A study on relationships between heuristics and optimal cuts in decision tree induction

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(RIB) based on Fayyad's method in order to eliminate situations where a single isolated instance is located amidst samples of another class. RIB further narrowed the detection range of cuts.

For most algorithms of building decision trees with continuous-valued attributes, their heuristic information functions are based on information entropy. This paper makes an attempt to investigate whether other heuristic information functions have the similar properties. Several kinds of heuristic information functions are discussed and a generalized form of heuristic information functions is proposed. Whether the generalized heuristic information function has the property that the optimal cuts are always located in boundaries is studied. An investigation to this relationship leads to a significant reduction of number of detected cuts and further an improvement of generalization for a decision tree.

The rest of this paper is organized as follows. In Section 2 we present the process of selecting optimal cuts. Section 3 introduces several typical heuristic information functions. In Section 4 we establish a relationship between heuristic information functions and optimal cut selection. Section 5 concludes this paper.

2. Optimal cut selection

Cut selection is a key step of generating decision trees with continuous-valued attributes. Cut point is a threshold value $T$. For a continuous-valued attribute $A$, all instances with $A \leq T$ are assigned to a sub-interval while all instances with $A > T$ are assigned to the other one. In this way, a continuous-valued attribute is discretized by using a cut to split its range into two intervals. A typical process of optimal cut selection includes four steps: sorting, getting cuts, evaluating cuts and splitting node [16].

(1) Sorting: All individual values of a continuous attribute are sorted in either descending or ascending order.

(2) Getting cuts: Generally, the midpoint between two adjacent samples in the sorted sequence is evaluated as a potential cut point. Assuming that all samples have distinct values $v_1, v_2, \ldots, v_N$, there are $N - 1$ candidate cuts to be evaluated.

(3) Evaluating cuts: Evaluating $N - 1$ candidate cuts based on a certain evaluation function for determining which cut is the optimal one. One can find numerous evaluation functions in the literature such as information gain, Gini-index and classification error.

(4) Splitting node: Splitting the range of continuous values into two intervals according to the optimal cut.

Repeating above operations for each node that has the continuous-valued attributes until a stopping criterion is met. The optimal cut selection is the main workload of generating a decision tree. Usually detecting all candidate cuts for a continuous attribute is time-consuming (although the decision tree generation algorithm has the computational complexity much less than other types of learning algorithms). The number of candidate cuts (we must evaluate) directly determines the efficiency of a decision tree learning algorithm.

3. Heuristic information functions

At each node to be extended, the extended attribute we choose is most beneficial for classifying samples. The selected heuristic information function plays an essential role in the process of extending a node. From literatures one can find many heuristic information functions and most of them are impurity-based functions [6–10]. Here, we review some of the most representative ones.

3.1. Information entropy

Quinlan proposed the ID3 decision tree algorithm in 1986 using information gain [5] and later the C4.5 algorithm in 1993 using gain ratio [7]. Each of the two heuristic functions is based on the information entropy. The information entropy, which measures the impurity of instances in a node with respect to the classes, is defined as

$$
\text{Entropy}(S) = -\sum_{i=1}^{k} p(C_i | S) \log_2 p(C_i | S),
$$

where $S$ is a data set (i.e., a node) to be extended, $k$ is the number of classes and $p(C_i | S)$ is the probability of an example belonging to class $C_i$ in the data set $S$. When all examples in $S$ belong to the same class, the entropy is zero. When the probabilities of an example belonging to different classes are identical, the entropy reaches its maximum $\log_2 k$.

3.2. Gini-index

One alternative measure that has been used successfully in generating decision trees is the Gini-index which was proposed by Breiman in CART [9] and employed in the following function:
\[ Gini(S) = 1 - \sum_{i=1}^{k} p^2_i(C_i|S) = \sum_{i=1}^{k} p(C_i|S)(1 - p(C_i|S)). \]  

The formula of Gini-index is quite similar to entropy. That is, Gini-index is zero if all examples in S belong to the same class and Gini-index reaches its maximum 1 – 1/k if all probabilities of an example belonging to different classes are equivalent.

### 3.3. Classification error

Classification error is also a kind of impurity-based measure. It is defined as follows:

\[ \text{Classification Error}(S) = 1 - \max(p(C_i|S)). \]  

This measure is similar to the two above-mentioned ones. It gets its minimum zero when all examples belong to the same class and gets its maximum 1 – 1/k when data set S contains the same number of examples for each class.

### 3.4. Ambiguity

Yuan and Shaw [17] used ambiguity as the attribute selection criteria for fuzzy decision tree. Let \[ \pi = (\pi(x)|x \in X) \] denote a normalized possibility distribution on \( X = \{x_1, x_2, \ldots, x_n\} \), the ambiguity measure is defined as

\[ \text{Ambiguity}(Y) = \sum_{i=1}^{n} (\pi_i' - \pi_{i+1}' - \pi_{i+1}' - \pi_i') \ln i, \]

where \( Y \) is a fuzzy variable and \( \pi' = \{\pi_1, \pi_2, \ldots, \pi_n\} \) is the permutation of the possibility distribution \( \pi = \{\pi(x_1), \pi(x_2), \ldots, \pi(x_n)\} \), sorted so that \( \pi_i' \geq \pi_{i+1}' \) for all \( i = 1, 2, \ldots, n \), and \( \pi_{i+1}' = 0 \). The ambiguity denoting a type of impurity can be re-written as

\[ \text{Ambiguity}(Y) = \sum_{i=1}^{n} (\pi_i' - \pi_{i+1}') \ln i, \]  

where \( p' = \{p_1, p_2, \ldots, p_n\} \) is a sorting of probability distribution \( p = \{p(x_1), p(x_2), \ldots, p(x_n)\} \), \( p_i = \frac{p(C_i|S)}{\max(p(C_i|S))} \), \( p_i' \geq p_{i+1}' \) for all \( i = 1, 2, \ldots, n \), and \( p_{i+1}' = 0 \).

### 3.5. Generalized heuristic information function

Given a data set \( S \) with positive and negative examples of a target concept which is represented as a Boolean function. As we show below, each of these impurity measures of \( S \) relative to this Boolean classification can be calculated as

\[
\begin{align*}
\text{Entropy}(S) & = -p(+) \log_2 p(+) - (1 - p(+) \log_2 (1 - p(+) ) \\
\text{Gini}(S) & = 1 - p^2(+) - (1 - p(+))^2 = 2p(+) (1 - p(+) ) \\
\text{Classification Error}(S) & = \begin{cases} 
    p(+) & 0.5 \leq p(+) \leq 1 \\
    1 - p(+) & 0 \leq p(+) \leq 0.5 
\end{cases} \\
\text{Ambiguity}(S) & = \begin{cases} 
    \frac{p(+) \ln 2}{1 - p(+) } & 0 \leq p(+) \leq 0.5 \\
    \frac{1 - p(+) \ln 2}{p(+) } & 0.5 \leq p(+) \leq 1 
\end{cases}
\end{align*}
\]

where \( p(+) \) is the proportion of positive examples in \( S \). 

\text{Fig. 1} shows the forms of the four heuristic information functions to a Boolean classification, where \( p(+) \) varies between 0 and 1.

Observing the specific forms of the four heuristic information functions, we can find their similarities and differences as follows.

Their differences mainly reflect in two aspects:

1. **These functions have different derivability at point \( p(+) = 0.5 \):** ambiguity and classification errors are derivable, entropy and Gini-index are non-derivable.
2. **The second-order derivatives of these functions are different in the derivable intervals:** The second-order derivatives of entropy and Gini-index are less than zero, classification error’s second-order derivative is equal to zero and ambiguity’s second-order derivative is greater than zero.

Their similarities mainly reflect in another two aspects:
These functions are symmetrical about point \( p(+) = 0.5 \), monotonically increasing in the left interval \([0,0.5]\), and monotonically decreasing in the right interval \([0.5,1]\). They get their maximum at point \( p(+) = 0.5 \) and their minimum at points \( p(+) = 0 \) and \( p(+) = 1 \).

These functions have the second-order derivatives in their derivable intervals \((0,0.5)\) and \((0.5,1)\).

Through summarizing these similarities and differences, we extract a general form of these functions as follows:

\[
F(x) = \begin{cases} 
  f(x) & 0 \leq x \leq \frac{1}{2} \\
  f(1-x) & \frac{1}{2} \leq x \leq 1
\end{cases}
\]

where \( x \) is the proportion of positive examples in \( S \). \( f(x) \) is such a function defined in \([0,1]\) with the properties: \( f(0) = 0 \), \( f(x) \) is continuous and monotonically increasing in interval \([0,0.5]\), and its second-order derivative exists in interval \((0,0.5)\). It is worth noting that the function \( f \) defined above can be regarded as a general form of the 4 measures given in Section 3.

\( F(x) \) is called the generalized heuristic information function which includes many existing heuristics such as the frequently used Entropy and Gini index as special cases. It is very practically useful for building decision trees to find a uniform (generalized) function summarizing diverse heuristics. The discussion about the generalized function is expected to make clear the impact of different heuristics on size of the generated decision tree. It is also to expected reveal some new key features of relations between the generalization capability and the size of a decision tree.

4. Relationship between generalized heuristic information function and optimal cut selection

For each node to be extended during the tree growing, we would like to select the attribute having the optimal cut as the extended attribute. Assume that \( S \) is the set of samples, representing the considered node, \( A \) is a candidate continuous-valued attribute, and \( T \) is a candidate cut of attribute \( A \). When we use \( F(x) \) as the heuristic function for decision tree generation, the cuts can be measured by using the following equation

\[
G_S(T) = \frac{|S_1|}{|S|} F(p(+|S_1)) + \frac{|S_2|}{|S|} F(p(+|S_2)).
\]

where set \( S \) is partitioned into the subsets \( S_1 \) and \( S_2 \) by cut \( T \), \(|| \) denotes the size of a data set, \( p(+|S_1) \) and \( p(+|S_2) \) are the proportions of positive examples in the two subsets (\( p_1 \) and \( p_2 \) for short).

For example, when \( F(x) \) is the information entropy, \( G_S(T) \) denotes the class information entropy of the partition induced by \( T \):

\[
G_S(T) = \frac{|S_1|}{|S|} \text{Entropy}(S_1) + \frac{|S_2|}{|S|} \text{Entropy}(S_2).
\]

Most decision tree generation algorithms select the extended attribute with the highest information gain. Maximizing information gain is equivalent to minimizing the average class entropy. We will select the optimal cut with the smallest average class entropy for continuous-valued attributes based on the generalized information function. Fayyad and Irani [12,13] proved that the cuts with minimum average class entropy are always boundaries. This result can narrow the range of the optimal cuts detection from all candidate cuts to boundary cute only, and therefore, improve the computational
efficiency of cut selection significantly. The key issue to be solved in this study is whether the optimal cuts based on generalized heuristic information function are also boundaries, that is, whether \( G_\delta(T) \) gets its minimum at boundaries. We have the following proposition.

**Proposition 4.1.** Suppose that \( G_\delta(x) \) gets its minimum at \( x = T \), then we have the following conclusions regarding the generalized heuristic information function and its optimal cuts

1. If \( f^\prime(x) < 0 \), then \( T \) must be a boundary point.
2. If \( f^\prime(x) = 0 \), then \( T \) can be a boundary point.
3. If \( f^\prime(x) > 0 \), then \( T \) must be a boundary or a point satisfying \( p_1 = p_2 \).

**Proof.** Let \( S \) be a samples set belonging to node to be extended and \( A \) be a continuous-valued attribute regarding \( S \). Sort the samples in \( S \) by increasing value of attribute \( A \). Assume that cut \( T \) occurs within a sequence of \( n \) examples of the same class, where \( n \geq 2 \). Without loss of generality, we assume this class being positive. Let \( T_1 \) and \( T_2 \) be the boundary points of \( n \) examples, and \( S_1 \) and \( S_2 \) be the subsets of \( S \) divided by \( T \). There are \( n_c \) examples that have values greater than \( T_1 \) and less than \( T \), where \( 0 < n_c < n \). Fig. 2 describes this situation.

The problem of judging the position of an optimal cut is converted to a problem of testing whether \( G_\delta(T) \) gets its minimum at \( T_1 \) or \( T_2 \). If \( G_\delta(T) \) gets its minimum at \( T_1 \) or \( T_2 \), then the optimal cut is a boundary; otherwise the optimal cut is not a boundary. Next, our main task is to obtain the position where \( G_\delta(T) \) gets its minimum according to the values of \( f^\prime(x) \).

Let there be \( N^+ \) positive examples in \( S \), \( nl \) examples in \( S \) with \( A \)-values less than \( T_1 \), where \( nl \) examples are positive, and \( nr \) examples in \( S \) with \( A \)-values greater than \( T_1 \) where \( nr \) examples are positive. Noting that \( 0 < nl \leq nl \), \( 0 \leq nr < nr \), and \( nl + nr = N^+ \). \( p_1 \) and \( p_2 \) are the proportions of positive examples in \( S_1 \) and \( S_2 \) respectively, we have:

\[
p_2 = \frac{N^+ - |S_1|p_1}{|S| - |S_1|}.
\]

\( G_\delta(T) \) can be written as an expression of \( p_1 \):

\[
G_\delta(T) = \frac{|S_1|}{|S|} F(p_1) + \frac{|S_2|}{|S|} F(p_2) = \frac{|S_1|}{|S|} F(p_1) + \frac{|S_2|}{|S|} F\left(\frac{N^+ - |S_1|p_1}{|S| - |S_1|}\right).
\]

While cut \( T \) moves from \( T_1 \) to \( T_2 \), \( p_1 \) increases and \( p_2 \) decreases monotonically. Because we cannot make sure the derivability on point 0.5, the change-intervals of \( p_1 \) can be divided into three kinds: the intervals are included within \( (0,0.5) \); the change-intervals of \( p_2 \) have the similar three cases.

Combining the change-intervals of \( p_1 \) and \( p_2 \), we can obtain the following 9 cases:

1. The change-intervals of both \( p_1 \) and \( p_2 \) are contained within \( (0,0.5) \).
2. \( p_1 \)’s change-interval is contained within \( (0,0.5) \), \( p_2 \)’s change-interval is contained within \( (0.5,1) \).
3. \( p_1 \)’s change-interval is contained within \( (0.5,1) \), \( p_2 \)’s change-interval is contained within \( (0,0.5) \).
4. The change-intervals of both \( p_1 \) and \( p_2 \) are contained within \( (0.5,1) \).
5. The change-intervals of both \( p_1 \) and \( p_2 \) contain point 0.5.
6. \( p_1 \)’s change-interval contains point 0.5, \( p_2 \)’s change-interval is contained within \( (0,0.5) \).
7. \( p_1 \)’s change-interval contains point 0.5, \( p_2 \)’s change-interval is contained within \( (0.5,1) \).
8. \( p_1 \)’s change-interval is contained within \( (0,0.5) \), \( p_2 \)’s change-interval contains point 0.5.
9. \( p_1 \)’s change-interval is contained within \( (0.5,1) \), \( p_2 \)’s change-interval contains point 0.5.

Below we discuss each of the 9 cases respectively.

1. The change-intervals of both \( p_1 \) and \( p_2 \) are included within \( (0,0.5) \).

In this case, we can rewrite the above expression as

\[
G_\delta(T) = \frac{|S_1|}{|S|} F(p_1) + \frac{|S| - |S_1|}{|S|} F\left(\frac{N^+ - |S_1|p_1}{|S| - |S_1|}\right).
\]

**Fig. 2.** A candidate cut \( T \).
Taking the first derivative of $G(jT)$ with respect to $p_1$, we have

$$
\frac{d(G(jT))}{dp_1} = \frac{|S_1|}{|S|} f'(p_1) + \frac{|S| - |S_1|}{|S|} f (\frac{N^* - |S_1| p_1}{|S| - |S_1|}) - \frac{|S_1|}{|S|} f'(p_1) - \frac{|S_1|}{|S|} f (\frac{N^* - |S_1| p_1}{|S| - |S_1|}) = \frac{|S_1|}{|S|} (f'(p_1) - f'(p_2)).
$$

(8)

We now discuss the minimum value of $G(jT)$ according to different values of the second-order derivative:

a. If $f''(x) < 0$, then $f'(x)$ is monotonically decreasing with respect to $x$. If $p_1 < p_2$, we have $\frac{d(G(jT))}{dp_1} = \frac{|S_1|}{|S|} (f'(p_1) - f'(p_2)) > 0$; if $p_1 > p_2$, we have $\frac{d(G(jT))}{dp_1} = \frac{|S_1|}{|S|} (f'(p_1) - f'(p_2)) < 0$. It then results in the following assertions:

(A1) If $p_1$ is permanently less than $p_2$, then $G(jT)$ is monotonically increasing and gets its minimum at boundary point $n_e = 0$.

(A2) If $p_1$ is permanently greater than $p_2$, then $G(jT)$ is monotonically decreasing and gets its minimum at boundary point $n_e = n$.

(A3) If $p_1$ is less than $p_2$ earlier and less than $p_2$ later, then $G(jT)$ is monotonically increasing earlier and decreasing later, and then, gets its minimum at boundary points $n_e = 0$ or $n_e = n$.

(A1)–(A3) imply that, no matter what relationship between $p_1$ and $p_2$, $G(jT)$ gets its minimum value at boundaries.

b. If $f''(x) = 0$, then $f(x)$ is a constant, $\frac{d(G(jT))}{dp_1} = 0$ for all $n_e = 0, 1, \ldots, n$. And therefore, no matter they are boundaries, $G(jT)$ is a constant.

c. If $f''(x) > 0$, then $f(x)$ is monotonically increasing with respect to $x$. We have $\frac{d(G(jT))}{dp_1} = \frac{|S_1|}{|S|} (f'(p_1) - f'(p_2)) < 0$ if $p_1 < p_2$ and $\frac{d(G(jT))}{dp_1} = \frac{|S_1|}{|S|} (f'(p_1) - f'(p_2)) > 0$ if $p_1 > p_2$, which imply that $G(jT)$ is monotonically decreasing and gets its minimum at boundary point $n_e = n$ when $p_1$ is permanently less than $p_2$; $G(jT)$ is monotonically increasing and gets its minimum at boundary point $n_e = 0$ when $p_1$ is permanently greater than $p_2$; and $G(jT)$ is monotonically decreasing earlier and increasing later, and gets its minimum at the point satisfying $p_1 = p_2$ when $p_1$ is greater than $p_2$ earlier and less than $p_2$ later. And therefore, we can see that $G(jT)$ gets its minimum value at boundaries or the points satisfying $p_1 = p_2$.

(2) $p_1$’s change-interval is included within $(0,0.5)$ and $p_2$’s change-interval is included within $(0.5,1)$.

In this case, we can rewrite expression (6) as

$$
G(jT) = \frac{|S_1|}{|S|} f (p_1) + \frac{|S| - |S_1|}{|S|} f \left(1 - \frac{N^* - |S_1| p_1}{|S| - |S_1|}\right).
$$

(9)

Taking the first derivative of $G(jT)$ with respect to $p_1$, we have:

$$
\frac{d(G(jT))}{dp_1} = \frac{|S_1|}{|S|} f'(p_1) + \frac{|S| - |S_1|}{|S|} f \left(1 - \frac{N^* - |S_1| p_1}{|S| - |S_1|}\right) \frac{|S_1|}{|S|} f'(p_1) + \frac{|S_1|}{|S|} f \left(1 - \frac{N^* - |S_1| p_1}{|S| - |S_1|}\right)
$$

$$= \frac{|S_1|}{|S|} (f'(p_1) + f'(1 - p_2)).
$$

(10)

$\frac{d(G(jT))}{dp_1} > 0$, for all $n_e = 0, 1, \ldots, n$, implies that $G(jT)$ is monotonically decreasing and gets its maximum at boundary point $n_e = 0$.

(3) $p_1$’s change-interval is included within $(0.5,1)$ and $p_2$’s change-interval is included within $(0,0.5)$.

Similarly to the case (2), it is easy to verify case (3).

(4) The change-intervals of both $p_1$ and $p_2$ are included within $(0.5,1)$.

In this case, we can rewrite expression (6) as

$$
G(jT) = \frac{|S_1|}{|S|} f (1 - p_1) + \frac{|S| - |S_1|}{|S|} f \left(1 - \frac{N^* - |S_1| p_1}{|S| - |S_1|}\right).
$$

(11)

Taking the first derivative of $G(jT)$ with respect to $p_1$, we have:

$$
\frac{d(G(jT))}{dp_1} = -\frac{|S_1|}{|S|} f'(1 - p_1) + \frac{|S| - |S_1|}{|S|} f \left(1 - \frac{N^* - |S_1| p_1}{|S| - |S_1|}\right) \frac{|S_1|}{|S|} f'(1 - p_1) + \frac{|S_1|}{|S|} f \left(1 - \frac{N^* - |S_1| p_1}{|S| - |S_1|}\right)
$$

$$= -\frac{|S_1|}{|S|} f'(1 - p_1) - f'(1 - p_2) = \frac{|S_1|}{|S|} (f'(p_1) - f'(p_2)).
$$

Noting that the expression above is the same to (8), we can obtain the same conclusion.

(5) The change-intervals of both $p_1$ and $p_2$ include point 0.5.

This combination is the most complex one. By dividing each of these change-intervals into two subintervals, the partition can be illustrated in Table 1. $p_1$ increases and $p_2$ decreases along with $n_e$ changes from 0 to $n$, so $p_1$ changes from values less
than 0.5 to values greater than 0.5 and $p_2$ changes from values greater than 0.5 to values less than 0.5. The change varies from state 2 to state 3 through the middle process state (1) or state (4).

The monotonicity of $p_1$ and $p_2$ in these subintervals are listed in Table 2 which has been discussed in the first four combinations. Noting that $G_0(T)$ is continuous in its domain and the monotonicity of $p_1$ and $p_2$ in state 1 is same as in state 4, we can get the position of $G_0(T)$'s minimum:

1. If $f''(x) < 0$, $G_0(x)$ gets its minimum value at one of the boundary points.
2. If $f''(x) = 0$, $G_0(x)$ gets its minimum value at more than one boundary point.
3. If $f''(x) > 0$, $G_0(x)$ gets its minimum value at a boundary point or the point with $p_1 = p_2$.

The other cases can be verified similarly to cases (1)–(5). We now end the proof.\footnote{Note. For particular engineering issue of building a binary decision tree in which the second-order derivative of the heuristic function is difficult to analytically evaluate, an approach to numerically estimating the second-order is necessary. For more details to numerical computation of derivative, one can see Ref. [18].}

The optimal cuts of information entropy and Gini-index are always on boundaries, while ambiguity gets its optimal cuts at boundaries or some special points. If the classification error function attains its minimum at non-boundaries, then it can attain the same minimum at boundaries. For a given heuristic information function, we can determine the positions of the optimal cuts according to the values of second-order derivatives. For example, if we use $\sin(x)$ as a heuristic information function, the optimal cuts are always boundaries because the second-order derivative of $\sin(x)$ in [0,1] is less than zero.

When the second-order derivative of the heuristic information function is greater than zero, optimal cut point may be a non-boundary point with $p_1 = p_2$.

$$p_{1(S)}^+ = \frac{|S_1| + |S_2|}{|S|} = p_1 \frac{|S_1| + |S_2|}{|S|} = p_1.$$ \hfill (12)

Noting that

$$p_1 = \frac{nl + nc}{nl + nc},$$ \hfill (13)

we have

$$nc = \frac{p_{1(S)}^+nl - nl^+}{1 - p_{1(S)}^+}.$$ \hfill (14)

If $n_c$ (the number of the points between $T_1$ and $T$) satisfies $0 < n_c < n$, then there exits a non-boundary point such that $G_0(T)$ reaches its minimum.

5. Numerical experiments

5.1. Experimental setting

Nine data sets are selected from UCI machine learning repository \[19\], which has been extensively used in testing the performance of diversified kinds of classifiers, LIBSVM available at http://www.csie.ntu.edu.tw/cjlin/libsvm and ELENA dataset available via anonymous ftp: ftp.dice.ucl.ac.be in the directory pub/neural/ELENA/databases. The sizes of data sets are from 683 to 19,020. The information about 9 data sets is summarized in Table 3.

5.2. Experimental objectives

It is to verify whether a decision tree learning system depends on its selection of heuristic function. The selected heuristic functions are required to meet the conditions given in Section 4. We selected 4 generalized heuristic information functions for our comparison. They are

<table>
<thead>
<tr>
<th>Subintervals</th>
<th>$p_1$</th>
<th>$p_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>State 1 (0,0.5)</td>
<td>(0,0.5)</td>
<td>(0,0.5)</td>
</tr>
<tr>
<td>State 2 (0,0.5)</td>
<td>(0,0.5)</td>
<td>(0.5,1)</td>
</tr>
<tr>
<td>State 3 (0.5,1)</td>
<td>(0.5,1)</td>
<td>(0,0.5)</td>
</tr>
<tr>
<td>State 4 (0.5,1)</td>
<td>(0.5,1)</td>
<td>(0.5,1)</td>
</tr>
</tbody>
</table>

Table 1: The change-intervals partition of $p_1$ and $p_2$. 

Note.
(1) \( f_1(x) = -x \log_2 x - (1 - x) \log_2 (1 - x) \). This special case is corresponding to the classical entropy heuristic information function.

(2) \( f_2(x) = x(1 - x) \). This special case is corresponding to the Gini index, another classical heuristic information function.

(3) \( f_3(x) = \begin{cases} \frac{1}{2} \log_2 \frac{1}{x(1-x)} & \text{if } 0 < x < 1 \\ x & \text{if } x = 0 \\ 1 - x & \text{if } x = 1 \\ \frac{1}{2} \log_2 \frac{1}{x(1-x)} & \text{if } 1 < x < \infty \end{cases} \). This case corresponds to the classical min–max heuristic.

(4) \( f_4(x) = \sin(\pi x) \). This is a case different from several classical heuristics.

Usually the used heuristic functions are smooth (such as entropy and Gini index) with expressions of elementary functions. Their second-order derivative is easy to evaluate. But for particular engineering problems in which the function is not smooth, a numerical method for computing the second-order derivative is necessary [18]. It is easy to directly evaluate the second-order derivatives of these 4 generalized heuristic information functions as follows:

\[
\begin{align*}
\frac{d^2}{dx^2} f_1(x) & = \frac{1}{x \ln 2} - \frac{1}{x(1-x) \ln 2}, \\
\frac{d^2}{dx^2} f_2(x) & = 0, \\
\frac{d^2}{dx^2} f_3(x) & = 0, \\
\frac{d^2}{dx^2} f_4(x) & = -\pi^2 \sin(\pi x).
\end{align*}
\]

A reason for selecting the 4 heuristics is to verify that (1) our proposed generalized heuristic information function can include many specific forms and (2) the frequently used classical heuristics, entropy and Gini index, can be considered as two special cases of our generalized function.

Sure, there are other forms of heuristics to be selected. Here we only would like to show such a statement that any function satisfying conditions of our generalized function (given in Section 3.5) can be selected as a heuristic for which the non-boundary cuts are not necessary to be evaluated during building the decision tree. (It is worth noting that there exist many heuristics for which all cuts (boundary and non-boundary) must be evaluated during building the decision tree.)

5.3. Experimental steps

The ten-fold cross-validation is performed for each data set. With the change of generalized heuristic information functions, we observe (1) the training accuracy, (2) the testing accuracy, and (3) the ratio of boundary-cuts to all cuts. The experiments repeat 5 times and the averaged values are recorded for each heuristic information function. The experimental records are summarized in Table 4 where the symbol NB represents Non-Boundary.

### Table 4

<table>
<thead>
<tr>
<th>Data sets</th>
<th>Training accuracy ( (f_1/f_2/f_3/f_4) )</th>
<th>Testing accuracy ( (f_1/f_2/f_3/f_4) )</th>
<th>Ratio of NB cuts (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pima</td>
<td>(0.7897/0.7991/0.7923/0.8163)</td>
<td>(0.7525/0.7636/0.7656/0.7893)</td>
<td>67.87</td>
</tr>
<tr>
<td>Breast cancer</td>
<td>(0.9542/0.9467/0.9502/0.9488)</td>
<td>(0.9213/0.9147/0.9322/0.9298)</td>
<td>78.23</td>
</tr>
<tr>
<td>Credit</td>
<td>(0.8636/0.8507/0.8644/0.8596)</td>
<td>(0.8029/0.8164/0.8211/0.8194)</td>
<td>75.56</td>
</tr>
<tr>
<td>Abalone</td>
<td>(0.6381/0.6504/0.6484/0.6391)</td>
<td>(0.6139/0.6014/0.6122/0.6087)</td>
<td>62.31</td>
</tr>
<tr>
<td>Clouds</td>
<td>(0.8774/0.8559/0.8354/0.8506)</td>
<td>(0.8697/0.8468/0.8432/0.8379)</td>
<td>70.81</td>
</tr>
<tr>
<td>SVMguide1</td>
<td>(0.7283/0.7455/0.7345/0.7301)</td>
<td>(0.7025/0.6765/0.6904/0.7117)</td>
<td>69.75</td>
</tr>
<tr>
<td>Waveform</td>
<td>(0.8485/0.8662/0.8421/0.8460)</td>
<td>(0.8348/0.8579/0.8334/0.8398)</td>
<td>72.66</td>
</tr>
<tr>
<td>Waveform + noise</td>
<td>(0.8406/0.8317/0.8385/0.8396)</td>
<td>(0.8259/0.8146/0.8164/0.8245)</td>
<td>73.59</td>
</tr>
<tr>
<td>MAGIC04</td>
<td>(0.7804/0.7826/0.7773/0.7801)</td>
<td>(0.7598/0.7461/0.7497/0.7588)</td>
<td>71.67</td>
</tr>
</tbody>
</table>
5.4. Experimental analysis

It is easy to view from Table 4 that the learning accuracy including training and testing is strongly dependent on the selection of generalized heuristic functions. For example, the heuristics 1 and 2 have the similar advantages regarding data sets Clouds and Waveform respectively. And the heuristic 4 has the advantages more than the other 3 heuristics with respect to the data set Pima. It is sure that the performance of learning is also dependent on the specific characteristic of the individual datasets, and it is interesting to give a specifically detailed analysis on relationship between individual datasets and their suitable heuristics.

Here, we select the Pima datasets for the analysis, on which the heuristic 4 obtains the better classification accuracy. Pima India diabetes data has 8 numerical attributes, and contains 768 cases related to the diagnosis of diabetes (268 positive and 500 negative). The local structure of Pima shows very nonlinear property. It is observed that there exist many cases that two samples are very near but their classes are different. It results in a boundary cut phenomenon. That is, a sample near boundary cuts usually has the statistical testing error more than a sample far from boundary cuts. Since the heuristic function with smooth second-order derivatives can bring more boundary cuts to some extent and then be adaptive to the highly nonlinear boundary, the bell shaped heuristics (such as heuristic 4) are suitable more than other type of heuristics for Pima dataset.

It is noted that robustness of a decision tree depends on the selection of heuristic information functions. Specifically we find that the decision trees generated based on heuristics 2, 3 and 4 respectively for Pima India diabetes data are more robust than the one based on heuristic 1. It can be seen that the testing accuracies obtained by decision trees with heuristics 2, 3 and 4 are all higher than the testing accuracy of decision tree with heuristic 1, which is the mostly-used heuristic in decision tree induction [5,7]. It is acknowledged that there are many noise data in Pima India diabetes dataset [20] but the heuristics 2, 3 and 4 enhance rather than degrade the classification performance of decision tree on Pima India diabetes dataset. This indicates that the heuristics 2, 3 and 4 are more insensitive to the noise data than heuristic 1.

We employ Wilcoxon signed-ranks test [21] to examine whether the difference among the 4 heuristics is significant. Wilcoxon signed-ranks test is safe and robust non-parametric test for statistical comparison of two classification methods [22]. In our experiment, 10-fold cross validation is repeated 5 times. There are 5 × 10 differences, and Wilcoxon signed-ranks test is distributed approximately normally. For a confidence level of 0.05 and regarding 6 pairs of heuristics, the tests give a result that the five differences are significant and one is not. It shows from the viewpoint of statistics that the learning accuracy is really dependent on the selection of heuristics.

From the last column of Table 4 one can see that the ratio of non-boundary cuts to all cuts is 0.7138 in average. It implies that, during the decision tree generation, around 71.38% computational load (which refers to the times of detecting candidate cuts) can be saved. The analysis on the second-order derivatives of generalized heuristic information functions really can really help reduce the computational complexity of generating a decision tree.

Although the decision tree learning system depends on the selection of heuristics, generally it is hard to say which kind of heuristic functions can significantly outperform other heuristics in decision tree learning from data with numerical attributes. It strongly depends on the local features of data. Our experiments confirm this conclusion.

6. Conclusions and future works

In this paper, we reviewed the process of decision tree induction with continuous valued attributes and several classical heuristic information functions. The expanded attribute for splitting a node to two sub-nodes is associated with a best cut. For classification problems in which the decision tree learning is based on finding best cuts, we have presented a generalized heuristic information function covering those existing frequently used heuristic information functions. We mathematically obtained a relationship between the second-order derivative of heuristic information functions and locations of optimal cuts, and further confirmed it experimentally. The relationship clearly indicates that the non-boundary cuts are not necessary to be detected when the generalized heuristic function meets some conditions related to the second-order derivatives. We statistically showed that the learning accuracy (including training and testing) is dependent strongly on the selection of heuristics. Considering the impact of this relationship on building a decision tree, we can significantly reduce the number of detected cuts, which indicates a big reduction of computational complexity for using cuts to generate a binary tree with continuous attributes. Furthermore, we experimentally showed that the generalization capability of the decision tree can be improved by incorporating this relationship into the process of decision tree generation, and the magnitude of improvement is generally dependent on the local characteristics of a specific data set.

Our future works regarding this topic will include how to categorize the generalized heuristic information functions such that a sub-category of heuristics can have better performance than other sub-categories with respect to a specified group of classification problems with continuous valued attributes.

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