On the problem of selecting categories and model subsets in decision trees
(October, 2006)

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Abstract

Discretization in data mining often centers on finding an appropriate discretization strategy. The problem of choosing the number of categories to create when discretizing is non-trivial and often accomplished with no theoretical or empirical justification. Frequently, problems contain too many possibilities to feasibly test various categorization strategies. We propose a comprehensive technique to discretize and compare datasets within decision trees. In addition, we investigate a variety of categories and present an information criterion for choosing among resulting model subsets within decision trees. This manuscript also presents a method to quantify opportunity losses among decision alternatives thereby providing decision-makers with a quantitative solution to evaluate alternative course of action. The proposed information criterion and opportunity loss measure provide decision support for the use of the new algorithm for optimizing choices in the face of uncertainty.
Introduction

Kyper, Lloyd, and Chin (2004) outlined the importance of discretization for use in data mining, specifically with rough sets and decision-tree induction where discretization is the process of transforming continuous data into ordinal categories. The most commonly used methods for discretization are equal width intervals and equal frequency intervals. Decision-makers often choose the number of categories to create based on convenience but without empirical, experimental or theoretical justification. The method of convenience often results in outputs not optimized for predictive accuracy or ease of interpretation. In this study, we present an information criterion to choose among decision tree model subsets created by testing multiple categorization schemes. The decision tree information criterion facilitates tree (or course of action) selection by directly comparing accuracy and complexities of decision trees in a given model subset. Efficient and accurate creation and comparison of multiple categorization schemes benefit decision-makers by precise results and knowledge of the opportunity losses among competing model subsets.

If decision-makers create categories based on convenience, they create equal width intervals having usually 4, 5, or 10 categories. Decision trees in this study rely upon continuous data discretized with an equal width interval algorithm. We choose equal width interval algorithms because it creates results that facilitate decision-making, is easy to use and understand, and is commonly available in statistical and decision tree software.

Successful managers normally have an intuitive understanding of the decision-making process (Simon, 1987). Managers understand the tradeoff between accuracy and complexity (Simon, 1977) and the principle of parsimony. This principle represents
managers' preferences, and we refer to it as Occam’s Razor (Bozdogan, 1987; Moody, 1967). The parsimony principle states that simpler models are preferable to complex models, *ceteris paribus*. If a decision-maker knows the accuracy requirement for a given problem domain, then decision-makers benefit by having the simplest model (most parsimonious) to fulfill that requirement. However, decision-makers often do not have the time to test multiple categorization schemes for a given dataset. In addition, decision-makers have a difficult time comparing the resulting models. The techniques below allow both the creation and comparison of multiple categorization schemes. As an example, requirements for accuracy known in advance are those that arising from legislation such as the Clean Air Act (1970) specifying air toxicity limits for industries.

Currently there is no comprehensive technique to discretize and compare datasets within decision trees. We propose an information criterion that automates the process of choosing among decision trees. Furthermore, we propose a system to integrate the discretization and decision tree construction processes together into a single decision-making process. Essential to this process is the ability for decision-makers to understand alternative decision trees and quantify the opportunity losses associated with their decisions. Opportunity loss is the difference between the realized benefit of a course of action and the benefit of the optimal course of action. Opportunity loss is defined as, $O = A_i - A_0$. Where $O$ is opportunity cost, $A_i$ is the cost of an alternative, and $A_0$ is the cost of the optimal alternative. To meet this latter requirement, we develop a metric to evaluate and quantify the opportunity losses between sub-models (decision trees) of a dataset.

We apply the proposed system to many commercial situations. For example, an insurance company call center generates various statistics from the incoming calls
including service levels and call volume. A decision tree provides information to quantify and rank the factors that influence service levels; this enables managers to focus their efforts. Decision trees also permit managers to forecast future service levels based on current performance. Attributes such as call volume are not categorical in nature, they must first discretize. The system proposed below provides a means to discretize, analyze, and choose between competing models based on an individual manager's needs.

There is a large body of research detailing discretization/categorization methods. Discretizing continuous data involves two factors: (1) the number of intervals and (2) interval width. The techniques discussed below are methods to determine intervals and width respectively. For a complete understanding of the discretization literature see (Berka and Bruha, 1995; Bryson and Joseph, 2001; Dougherty, Kohavi and Sahami, 1995; Ishibuchi and Yamamoto, 2003; Kurgan and Cios, 2004; Kwedlo and Kretowski, 1999; LiuWong and Wang, 2004; Postema, Wu and Menzies, 1997; Ventura and Martinez, 1995).

We organize the remainder of this study as follows; a discussion of the current decision-making literature and methodologies, model subset selection, decision tree information criterion for decision trees, opportunity loss, and conclusion.

**Decision-Making Literature/ Discretization Methodology**

Choosing an appropriate discretization or categorization scheme is a non-trivial task that requires time and experience on behalf of the decision-maker. Moreover, statistical software, e.g., SAS SPSS, Minitab and Statistica among others, have limited functionality for categorizing data beyond creating equal width intervals or equal width frequency. Using equal width intervals, we write a simple routine to repeatedly categorize
a dataset into an increasing number of categories. Appendix A contains a sample of how to create multiple categories of equal width in Statistica\(^1\) (this routine would be with minimal changes applied to SAS, SPSS, and Minitab). Once the dataset is categorized, our solution offers a simple way to then choose a resulting model that best fits the decision-makers specific needs.

According to Simon (1977, pp. 57-58) the general process for using any mathematical tool in management decision-making contains the following steps:

1. "Construct a mathematical model that satisfies the conditions of the tool to be used and which, at the same time, mirrors the important factors in the management situation to be analyzed. For success, the basic structure of the tool must fit the basic structure of the problem, although compromise and approximation are often necessary to fit them to each other.

2. Define a criterion function, a measure to use for comparing the relative merits of various possible courses of action.

3. Obtain empirical estimates of the numerical parameters in the model that specify the particular, concrete situation to which it is to apply.

4. Carry through the mathematical calculations required to find the course of action, which, for the specified parameter values, maximizes the criterion function. With each of the tools are associated computational procedures for carrying out these calculations efficiently."

\(^1\) Statistica 7.1, copyright© Statsoft, Inc. 1984-2005, see http://www.statsoft.com
The above process outlines the steps used in this research. Once the collected data is in a format appropriate for analysis (discretized/categorized continuous variables), construction of decision trees begins. Step One above defines the important factors for study as accuracy and complexity. Step Two defines a criterion function; the information criterion presented below meets this requirement. Step Three requires the collection of empirical estimates for the criterion function parameters. We complete Step Three by collecting user preferences for evaluating between models as applied to their particular problem domain. Step Four applies calculations required to determine the desired course of action.

**Model Subset Selection**

If multiple categorization schemes are implemented the decision-maker has the real problem of choosing the appropriate model from the subset of models created. An often-cited solution in forecast evaluation is Akaike’s Information Criterion (AIC). Akaike (1976) developed a criterion that chooses the simplest model for a given level of accuracy, thereby leading to parsimony. It is useful to briefly review Akaike’s solution as a basis for comparison with the decision tree information criterion presented in the next section.

AIC selects from nested econometric or predictive models. The criterion is \( AIC = \ln (s_m^2) + 2m/T \), where \( m \) is the number of parameters in the model; \( s_m^2 \) is the estimated residual variance (in an autoregressive example), and \( T \) is the number of observations. The criterion minimizes over choices of \( m \) forming a tradeoff between model fit and model complexity (measured by \( m \)) (Wei, 1993). The basic components of this model are accuracy and complexity, measured by \( s_m^2 \) and \( m \) respectively. Finally, AIC selects the simplest model subset having the greatest accuracy.
To calculate a measure of parsimony for decision trees the proposed information
criterion (referred to from now on as IC) evaluates decision tree accuracy and complexity
respectively. One possible method to measure decision tree complexity is through an
implementation of Shannon’s information theory research (Shannon, 1948). Information
theory specifies the measurement of complexity of information when choices are not
equally likely. Shannon developed the method to measure the average number of bits
required to describe an entity. In the simplest form $M$: bits $= \log_2 M$, where $M$ is the number
of choices. In decision trees, a binary decision one makes at each non-terminal node. This
paper uses the criterion developed by Shannon to measure complexity in decision trees.
The number of non-terminal nodes now represents the number of possible choices.
Therefore, decision tree complexity becomes $\log_2 N$, where $N =$ number of non-terminal
nodes.

Statistica provides the mean square error (MSE) as a measure of accuracy with
predictive decision trees. Traditional prediction methods, for example ordinary least
squares regression, employ $R^2$, the coefficient of determination (proportion of total
variation explained by the model), as a measure of accuracy. While not generally
associated with decision trees, there exists no statistical obstacle to calculating $R^2$.

$$R^2 = \frac{\sum_{i=1}^{n} (\hat{Y} - \bar{Y})^2}{\sum_{i=1}^{n} (Y - \bar{Y})^2},$$

where $\hat{Y}$ is the predicted value, $Y$ is the observed value, and $\bar{Y}$ is
the mean of the observed values. We provide the required predicted and observed values
for these decision trees. Additionally, $R^2$ is bound to $(0 \leq R^2 \leq 1)$, making the interpretation
of the IC straightforward. Thus, it is a measure of relative accuracy where 1 is perfect
accuracy. With working measures for accuracy and complexity, one constructs a ratio. We
detail the calculation of this ratio in the next section.

**Decision Tree Information Criterion**

Once we define measures of accuracy and complexities, it is possible to construct a
ratio of accuracy to complexity (similar to AIC). It is easier to define the functions for
accuracy and complexity independently than to construct the IC measure right away.

The accuracy function chosen in this paper is 1-\(R^2\), "the numerator", (decreases
with \(R^2\)). This function is a complement of \(R^2\), making low IC values desirable. This
means that the numerator will have low values at high levels of accuracy. In this case,
perfect accuracy (\(R^2 = 1\)) would have a numerator of zero and a total lack of accuracy
would have a numerator of 1.

The complexity function chosen in this paper is \(N/ (1-\log_2 N)\). This function
decreases with \(N\). This has implications for constant levels of accuracy. As \(N\) increases, the
complexity function decreases and correspondingly the IC function will increase. This is a
penalty since low values of IC are desirable.

The IC measure is \(\text{COMPLEXITY} \times \text{ACCURACY} = (1 - R^2)/ (1-\log_2 N)\). This
expression yields negative values, so its complement is taken, yielding positive values to
facilitate interpretation: \(1 - N (1-R^2)/ (1-\log_2 N)\). Taking the common denominator \(1-\log_2 N\)
yields

\[
IC = \frac{[1 - \log_2 N - N(1-R^2)]}{[1 - \log_2 N]} \\
(1)
\]
To encapsulate the decision-maker’s input, we add two additional parameters to the equation resulting in

\[
IC = \frac{[1 - \log_2 \kappa(N)] - [(N)(1 - \psi R^2)]}{1 - \log_2 \kappa(N)}
\]  

(2)

For values greater than zero, \(\psi\) parameter adjusts the benefit of accuracy and the \(\kappa\) parameter adjusts the penalty of complexity. To examine the function in each dimension, we find the derivatives of the function. Graphical representations of the function follow the discussion on derivatives.

Derivatives:

Let \(u = 1-\log_2\kappa N\). Equation is then

\[
DTIC = \frac{[u - N(1 - \psi R^2)]}{u}
\]

The partial derivative with respect to \(R^2\) (< 0 for all \(\kappa N \geq 2\)) is

\[
\frac{\delta IC}{\delta R^2} = \frac{N}{u} \frac{N \psi}{(1 - \log_2 \kappa N)}
\]

(3)

Note that the rate of change of IC with respect to \(R^2\) (the above derivative) is negative and a function of \(N\). More precisely, \(u\) is negative for \(\log_2 \kappa N > 2\), so \(N/u\) is negative for the same value. Lower values of IC indicate better accuracy, and the response of the function to \(R^2\) increases with \(N\). The implications are that for constant levels of accuracy (\(R^2\)), as complexity increases (\(N\)), the values of IC increase (becoming less desirable).

Second partial derivative with respect to \(R^2\) (slope with respect to \(R^2\) is constant):

\[
\frac{\delta^2 IC}{\delta^2 R^2} = 0
\]

(4)

This confirms that the slope of the previous derivative does not change. This indicates that the response of the function to \(R^2\) does not change as \(N\) changes.
First partial derivative with respect to \( N \):

\[
\frac{\delta IC}{\delta N} = \frac{[u - N(1 - \psi R^2)]du - u[du - (1 - \psi R^2)]}{u^2} = 0
\]

This has an extremum at \( u - Ndu = 0 \), or \( u = Ndu \)

Second partial derivative with respect to \( N \):

\[
\frac{\delta^2 IC}{\delta N^2} = \frac{(1 - \psi R^2)[(u - Ndu)(2udu) - u^2(du - (N\psi R^2 + du))]}{u^4} = 0
\]

\[
\frac{(1 - \psi R^2)(2u^2du - 2Ndu^2 - u^2du + u^2Nd^2u + u^2du)}{u^4} = 0
\]

\[
\frac{(1 - \psi R^2)(2u^2du - 2Ndu^2 + u^2Nd^2u)}{u^4} = 0
\]

The above expression evaluated at \( u = Ndu \), with \( du = \frac{\log e}{N} \) and \( d^2u = \frac{\log e}{N^2} \)

yields:

\[
\frac{(1 - \psi R^2)(\log e)^2}{N} (- \log e + 2N)
\]

which is > 0 for \( N \geq 1 \), MINIMUM at \( u = Ndu \).

Note that the rate of change with respect to \( N \) is a function of both \( N \) and \( R^2 \); it has a minimum at \( U = Ndu \), (which is at \( N = (1/\kappa)2^{\log 2e + 1} = 5.432/\kappa \)) and increases thereafter.

The slope is negative before, zero at the point \( u = Ndu \), and positive thereafter resulting in a minimum shaped like a valley (see Chart 2). The IC function has a local minimum of
5.4/κ when N = 5. However, there is a global minimum at IC = 1 when we achieve [R^2 = 1/ψ].

To visualize the behavior of the function, the breadth (dimension) is modeled separately in three directions. Figure 1 below shows the shape of the gain function (fixed complexity). Input tables for Figures 1 thru 3 are in Appendix B. The gain function is decreasing linearly, with a minimum of IC = 1 at R^2 = 1. This demonstrates that greater values of R^2 result in lower IC values, and that perfect accuracy results in a global minimum IC of 1.0.

![Graph](image)

Figure 1: Accuracy function holding complexity constant

Figure 2 below shows the shape of the penalty function, which demonstrates that for nodes greater than 5, increasing complexity results in greater values of IC.
Figure 2: Complexity function holding accuracy constant

Figure 3: Simultaneously varying complexity and accuracy
Figure 3 demonstrates the J-shaped curve frequently produced by the measurement function (Appendix B provides empirical evidence to support this). In all cases, the IC function produces a global minimum. In the above case, a model with six nodes (barring any decision-maker input) has the optimal tradeoff between accuracy and complexity as defined by the IC. This demonstrates the measurement's natural tendency towards more parsimonious models for a constant increase in accuracy and complexity. In practice, the increases in accuracy and complexity are not always linear. This creates no problems in calculating the IC or modeling decision trees, but means that the IC function does not behave monotonically with changes in $R^2$ and the number of non-terminal nodes.

**Opportunity Loss**

Cyert, Simon, and Trow (1956, pp. 237) outline the importance of choosing between alternatives in decision-making. They describe an economic rational choice process as:

1. "An individual is confronted with a number of different, specified alternative courses of action.

2. To each of these alternatives is attached a set of consequences that will ensure if that alternative is chosen.

3. The individual has a system of preferences or "utilities" that permit him to rank all sets of consequences according to preference and to choose that alternative that has the preferred consequences. In the case of business decisions, the criterion for ranking is generally assumed profit."

However, according to Cyert, Simon, and Trow (1956, pp. 237) several missing elements must be incorporated into the above process. These missing elements are:
1. "The alternatives are not usually "given" but must be sought, and hence it is necessary to include the search for alternatives as an integral part of the process.

2. The information as to what consequences are attached to which alternatives is seldom "given," but, instead, the search for consequences is another important segment of the decision-making task.

3. We do not make comparisons among alternatives in terms of simple, single criterion like profit maximization. One reason is that there are often important consequences that are so intangible as to make an evaluation in terms of profit difficult or impossible. In place of searching for the "best" alternative, the decision-maker is usually concerned with finding a satisfactory alternative - one that will attain a specified goal and at the same time satisfy a number of auxiliary conditions.

4. Often, in the real world, the problem itself is not a "given", but, instead, searching for significant problems to which organizational attention should be turned becomes an important organizational task."

The IC presented above is effective choosing between alternative decision trees and satisficing a decision-maker's preference for either accuracy or parsimony. Satisficing decides on a course of action that meets the minimum requirements to achieve a goal. To compare the consequences of choosing one decision tree over another requires a new yet undefined measure. To state the consequences in terms of profit, an intimate understanding of the problem domain is needed, but not likely known. The IC is robust enough to be
applied across most, if not all, problem domains. The measure of consequences then must share the same quality.

Applying the concept of opportunity loss (Petersen and Lewis, 1999, Clemen and Reilly, 2001 discusses the same problem using the concept of imperfect information) creates a generalizable measure of the consequences between trees which is easy for decision-makers to understand. The difference in mean values of the response variables between trees (model subsets) is often very small, resulting in a poor measure of opportunity loss. Even with small differences in mean response values, the variance of the individual means within a tree differs a great deal between model subsets. Calculating the difference in root mean square errors (RMSE) for the model with the lowest IC and the competing models, accounts for the cost of choosing between alternative models. The RMSE is calculated as 

$$\sqrt{\frac{1}{N} \sum (\hat{y} - y)^2},$$

where $\hat{y}$ are the predicted values, $y$ are the observed values, and N is the number of observations (McClave, Benson and Sincich, 2001). The RMSE is the residual after we define all modeled relationships. We apply this when looking for differences between sub-models. Positive values indicate the competing model has response values with greater variation. Negative values indicate the competing model has response values with less variation.

While the IC is capable of measuring the tradeoff between accuracy and complexity of decision trees (parsimony), comparing IC values has little meaning for decision-makers. This is because the IC values represent a complex relationship between accuracy and complexity, and are extremely difficult to comprehend in any sense other than knowing some trees had higher values than others did.
R² is calculated for each decision tree. This gives a precise measure for goodness of fit for each tree. However, it is difficult for a user to convert that measure of goodness of fit into actual differences in response values between trees. The differences in RMSE between trees simplify arriving at a decision by indicating the accuracy of prediction of mean values at each non-terminal node.

**Conclusion**

We provide a unique information criterion for evaluating decision trees because it provides an effective and efficient method for model selection. This will enable decision-makers to choose among different decision alternative (trees) constructed from the same data set. The ability to compare and contrast separate decision trees enables decision-makers to select a model that suits their individual needs. Calculating the opportunity losses among decision trees aids the decision-making process by providing information about the differences in alternative models. To date there is no competing technique that allows a decision-maker to compare decision trees with different categorization schemes based on the same initial dataset.

Traditionally, information was a scarce factor in decision-making (Simon, 1998). Now, information is plentiful and filtering through it is a challenge. The processes of applying the presented IC and opportunity loss calculations are extremely time consuming. Future work will aid decision-makers in the process of finding a satisfactory decision tree, that is, we plan to develop a program to conduct decision tree simulations based on a dataset. We plan to apply it the IC and opportunity loss calculations to a sample dataset.
and provides a prototype application for use in decision-making. Additionally, it creates a starting point for continuations of this research.

References


Appendix A

Display open file dialogue to user;
Get file name for statistica input file;
If filename is valid statistica datasheet {
  Open statistica data file;
  Prepare data for analysis{
    Display user dialogue for variable selection from statistica data file {
      Select continuous variables;
      Select categorical variables;
      Select dependent variable;
    }
    Display user dialogue for discretization parameters {
      Select minimum number of discretization categories;
      Select maximum number of discretization categories;
      Select discretization category increment value;
    }
    For each variable to be discretized {
      Sort variable;
      For each category {
        Determine category cutpoints;
        Add new discretized variable to statistica data file;
      }
    }
  }
}
### Appendix B

#### Input for Tables 1 thru 3

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Table 1: Inputs and DTIC values for Figure 1

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Table 3: Inputs and DTIC values for Figure 3

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Our responsibility is to provide strong academic programs that instill excellence, confidence and strong leadership skills in our graduates. Our aim is to (1) promote critical and independent thinking, (2) foster personal responsibility and (3) develop students whose performance and commitment mark them as leaders contributing to the business community and society. The College will serve as a center for business scholarship, creative research and outreach activities to the citizens and institutions of the State of Rhode Island as well as the regional, national and international communities.

Mission

The University of Rhode Island started to offer undergraduate business administration courses in 1923. In 1962, the MBA program was introduced and the PhD program began in the mid 1980s. The College of Business Administration is accredited by The AACSB International - The Association to Advance Collegiate Schools of Business in 1969. The College of Business enrolls over 1400 undergraduate students and more than 300 graduate students.

The creation of this working paper series has been funded by an endowment established by William A. Orme, URI College of Business Administration, Class of 1949 and former head of the General Electric Foundation. This working paper series is intended to permit faculty members to obtain feedback on research activities before the research is submitted to academic and professional journals and professional associations for presentations.

An award is presented annually for the most outstanding paper submitted.