mathbf{x},\mathbf{y}} P(\mathbf{x},\mathbf{y}) \log\left(\frac{P(\mathbf{x},\mathbf{y})}{P(\mathbf{x})P(\mathbf{y})}\right).$$

Applying the this weight to the edges allows us to construct a minimum spanning tree of the graph. We can then make the spanning tree directed by choosing a root node and setting the direction of all edges to be outward from it. The result is exemplified in Figure 2. Using this representation, we can calculate the analog

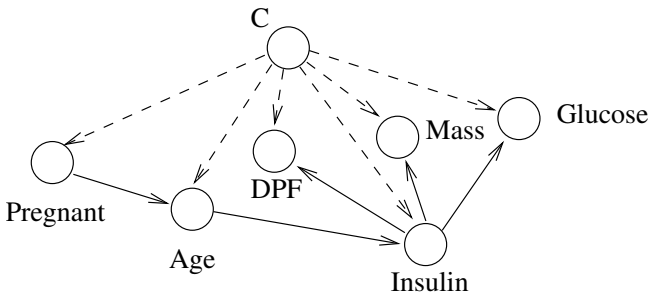

Figure 2: *An example of the directed minimum spanning tree produced by TAN. Dashed lines represent the original naive Bayes representation and the solid lines represent the spanning tree [Friedman et al., 1997].*

of equation 1, the probability distribution using the expression given by [Zheng and Webb, 2010]

$$\mathbf{P}(C|x_1,...,x_n) = \alpha\mathbf{P}(C)\prod_i \mathbf{P}(x_i|C,\pi(x_i)) \tag{2}$$

where $\pi(x_i)$ is the parent of the attribute x_i in the directed minimum spanning tree. Then, using a similar process to that described in Section 3.2 we can classify a set of attributes by selecting the class with the highest probability calculated from equation 2.

3.3.2 Design Implications

To develop the TAN algorithm, we will need to implement a tree structure to represent the naive Bayesian network and the associated minimum spanning tree. To find the minimum spanning tree we will need an implementation of Prim's algorithm. If appropriate we will use the implementation of Prim's algorithm provided in the Boost C++ libraries, otherwise we will develop our own implementation of Prim's algorithm. Once the minimum spanning tree is constructed we can appropriate the probability calculations developed for naive Bayes to calculate the value of equation 2 for classification.

3.4 ID3

3.4.1 Description

Iterative Dichotomiser 3 (ID3) is an algorithm that creates a decision tree and uses it to make inductive inferences about a set of data. The decision tree approach to making these inferences is a fairly obvious one. Make a decision tree that correctly classifies all the individuals in the training data. Since the goal of this solution is to generalize classification, it makes sense to use the smallest tree that can still correctly classify all of the training data. The naive way of finding the shortest tree would be to generate all possible trees and select the shortest one[Quinlan, 1986]. The problem that one encounters is the very large, but finite, number

of decision trees that are capable of correctly classifying all data. The computation required to do this is unfeasible large. ID3 provides a good, but not optimal, solution to this problem.

ID3 is an iterative process that generates a short tree by splitting the tree one attribute at a time. The first attribute to be used is the one with the most information gain. Information gain is a metric that tells you how well that attribute splits the data into the correct classes. The equation for finding the gain in an $n - ary$ classification system is as follows

$$H(S) = \sum_{i=1}^{n} \left(-p_i \log_2 p_i\right).$$

One bias that ID3 introduces is the fact that attributes that have a large amount of possibilities will naturally have a higher gain and, therefore, will be chosen first. To combat this we will use gain ratio instead. Gain ratio takes into account the number of possibilities for each algorithm.

Another problem is that the tree still might not be general enough and could be trimmed down further. To help with this we will implement reduced error pruning. The general idea is to fully create a tree and then prune branches while checking if the missing branch reduces the accuracy of its classifications of a validation set.

3.4.2 Design Implications

This algorithm will affect the structure of our code greatly. A special tree structure will have to be created that can contain subsets of the training set and also leaf values for when a classification is found. In addition the training set is going to have to be divided to get a validation set to perform reduced error pruning. The main body of the learning part of the algorithm will be in a while loop with the conditions above. The search part of the algorithm will just consist of transversing the tree according to the attributes belonging to the query.

4 Software Architecture

To reliably compare the four machine learning algorithms on five different datasets, we will use inheritance and C++ virtual classes that allows us to perform algorithm- and dataset-independent analyses on the MLAs. The inheritance structure is described in Figure 3. Each of the datasets will be encapsulated in an associated class, e.g. the Glass Identification Database will be stored in a class denoted `GlassDataset`. This class will inherit from the virtual class `Dataset`, which defines a dataset as a vector of integers, and also a set of associated functions for selected subsets of the dataset, printing the dataset, etc.

We will also implement a virtual class called `Learner`, which operates on a single training dataset. `Learner` defines the two functions `learn()` and `answer()` which will be used to perform training and testing respectively. Therefore, each of the four MLAs will inherit from learner and implement the two functions `learn()` and `answer()` based on the algorithm descriptions in Section 3.

To relate MLAs to datasets, we will define a `Teacher` class that is responsible for training and validating the MLAs, and measuring their performance. This class will also be responsible for performing the convergence measurement described in Section 5.3.

Not depicted in Figure 3 is a class called `Validation`. This class will be responsible for the 10-fold cross validation described in Section 2.3. `Validation` will partition the datasets into training and testing datasets and provide them to the `Teacher` to train and validate the MLAs.

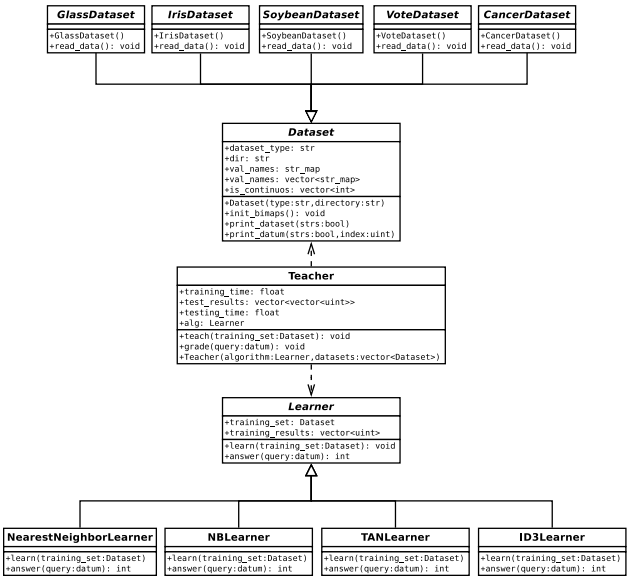

Figure 3: *A high-level description of the program architecture in UML.*

5 Experiment Design

5.1 Algorithm Accuracy

5.1.1 Precision

Precision is the proportion of results that are relevant[Russel and Norvig, 2010]. It is represented by the equation:

This is a good metric to look at because it tells you what proportion of the datums were correctly classified.

5.1.2 Recall

Recall is the proportion

5.1.3 Confusion

5.2 Algorithm Time-Complexity

5.3 Algorithm Convergence

References

[Friedman et al., 1997] Friedman, N., Geiger, D., and Goldszmidt, M. (1997). Bayesian network classifiers. *Machine Learning*, 29(2):131–163.

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[Zheng and Webb, 2010] Zheng, F. and Webb, G. I. (2010). *Tree Augmented Naive Bayes*, pages 990–991. Springer US, Boston, MA.