A Massive Local Rules Search Approach to the Classification Problem

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Abstract. An approach to the classification problem of machine learning, based on building local classification rules, is developed. The local rules are considered as projections of the global classification rules to the event we want to classify. A massive global optimization algorithm is used for optimization of quality criterion. The algorithm, which has polynomial complexity in typical case, is used to find all high–quality local rules. The other distinctive feature of the algorithm is the integration of attributes levels selection (for ordered attributes) with rules searching and original conflicting rules resolution strategy. The algorithm is practical; it was tested on a number of data sets from UCI repository, and a comparison with the other predicting techniques is presented.

Keywords: Classification rules, Lazy learning, Global optimization, Conflicting rules resolution strategy.

1. Introduction

Extraction of structural information from raw data is a problem which is of great interest for both fundamental and applied studies. This paper will focus on one specific example of this problem — classification. The goal is to predict a class of a particular event. This problem was approached from a number of different disciplines, including Statistical Data Analysis (Dobson, 1990; Limnios and Nikulin, 2000), Machine Learning (Carbonell et al, 1983; Shavlik and Dietterich, 1990; Aha, 1997; Mitchell, 1990), Fuzzy Logic (Hellendoorn and Driankov, 1997), Operations Research (Walker, 1999) and Data Mining (Pitaetsky and Frawley, 1991; Fayyad et al, 1996). As a result, a variety of learning techniques was developed. The result of learning can be represented in a number of different forms. The form that we are interested in working with is a set of rules. It should be stressed that some other forms (such

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as decision trees, fuzzy models and many others) are equivalent to a set of rules.

A set of rules (or any other form to which it is equivalent) is often a preferred form of knowledge representation because it allows for a simple answer to the question, "What was learned?" This specific set of rules was learned from the data. For an algorithm, which produces only an answer, it is often impossible to understand what was really learned and why this specific answer was produced. (The two mentioned knowledge representations differ as follows: in the case that the result is a rule, the learned knowledge is represented in a language which is richer than one used to describe the dataset; in the case that the result is a value, the learned knowledge is represented in the same language as the one used to describe the dataset (Quinlan, 1993).)

The model–based techniques, such as developed in (Quinlan, 1992; Riddle et al, 1994), take training data as input and produce a set of rules (or statements which are equivalent to rules) which can classify any event. The lazy instance–based techniques, such as developed in (Aha et al, 1991; Aha, 1997; Quinlan, 1993), return a result tailored to the specific event we want to classify. With such techniques the events similar to the given one are usually found first, then a prediction based on found instances is made. An interesting attempt to combine model based and lazy instance based learning was presented in (Melli, 1998). In (Melli, 1998) a greedy lazy model–based approach for classification was developed in which the result was a rule tailored to the specific observation. While such an approach gives a simple rule as an answer (which is often much easier to understand than a complex rules set) and often works faster for classification of a single event, it–as every greedy algorithm–is not guaranteed to find the best rule, because the algorithm may not reach the global maximum of the quality criterion and a sub–optimal rule may be returned.

In the work (Riddle et al, 1994) an approach based on the brute force of rule–space scanning was developed. It was used for finding the "nuggets" of knowledge in the data (each nugget is a rule with a high degree of correctness). In contrast with greedy type algorithms, massive search algorithms are guaranteed to find the best rule(s).

In our early work (Malyshkin et al, 1999) we presented an approach which combined the massive model–based rule search approach with lazy instance–based learning. In that work we were also interested in "nuggets" of knowledge, but only those which were applicable for the instance we wanted to classify. The result was a set of rules which were applicable for classification of the given event. One may think about these rules as a projection of a global classification rules set to the given instance of the event.

In the current paper this approach is taken to the next level, and a practical algorithm, applicable to a variety of problems, is presented. A number of significant improvements have been made since that early version. The current algorithm includes the following new features: 1. highly optimized rule–space scanning, which allows problems with significant number of attributes to be solved; 2. integration of levels selection procedure for ordered (continuous and literal) attributes with the rule search algorithm; 3. information about dependent attributes directly included into the tree search algorithm thus significantly reducing computational complexity; and 4. an original conflicting rules resolution strategy which was especially built to work with automatically generated rules.

To create a practical algorithm, the three aspects — logical, statistical and computational complexity need to be addressed. In section 2 we formulate the problem and discuss the logical formulas which represent the rules we are interested in finding. In section 3 we discuss the statistical quality criterion which can be used for evaluation of rule quality and specify the criteria which we use in this work. We also present a conflicting rules resolution strategy for automatically generated rules. At the end of section 3 a sketch of the algorithm is presented. In section 4 we discuss the selection of attributes for analysis; it should be stressed that some attributes as they are built in section 4 are not independent, and this fact is known in advance. In section 5 we discuss computational complexity issues; an approach which includes information about dependence of the attributes into the algorithm is proposed. In section 6 we discuss error estimation. In section 7 we present the data analysis results and compare our results with the results of C4.5R8 (Quinlan, 1992). In section 8 a discussion is presented.

2. Logical formulas as a result of statistical analysis

In this section we describe logical formulas obtained as a result of data analysis. Representation of knowledge after it has been learned from the data, can vary depending on the approach used. However, different forms of knowledge representation(decision tables, decision trees, rules list, etc.) are equivalent to some logical formulas. Formulas obtained during data analysis are usually quite complex when applied to prediction or classification. This complicates the understanding of the results. The major source of complexity is the fact that the formulas are usually built to be applicable to all data observations. As we show below the complexity of the rules can be significantly reduced if, instead

of building global rules, we build local rules which are defined on a subset of observation data; this subset must include the data point where we want to perform a prediction/classification. Such an approach combines the best of both instance–based and model–based learning. It can be described as an approach working with projections of global formulas to local observations. A drawback of such an approach is the need to recalculate the rules for every event we want to classify. This is the cost of using simple local rules instead of complex global rules.

In the simplest form the problem can be represented as the following: We have a random variable g (consequent) and a random vector $\mathbf{x}$ (antecedent) of M components $x^{(m)}, m = 1 \dots M$. Random variables g and $x^{(m)}$ are assumed to take two different values: $true$ and $false$ (Note that this does not limit us in using other types of input data. The detailed process of g and $\mathbf{x}$ selection will be described in section 4.) We have a finite number of observations $N + 1$, each observation gives specific values of $x_n^{(m)}$ and g_n. Index $n = 0 \dots N$ numerates the observations. The value of antecedent $x_n^{(m)}$ is known for $n = 0 \dots N$, the value of consequent g_n is known for $n = 1 \dots N$, at the point $n = 0$ the value of consequent is unknown. The problem is predicting the value of g at $n = 0$. Again, we are interested in finding a prediction of g only at one point $n = 0$, not in building a universal prediction formula which is applicable at any n. This allows us to build a prediction which is easier to build, understand, and interpret.

The prediction is represented as a set of conjunctive forms which are correct with a high degree of confidence; this set of conjunctives may be considered as a distinctive conjunctive form of a logical formula. The criterion of acceptance/rejection will be described in section 3. Consider all possible expressions of the form:

$$f = \prod_{m \in \{\mu\}} x_n^{(m)} = x_0^{(m)} \tag{1}$$

In the Eq. (1) each term is a match of $x^{(m)}$ antecedent component at a given point n, with the value of the $x^{(m)}$ at the point we want to make a prediction: $n = 0$; index m belongs to a given set of indexes $\{\mu\}$; we have logical "and" in between all these terms, i.e. the formula (1) represents a fact of simultaneous matches of several antecedent components (those with indexes in $\{\mu\}$ set) with their values at the prediction point $n = 0$. Each formula of (1) type is completely defined by a set $\{\mu\}$. In total there are 2^M possible $\{\mu\}$ sets.

The goal is to find the conjunctive of form (1) which can give an implication with high degree of confidence.

$$\left(\prod_{m \in \{\mu\}} x^{(m)} = x_0^{(m)} \right) \rightarrow g = g_0^{(pr)} \tag{2}$$

Formula (2) represents an implication rule when a simultaneous match of given antecedent components (those in $\{\mu\}$ set), with their values at a point to predict $n = 0$, gives specific values of consequent. The value $g_0^{(pr)}$ is the value that the rule (2) predicts. Note that the rule of form (2) is defined on a subset of all available observations (on observations on which (1) is true). We do not consider the rules (even if they have very high confidence) which can not be applied at $n = 0$. This drastically reduces the number of rules we may accept.

In the next section we discuss statistical criteria used for the evaluation of each rule quality and for resolving the problem of conflicting rules(when several high confidence rules predict different values of g).

3. Local prediction rules: statistical evaluation of quality and conflicts resolution

Quality evaluation of a rule is based upon its statistical characteristics. In this paper we use canonical statistics: statistics which can be expressed via components of matrix of joint distribution (f, g):

$$\begin{pmatrix} P(f = false, g = false) & ; & P(f = false, g = true) \\ P(f = true, g = false) & ; & P(f = true, g = true) \end{pmatrix} \tag{3}$$

Here g is the consequent and f is a logical formula; for example, one from Eq. (1); the (3) is 2x2 matrix (because both f and g take two different values). Probability P can be defined in a number of different ways. In this paper the probability is defined in a standard combinatoric way (the number of favorite outcomes divided by the total number of outcomes). Almost any of the commonly used (coverage,correctness) type of criteria can be expressed via the components of a matrix (3).

There are many different statistics which can be used for quality evaluation of a logical formula. In the work (Hájek and Havránek, 1978) an approach of logical formulas transformation was developed which may solve an exponential complexity combinatoric problem in polynomial time. A similar approach was developed in (Lyashenko, 1989), where only statistics allowing formula transformations increasing quality criterion were used.

A statistic commonly used as a quality criterion is information gain (Shennon, 1948). The information gain based criterion was used in a number of machine learning studies. This criterion usually works well for the evaluation of global rules, but much less effectively for local rules. In the case of local rules the major problem with information gain criterion is the fact that $f \to g$ and $\neg f \to \neg g$ are equally important for this criterion. For the rules of (2) type we know in advance that $f = true$ and this asymmetry should be included into the quality criterion. Information gain criterion work well in the case of a seldom event. For example, for an event which happens in 1 out of 100 cases a rule which predicts that the event will never happen has 0.99 correctness. At the same time, an information gain based criterion gives no value to such a rule because we get no extra information beyond what we already know.

The most widely used statistics for estimation of a logical formula quality are ones of (coverage, correctness) type; the coverage is defined as $P(f = true; g = g_0^{(pr)})/P(g = g_0^{(pr)})$, and the correctness is defined as $P(f = true; g = g_0^{(pr)})/P(f = true)$. In (Riddle et al, 1994) a criterion based on high correctness (the coverage considered to be secondary) has been used. A criterion based on the F–measure (which combines precision and recall into one number) from information retrieval theory (van Rijsbergen, 1979) can also be used as a quality criterion. An important characteristic of the F–measure is the presence of a parameter allowing the adjustment of relative importance of coverage and correctness.

In this paper we use a quality criterion which has properties similar to one of (coverage,correctness) type. The quality α of implication rule is defined as following:

$$\alpha = \lambda \frac{P(f \neq true; g \neq g_0^{(pr)})}{P(g \neq g_0^{(pr)})} + (1-\lambda)\frac{P(f = true; g = g_0^{(pr)})}{P(g = g_0^{(pr)})} \quad (4)$$

$$g_0^{(pr)} \ : \ P(f = true; g = g_0^{(pr)}) \text{ is maximal} \quad (5)$$

In this paper we focus on predicting the events, not the probabilities, so for a given f we first select the value (of two possible values) of $g_0^{(pr)}$ which gives maximum of $P(f = true; g = g_0^{(pr)})$, Eq. (5), then evaluate the quality of implication rule using quality criterion (4). The value of α is equal to 1 for implications (2), giving totally correct predictions for every observation. For implications with non–perfect correctness and/or coverage the value of α is lower than 1. The parameter $0 \leq \lambda \leq 1$ determines the relative importance of coverage and correctness. The value $\lambda = 0.5$ makes coverage and correctness equally important

characteristics of a rule. The values $\lambda > 0.5$ make correctness more important than coverage.

While different statistics give very similar results on data which does not produce conflicting rules, the difference between different statistics may become significant when analyzing data producing conflicting rules. Our experiments with different types of data have shown that quality criterion (4) works well for the different data that we tested. To resolve a problem of conflicting rules we separate the process of making a prediction on two steps. On the first step we do not predict the specific value of g, we just find all implication rules of high quality. On the second step we use all found implication rules to obtain a prediction. Let us assume we found all rules of high enough quality; for example, with a quality better than a given acceptance level α_0. Each rule predicts its own $g_0^{(pr)}$ at $n = 0$. If we have no conflicting rules (all accepted rules predict the same value of $g_0^{(pr)}$) everything is very simple: this value is the value we predict at $n = 0$. If we have conflicting rules (rules which predict different values of g), the situation is more complicated, and a conflict resolution strategy must be developed. This is a special problem which has been considered in a number of publications. (See Refs. (Brownstown et al, 1985; Durkin, 1994; Lucas and Van Der Gaag, 1991) for review.) Most studies focus on resolving conflicts between hand–crafted, rather than automatically generated rules. The conflict resolution of automatically generated rules has its own specifics. The simplest approach is to accept only one (the best) rule. The problem is the fact that it is common to have a number of rules of similar quality, and the idea of taking a single rule and leaving a number of rules of similar quality out of consideration often causes a significant bias in data analysis. An approach often used to resolve such conflicts is the idea of ordering rules, but it gives away an extremely useful property of rules–based predictions — the ability to evaluate rules in arbitrary order.

The approach we use in this paper differs from the ones mentioned above in a very significant way. We assume that all accepted rules must be incorporated into the prediction formula. If we do not have conflicting rules prediction quality usually increases by combining all rules. If we do have conflicting rules, prediction quality may decrease (often in a very significant way) when the rules are combined.

For resolving the problem of conflicting rules consider the following problem: Let s be a set of observations on which the value of f from (1) is true. The $P(s)$ is the probability of an observation to give true value of f and $P(g = g_0^{(pr)} \Big/ s)$ is the probability of an observation to have g equal to $g_0^{(pr)}$ under the condition that the observation belongs

to s. Note that these two probabilities are just equal to $P(f = true)$ and $P(g = g_0^{(pr)} \Big/ f = true)$ respectively, but for conflict resolution it is much more convenient to work with a set of observations than with individual rules. The problem of resolving conflicting rules is equivalent to the following: For a number of sets s_q, $q = 1 \dots Q$ determines probabilities of different outcomes of g under the condition that all s_q are true. For a single rule ($Q = 1$) the answer is trivial: this is either $P(g = g_0^{(pr)} \Big/ s)$ or $P(g = g_0^{(pr)})$ depending on whether we accepted or rejected a rule. For more than one rule ($Q > 1$), a formal answer can be also written: this is either $P(g = g_0^{(pr)} \Big/ s_1 \cap s_2 \cap \dots \cap s_Q)$ or $P(g = g_0^{(pr)})$ depending on whether we accepted the rules or not. The problem is that the probability $P(g = g_0^{(pr)} \Big/ s_1 \cap s_2 \cap \dots \cap s_Q)$ cannot even be estimated because the set $s_1 \cap s_2 \cap \dots \cap s_Q$ often has few observations, insufficient for probability calculation. There is an example of this: Assume we have 100 observations of g and 101 observations of $x^{(m)}, m = 1 \dots 2$, in the point to predict antecedent $\mathbf{x} = (true, true)$. Let g take the value of $true$ on 50 observations and $false$ on the other 50. Suppose we have two implication rules $(x^{(1)} = true) \to (g = false)$ and $(x^{(2)} = true) \to (g = true)$; both give perfect prediction (correctness and coverage are equal to 1) on these 100 observations. What will be the probability of different values of g in the point to predict $\mathbf{x} = (true, true)$? We have two perfect rules. The first one predicts $g = false$, and, the second one predicts $g = true$. The probability $P(g = g_0^{(pr)} \Big/ s(x^{(1)} = true) \cap s(x^{(2)} = true))$ cannot be calculated because we have no observation with known g when $x^{(1)} = true$ and $x^{(2)} = true$ simultaneously.

To resolve such conflicts we build a set S from all s_q sets and then apply a quality criterion to a single "combined" rule which is defined on S. This way the problem of conflicting rules is resolved by introducing a new, "combined" rule, and the answer is the same as the one mentioned above for a single rule: The probability is either $P(g = g_0^{(pr)} \Big/ S)$ or $P(g = g_0^{(pr)})$ depending on whether we accepted or rejected a combined rule. Having only one rule we may use a number of different criteria to evaluate this "combined" rule quality; for example, in addition to criterion (4) we may use χ^2 criterion or any other criteria. Different criteria usually give similar results in the case of a single rule (because adjustment of acceptance level does not affect how many rules will be accepted/rejected: we have only one rule to consider). It should be stressed here that the quality of combined rule may be lower than

individual rule quality. If this happens this often indicates the presence of rule conflicts or data overfitting.

The only problem left to discuss is how to obtain the set S from individual sets s_q. There is no universal way to do this, because the sets s_q are sensitive to the quality criteria.

The simplest way is to choose the set S as a union of all s_q

$$S = s_1 \cup s_2 \cup \ldots \cup s_Q \tag{6}$$

Returning to a simple example above with two perfect conflicting rules: the set $S = s(x^{(1)} = true) \cup s(x^{(2)} = true))$ covers all 100 observations and the criterion (4) produces 0.5 value (0.5 correctness with 1.0 coverage), which is a very low value. The "combined" rule must be rejected and unconditional probabilities $P(g = g_0^{(pr)})$ should be used for prediction. This is what we intuitively expect in such an extreme case of conflicting rules. There are several other ways to select the set of observations S. We will not discuss all the variants here. The way to select S in (6) form seems to work the best for the quality criterion (4). In addition to that the (6) way to select S is well protected against data overfitting, because overfitted rules often produce different values of g which drastically reduce combined rule quality.

Let us return to the original problem we formulated in the beginning of section 2. Now we can present an algorithm for predicting the value of consequent at $n = 0$.

1. Select acceptance level α_0.
2. Initialize set S to an empty set.
3. For every set of antecedent indexes $\{\mu\}$ (totally there are 2^M sets) do:
   a) Build implication (2) and evaluate quality α of it.
   b) If $\alpha > \alpha_0$ add all observation points for which f from Eq. (1) is true to the set S.
4. Evaluate the quality of a "combined" rule: the rule which is defined on observations from S. This can be done by using the same criterion (4), χ^2 or any other type of criterion. If the combined rule is accepted use $P(g = g_0^{(pr)} \Big/ S)$, if rejected use $P(g = g_0^{(pr)})$ probability to predict the fact of g taking value $g_0^{(pr)}$ at $n = 0$. The predicted value $g_0^{(pr)}$ corresponds to the event with maximal probability.

The algorithm described above is of exponential complexity (one needs to check 2^M possible implication rules). As we will show in section 5 the

complexity may be significantly reduced in an average case. Before we start discussing computational complexity let us discuss the procedure of attributes selection for antecedent and consequent.

4. Selection of attributes for analysis

In all of the considerations above, we always assumed that consequent g and antecedent components $x^{(m)}$ are Boolean attributes. There are many cases in which the data contain attributes of other types. In addition to Boolean variables in this paper we consider continuous variables (variables taking values from an interval) and discrete (literal) variables (variables taking values from a finite set of possible values). The requirement of ordering (so we can compare the values which the variable takes) is very important for analysis, because this allows us to build an effective algorithm of levels selection. The case with non–ordered values is much less interesting, because in this case for a descrete variable the algorithm described above will use the following Boolean attribute: whether the value of the attribute is equal to its value at $n = 0$ or not.

Let us consider a variable (continuous or discrete) r_n (index $n = 0 \dots N$ enumerates the observations) taking values from some ordered set (for example an interval). We convert r_n to a number of Boolean attributes which will be used as the components of vector $\mathbf{x}$. This transformation is performed by selecting a grid $y_l, l = 1 \dots L$ and comparing the value of r with levels y_l, that gives antecedent components $x_n^{(m(l))} = r_n \leq y_l$. The question is how to select levels y_l to use in implication. The most commonly used approach is to take a single level. People usually do this because an increase in the number of levels increases the number of antecedent components that can drastically increase computational complexity. The most common criterion used for selection of the split level is information gain criterion. In several works (Dougherty et al, 1995; Quinlan, 1996) this criterion was successfully applied for determination of levels of comparison.

We propose a new approach for antecedent attributes selection. The major new characteristics of proposed approach is integration of two usually independent steps into one step, so the inference algorithm described in section 3 will perform not only data analysis, but will also select levels to compare.

We do not limit ourselves to one or two levels that we can compare with; we use a number of levels (the value of L can be chosen pretty high) and determine the real levels to use directly during data analysis.

One may think about this as automatic selection of levels in singleton Mamdani rules in fuzzy logic, see (Mamdani and Assilian, 1975).

The first step is to take an ordered ($y_l < y_{l+1}$) grid $y_l, l = 1 \dots L$, which has many different levels. (The levels y_l, may be selected as all possible values of r or by using any of supervised or unsupervised discretization techniques (Dougherty et al, 1995). These levels are only "initial" levels. The inference algorithm will select from these the "real" levels which will be used in implication rules.) Then we obtain L antecedent components $x^{(l)} = r \leq y_l$. The attributes $x^{(l)}$ are not independent. From the fact of ordering of y_l follows that if $x_n^{(l)}$ is true then $x_n^{(p)}$ is also true for $p > l$. Also if $x_n^{(l)}$ is false then $x_n^{(p)}$ is also false for $p < l$.

The second step is to find the highest index l for which $r_0 < y_l$ is false (r_0 is the value of r in the point to predict $n = 0$), and mark this index as h. Then y_l with $l = h, h-1, h-2, \dots, 1$ may be considered as lower boundaries of r and y_l while $l = h+1, h+2, \dots, L$ may be considered as upper boundaries of r. These upper and lower boundaries can be considered as fuzzy levels for r. Instead of determining specific values for upper/lower levels from some *ad hoc* special procedure, we select them during data analysis by using the inference algorithm we described in the previous section. Such integration allows us to automatically select the best level for a rule. While it may look like we have increased the number of antecedent components and exponentially increased computational complexity, this is not really the case. The difference between standard approach (Witten and Frank, 1999) p.246, when a k–valued variable is replaced by $k-1$ synthetic Boolean variables, and our approach is that we incorporate the knowledge about the dependence of these $k-1$ variables into the inference algorithm, In section 5 we show that this knowledge can drastically reduce computational complexity in average case.

The problem of consequent variable selection is usually more straightforward than that for antecedents. If consequent j is a Boolean (literal variable with two values) nothing special should be done about consequent selection and we use j as consequent g. If j is an ordered (continuous or discrete) variable then we take a grid $y_l, l = 1 \dots L$, $y_{l+1} > y_l$ and just run the analysis for every $g = (j < y_l)$. Additional testing on monotonic increase of the predicted probability of $true$ value of g with increase of l may be performed to test the consistency of the predictor. The algorithm in section 3 can also be applied to g taking more than two values, because the quality criterion (4) may be generalized to such g.

5. Estimation of computational complexity for brute force rules analysis

As we showed in section 3, a brute force algorithm is of exponential complexity (it requires 2^M rules evaluation). However, the implication rules we consider are not independent. It is often possible to determine from one rule's characteristics that a set of rules does not have a member of required quality, so that set of rules can be taken out of consideration. The requirement of preventing data overfitting also helps because it eliminates rules that are too complex. In addition some optimization techniques can be applied. This way we can often perform brute force analysis for a problem with a significant number of components.

Let us discuss the properties which allow us to reduce computational complexity.

1. Preventing data overfitting. This usually requires taking out of consideration overly complex rules. We do this by considering only rules with less that M_{max} terms ($M_{max} < M$) in implication (2). This immediately reduces the number of rules to consider from 2^M to $C_M^0 + C_M^1 + \ldots + C_M^{M_{max}} \approx \frac{M^{M_{max}}}{M_{max}!}$ which is still too high.

2. Taking into account dependent antecedent components. In this paper we consider the simplest case: upper and lower boundary antecedent variables as we build them in section 4.

   Antecedent attributes as we build them in section 4 from variable r (which takes values in some ordered set) are not independent. For example the components of lower boundary $r_n < y_l$ with $l = h, h-1, h-2, \ldots, 1$ have the following property

$$\left(x_n^{(m(l_1))} = x_0^{(m(l_1))}\right) \& \left(x_n^{(m(l_2))} = x_0^{(m(l_2))}\right) = \left(x_n^{(m(l_3))} = x_0^{(m(l_3))}\right) \tag{7}$$

$$l_3 = \max(l_1, l_2) \tag{8}$$

   The property (7) follows from the fact of ordering of y_l, the way of h selection which leads to $x_0^{(m(l_1))} = x_0^{(m(l_2))} = false$ and the following equation:

$$(r < a)\&(r < b) = (r < \min(a, b)) \tag{9}$$

   An equation very similar to (7) can be also written for upper boundary set $r_n < y_l$ with $l = h+1, h+2, \ldots, L$. This means that only one attribute from the upper(lower) boundary set needs to be included

in implication (2). If we put two components from the upper(lower) boundary set of attributes then, by applying a (9) type of transformation, we can always replace two terms by a single one. This property, which is known directly from the antecedent, allows us to reduce the number of implications we need to consider. Increase in computational complexity when adding one set with n_d dependent antecedent components selected as described above in terms of computational complexity is equivalent to adding much fewer (about $\log_2(n_d+1)$) independent components. This is why we can integrate selection of fuzzy levels with the inference algorithm without much increase in computational complexity. Addition of L levels to test is equivalent to adding about $\log_2(h+1)+\log_2(L-h+1)$ independent Boolean attributes.

3. If an implication rule of (2) form has a perfect (or close to perfect) correctness, then the quality of this rule can not be improved by adding more elements to set $\{\mu\}$ (see (Riddle et al, 1994)), because by adding more conditions we just decrease coverage while correctness cannot be further improved. This means we do not need to consider the subsets of rules with close to perfect correctness.

4. As it has been shown in (Riddle et al, 1994), an implication rule (and all rules which include it) with coverage below some level cannot produce a rule of the required quality. This requirement can be slightly improved by using minimal probability $p^{(v)}$ for every consequent value (the $v \in \{true, false\}$ is one of two possible consequent values). Specifically, for at least one v we must have $P((g = v)\&(f = true)) > p^{(v)}$. If we have no single v for which this condition holds, then the implication (and all rules which include it) cannot produce a rule of the required quality. For the quality criterion (4) the value of $p^{(v)}$ can be easily obtained

$$p^{(v)} = \frac{(\alpha_0 - \lambda)P(g = v)}{1 - \lambda} \tag{10}$$

5. An implication rule must not have redundant conditions. An extreme example of redundant condition is a situation when a term $x_n^{(m(l))} = x_0^{(m(l))}$ is added to implication (2) twice. This does not change any property of a rule, it just increases the complexity of it. To check for redundancy of a rule with m conjunctions we may compare the rule with m rules obtained by taking out one condition from the original rule, see section 7.3.13 (page 318), Ref. (Hájek and Havránek, 1978). Specifically in our case this criterion can be formulated as following: Having a $\{\mu\}$ set with m elements consider

m formulas f_m of (1) type, each one is obtained by taking out one of m element. If for at least one f_m there is no v for which the condition $P((f_m = true)\&(f = false)\&(g = v)) > p^{(v)}_{mism}$ holds, then this rule (and all rules which include it) have redundant conditions and should not be considered. The value of $p^{(v)}_{mism}$ can be obtained from the same formula (10) which was used for $p^{(v)}$. The only difference is the different value of threshold α_0. For mismatches, the threshold α_1 is usually chosen lower that α_0.

The five properties presented above allow us to build an algorithm of polynomial complexity. This comes from the fact that we are interested only in rules applicable at $n = 0$, what reduces the number of rules to consider from 2^{2^M} to 2^M and from the properties 4 and 5 which limit the maximal tree depth in a typical case. In the worst case the tree depth is limited by the value of M_{max} from item 1. The other properties reduce the complexity further. This algorithm, which in typical case is of polinomial complexity on N and M, can be applied for solving a variety of practical problems.

The algorithm can be applied to a brute force analysis for a problem with a significant number of components. A sketch for the algorithm is the following: All possible implication rules may be represented as a tree. Each node has an antecedent index assigned to it. Every node can be mapped to a $\{\mu\}$ set (by taking indexes of this node and all its ancestors). This property means that if node A is an ancestor of node B, then $f_B = f_A\&X$ where f_A and f_B are formulas of (1) type obtained from a $\{\mu\}$ set corresponding to nodes A and B respectively, that allows us to implement the algorithm as a recursive tree scanning algorithm and directly incorporate five properties above as indicators for a branch not having a rule of the required quality. We discuss different applications in section 7.

6. Predictor: error estimation

An estimation of predictor correctness usually involves building a global rule on training data and then evaluating this rule's quality on testing data. While this testing approach suits well for testing global rules, it is not very convenient when considering local rules, because for every prediction point we may have different local rules. It is nice to know the quality of a local rule, but this information is not useful for error estimation at the other prediction points.

The best way to perform testing in such a case is to test the average performance of the predictor. One may consider a predictor as some

kind of "global rule" and estimate its quality. The quality of such a "global rule" is equivalent to the predictor average quality.

A common problem of errors estimation is the limited number of observations. Techniques such as bootstrap and cross–validation are commonly used for performing error estimation with a limited number of observations.

For local predictors, a leave–one–out type of cross–validation is very promising when working with a limited number of observations. This type of testing includes creation of a set with $N-1$ observations and this data is used for predicting the value at one left point with known value of g. The procedure is repeated N times and average predictor performance is obtained. Mentioned in (Witten and Frank, 1999) the non–stratification problem of testing data (the data in every testing set has only one observation and does not have the right proportions of observations with different values of g) is much less an issue in the case of local predictions than in the case of global predictions, because the predictor was specifically built to be applicable at the point where it tested.

In case we have plenty of data, we can estimate predictor average performance without leave–one–out cross–validation. The fact of the local nature of the predictor should be taken into account when performing the tests. Assume we have a training set of N observations and testing set of T observations. To determine predictor average performance we predict the value for every observation in a testing set using all the observations from the training set. In total we run predictor T times (for every observation from testing set) each time using the same training set with N observations and estimate predictor average performance from these T predictor runs. Predictor average correctness C is defined as:

$$C = \sum_{j=true,false} p_{jj} \tag{11}$$

$$p_{jk} = \frac{t\left((g=j)\&(g^{(predicted)}=k)\right)}{T} \tag{12}$$

The probabilities in (11) are calculated in the testing space; the value of $t\left((g=j)\&(g^{(pr)}=k)\right)$ is the number of tests (totally there are T test runs) when the value of the consequent which really happened was equal to j and the predicted value was k.

One of the problems with (11) and similar types of criteria is its dependence on unconditional probabilities of different outcomes of g. For example, if we have an event which happens in 1 out of 100 cases,

then a predictor predicting that the event will never happen has 0.99 correctness. This high value of correctness is not a result of predictor quality but of the distribution of g. One may use information gain based criteria, but using several criteria simultaneously complicates the analysis. This problem does not arise when the (11) criterion is used for relative comparison of different predicting techniques on the same data, because in this case we have identical distribution of g.

7. Results of data analysis

The real algorithm has a number of features not presented in the basic algorithm description which we gave in sections 3, 4 and 5. These are some of them:

1. The acceptance level α_0 is dynamically adjusted. First we set an initial acceptance level. Then, during tree scanning, required acceptance level gets automatically increased to $\kappa\alpha$ if we find a rule with quality α such us $\alpha_0 < \kappa\alpha$, i.e. we keep only rules with quality better than κ fraction of the best rule quality; all rules with the quality below this value are pruned. The value $\kappa = 1$ corresponds to the case when only the best rule is accepted.

2. Dependent variables are also handled in a slightly more complex way than described because of additional optimization.

These and other details which are not described here make the algorithm practical. This algorithm was implemented in the MLS program (Massive Local Search), the complete source code of which is available from (Malyshkin, 2000).

The following parameters were used during all trials. The parameter λ in quality criterion (4) was set to 0.75 making correctness more important than coverage. The maximal tree depth M_{max} was set to 8. The c_{min} was set to 0.08, i.e. we accept only rules with quality better than the quality of a perfectly correct rule covering 0.08 of positive samples (with the exception of Chess, Mushroom, Spambase for which $c_{min} = 0.17$ was used). The minimal number of mismatches (item 5 in section 5) was also determined on a base of minimal coverage; the value of $c_{min}^{(mism)}$ was set to 0.02 (with the exception of Chess, Mushroom, Spambase for which $c_{min}^{(mism)} = 0.1$ was used). This threshold stayed the same during tree scanning and was not adjusted as it was for the matches.

For non–ordered input variables antecedent components were built as a fact of the exact match of variable value with its value at a point to predict. For ordered input variables (with the exception of Ionosphere and Spambase for which we used exact match variables) antecedent

components were built as described in section 4. For ordered literal variables we used all possible values as initial levels y_l, $l = 1 \dots L$. For continuous variables a discretization was performed first to build ordered literal variables, then the same attribute selection procedure used for ordered literal variables was applied. The initial levels for continuous attributes may be selected in a number of different ways, for sufficiently big L different supervised and unsupervised techniques give very similar results for predictor quality. From a computational complexity point of view it is good to have low values of L. The entropy based discretization (Dougherty et al, 1995) gives a very good balance of quality and levels numbers. In this work the entropy based discretization from (Dougherty et al, 1995) was used for initial selection of levels y_l for continuous variables, then the procedure described in section 4 was applied. The utility we used is available from (Kohavi et al, 1997).

A rich collection of data from UCI repository (Blake and Merz, 1998) allows a comprehensive data analysis on data from different domains to be performed. Predictor correctness was estimated using 3–fold cross–validation with stratification. Obtained results were compared with ones produced by widely used program C4.5R8 (Quinlan, 1992) with default settings. In Table I we present the comparison of MLS with C4.5R8. For comprehensive comparison with the other predicting techniques we refer to (Lim et al, 2000; Zheng and Webb, 2000; Gama and Brazdil, 2000), where a variety of predicting techniques were tested on the same data from UCI repository. The error estimation from these works can be directly compared with ones from Table I of this paper, which allows our technique to be easily compared with the other predicting techniques.

The exceptions mentioned above in algorithm parameter values for some datasets (Chess, Mushroom and Spambase) were required to reduce computation time. The higher values of c_{min} and $c_{min}^{(mism)}$ the earlier tree scanning algorithm, will reach termination criteria.

The first column of Table I identifies the data set. The second and third columns contain predictor correctness C for C4.5R8 and our program MLS respectively. The fourth column contains the total number of observations. (These are needed for calculation of correctness error due to the finite number of tests run. For a given confidence level and number of tests run the lower boundary of C can be estimated using standard statistical technique (Schervish, 1995). We do not demonstrate this analysis here because we are interested only in comparison of two predicting techniques.) The number of antecedent variables is presented in the last column. This value is for estimation of computational complexity. (Note that the number of antecedent components typically higher than the number of variables because the methodology

Table I. MLS and C4.5R8 performance comparison.

data	C4.5R8	MLS	$N_{observations}$	$N_{variables}$
Monk1	1.0	1.0	432	6
Monk2	0.65	0.71	432	6
Monk3	1.0	0.972	432	6
Breast-cancer	0.73	0.69	286	9
Chess	0.99	0.90	3196	36
Crx	0.82	0.86	690	15
Diabetes	0.74	0.78	768	8
Hepatitis	0.75	0.86	155	19
Horse-colic	0.8	0.81	368	22
Ionosphere	0.90	0.90	351	34
Labor-neg	0.72	0.81	57	16
Mushroom	1.0	0.96	8124	22
Pima	0.74	0.77	768	8
Spambase	0.92	0.87	4601	57
Tic-tac-toe	0.985	0.99	958	9
Vote	0.96	0.96	435	16

from section 4 usually gives several antecedent components for a single variable.)

The trials are usually executed much faster in C4.5R8 than MLS. First, because C4.5R8 is written in C while our program MLS is written in Java. Second, because we need to re–run the predictor for every test (lazy learning), while C4.5R8 does this only once (eager learning). This slowdown is important only when doing predictor testing, because we are especially interested in the tasks when just a few predictions, not about the same number as the training set, is necessary. Third, massive search algorithms are generally slower than decision tree "divide and conquer" type of algorithms. Despite running more slowly, the proposed algorithm is fast enough to solve practical problems.

The Monk1, Monk2 and Monk3 are the problems usually tried first by different predictor algorithms. From Table I it follows that on monk tests MLS performs about the same or slightly better than C4.5R8.

On Chess MLS performs noticeably worse that C4.5R8. This is because the values of c_{min} and $c_{min}^{(mism)}$ used for this trial effectively reduce maximal tree depth to a value of about 4. At the same time, C4.5R8 generates a number of rules with more than 10 conditions. This Chess problem is an example of a problem for which massive search approach

is not effective: a large number of attributes produce complex rules. A similar effect (but to much lower degree) occurs in the Mushroom trial.

On Crx, Diabetes, Hepatitis, Horse-colic, Labor-neg, Pima, Tic-tac-toe and Vote MLS performs about the same as or better than C4.5R8. These trials also have significant number of attributes, but the rules do not have too many conditions, and global optimization algorithm easily catches the best rule(s) without any major slowdown in calculations.

Our tests also show that in some trials different values of c_{min} (minimal coverage) and parameter $\lambda = 0.75$ from Eq. (4) (relative importance of quality and correctness) may result in better correctness than presented in Table I. The higher c_{min} the higher is the required quality for a rule to be accepted. As shown in section 5, the value of c_{min} affects computational complexity. The increase of c_{min} and $c_{min}^{(mism)}$ decreases computational complexity by reducing the effective tree scanning depth. We expect that automatic adjustment of parameter λ and required minimal coverage c_{min} based on available data will make noticeable improvement to MLS.

In addition to predictor quality on different datasets another thing we are interested in testing is an effect of attribute selection methodology from section 4 to predictor quality. To test this we ran the predictor twice on some datasets: the first time all antecedents were selected as a fact of exact match of variable value with its value at a point to predict, and the second time all antecedent components (even if they correspond to non–ordered attributes) were selected as a comparison with upper and lower levels in the way described in section 4. Note that the former selection can be always obtained from the latter one because the condition $r = a$ is the same as $(r \leq a)\&(r > a - 1)$ (here the variable r assumed taking integer values from an interval). This way we tested how the quality of a predictor is affected by the increase of rule expressive power when we go from "exact match" type of attributes to the type of attributes built in the way described in section 4. We performed this testing on five datasets with ordered attributes (in Monk1, Monk2 and Monk3 the structure of attributes values allows the variables being considered as ordered, and in Pima and Diabetes the attributes are ordered), and two datasets with literal non–ordered attributes (Tic-tac-toe and Vote). The results are presented in Table II

From these trials it follows that for datasets with ordered attributes (Monk1, Monk2 and Monk3) the transition from "exact match" to "levels comparison" may significantly increase predictor quality. In Monk2 no single rule found for an exact match (because we require high enough minimal coverage for a rule), but increased expressive power of generated rules allows us to generate high quality rules which obey the condition of minimal coverage. At the same time in trials where

Table II. Predictor results for "exact match" and "level comparison" type of attribute selection for MLS.

data	Exact Match	Levels Comparison
Monk1	1.0	1.0
Monk2	-	0.71
Monk3	0.972	0.972
Pima	0.76	0.77
Diabetes	0.78	0.78
Tic-tac-toe	0.99	0.82
Vote	0.96	0.94

antecedent attributes were obtained as a result of entropy discretization (Diabetes and Pima) there is no strong effect of automatic selection of upper/lower boundaries. Because of computational complexity for Ionosphere and Spambase we did only "exact match" type of attribute selection trials, but preliminary results show that "exact match" type of attributes may produce even better results than "levels comparison".

For the datasets with non-ordered attributes (Tic-tac-toe and Vote, for which we forced non-ordered variables being considered as ordered) such transition may either not affect or even decrease predictor quality. This is because increased expressive power of the rules may cause an effect similar to data overfitting. The most clear example is Tic-tac-toe trial, where the global optimization algorithm finds many "false rules", a combination of conditions which by chance happened to give a high value of quality criterion. Such "false rules" can be significantly reduced by increasing the value of minimal coverage.

From these trials it follows that the approach to antecedent attributes selection from section 4 may give better results only for ordered attributes, and even in this case an "exact match" of attributes may produce better results in some instances.

Presented test trials show that the massive search algorithm often performs about the same or better than C4.5R8 on many datasets. We attribute this to global optimization. There are also cases when MLS is less effective than decision tree "divide and conquer" type of algorithms. This usually happens on the datasets with a large number of attributes producing complex rules.

8. Discussion

The described approach proves that a massive local rules search global optimization algorithm can be applied to problems with a significant number of attributes. The computational complexity can be greatly reduced by building rules which are specific to a prediction point and by using the optimization technique described above. The massive search algorithm is guaranteed to find the global maximum which makes it especially valuable for testing various predicting systems.

In this work we have shown that the process of attributes selection can be integrated with the process of rules search. This allows us to perform data analysis in a uniform way without separation of the attribute selection and the rules search stages. From a fuzzy logic approach this may be considered as automatic selection of levels in singleton Mamdani rules (Mamdani and Assilian, 1975). Such a method of attribute selection usually allows us to build more "expressive" rules. This is related to the fact that in many problems the comparison of the value with a level is a natural method of attribute selection for the problem.

Another distinctive feature of the proposed algorithm is a conflicting rules resolution strategy. We accept a number of rules, then build a single rule for prediction based on accepted rules. The quality of this single rule may significantly decrease if accepted rules predict different values of consequence.

While the described approach is already practical and was applied in the solution of a number of different problems, it can be further improved. From our point of view there are two improvements which would improve the algorithm. Firstly, the quality criterion (4) is different than commonly used criteria. The major advantage of the criterion is the fact that its calculation can be optimized. The problem of probability calculation of a logical expression is a problem actively studied from a computational complexity point of view, see (Abraham, 1979; Heidtmann, 1989; Bertschy and Monney, 1996; Gorodetsky and Dubarenko, 1997; Anrig, 2000) and references therein. Because calculation of (4) is equivalent to calculation of a probability various optimizations used in reliability theory (Limnios and Nikulin, 2000) can be applied. Another improvement which can be added to the algorithm is automatic selection of minimal coverage c_{min} and relative importance of coverage and correctness λ. A flexible selection of these parameters often improves the results. These improvements, in our opinion, can further increase the correctness and decrease the computational complexity of the algorithm.

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