Robust Rule-based Prediction

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Abstract

This paper studies a problem of robust rule-based classification, i.e. making predictions in the presence of missing values in data. This study differs from other missing value handling research in that it does not handle missing values but builds a rule based classification model to tolerate missing values. Based on a commonly used rule-based classification model, we characterise the robustness of a hierarchy of rule sets, *k*-optimal rule sets with the decreasing size corresponds to the decreasing robustness. We build classifiers based on *k*-optimal rule sets and show experimentally that they are more robust than some benchmark rule-based classifiers, such as C4.5rules and CBA. We also show that the proposed approach is better than two well known missing value handling methods for missing values in test data.

keywords: Data mining, rule, classification, robustness.

1 Introduction

Automatic classification has been a goal for machine learning and data mining, and rule-based methods are widely accepted due to their easy understandability and interpretability. In the last twenty years, rule-based methods have been extensively studied, for example, C4.5rules [20], CN2 [7, 6], RIPPER [8], CBA [16], CMAR [15], and CPAR [23].

Most rule-based classification systems make accurate and understandable classifications. However, when a test data set contains missing values, a rule-based classification system may perform poorly because it may not be robust. We give the following example to show this.

Example 1 Given a well-known data set listed in Table 1, a decision tree (e.g. ID3 [19] can be constructed as in Figure 1.

No	Outlook	Temperature	Humidity	Wind	Play
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

Table 1: A training data set

The following 5 rules are from the decision tree.

- 1. If outlook is sunny and humidity is high, then do not play tennis.
- 2. If outlook is sunny and humidity is normal, then play tennis.



Figure 1: A decision tree from the training data set

- 3. If outlook is overcast, then play tennis.
- 4. If outlook is rain and wind is strong, then do not play tennis.
- 5. If outlook is rain and wind is weak, then play tennis.

We note that all rules include the attribute outlook. Suppose that the outlook information is unknown in a test data set. This rule set makes no predictions on the test data set, and hence is not robust. It is possible to have another rule set that makes some predictions on the incomplete test data set.

In real world applications, missing values in data is very common. In many cases, missing values are unrecoverable due to unrepeatable procedures or high cost of experiments or surveys. Therefore, a practical rule-based classification system has to be robust for missing values.

One common way to deal with missing values is to estimate and replace them [18], called imputation. Some typical imputation methods are: mean imputation, prediction imputation, and hot deck imputation [3]. Imputation methods are dominating in classification. For categorical attributes, the following three imputation methods are commonly used: most common attribute value substitution [7], local most common attribute value substitution [20]. In a recent study [3], k-nearest neighbor substitution method is shown as the most accurate

imputation method.

In this paper, we discuss an alternative approach to deal with missing values. Instead of imputing missing values, we propose to build robust rule based classification models to tolerate missing values. An imputation method is to "treat" missing values, but the proposed method is to make a system "immunise" from missing values to certain degree.

Treating missing values can be effective when users know the data very well, but may lead to misleading predictions when a wrong value is imputed. For example, when a missing value female is imputed by value male, misleading prediction on the record may occur. In the worst case, the errors of a classification model and the errors of an imputation method are additive. In contrast, the proposed method does not impute missing values, and hence does not incur errors from the missing value estimation.

We will discuss how to build robust rule-based classifiers that tolerate missing values. A rule based classifier built on our method has been shown to be more accurate than two benchmark rule based classifications systems, C4.5rules [20] and CBA [16] on incomplete test data sets. We also show that the classifier is more accurate than C4.5rules plus two imputation methods respectively. A preliminary study appeared in [14], and this is a comprehensive report with a significant extension.

This paper primarily characterises the relationships between the size of rule sets and their tolerative capability for missing values in test data. The theoretical conclusions are very useful for selecting right rule sets to build rule based classifiers. The paper also shows that building robust classifiers is a good alternative to handling missing values.

The rest of the paper is organised as follows: Section 2 defines class association rules and their accuracies. Section 3 defines the optimal rule set and discusses its robustness. Section 4 defines k-optimal rule sets and discusses their robustness. Section 5 presents two algorithms to generate k-optimal rule sets. Section 6 demonstrates

k-optimal rule set based classifiers are more robust than some benchmark rule-based classifiers. Section 7 concludes the paper.

2 Class association rules and accuracy estimation

In this section, we define class association rules and discuss methods to estimate their accuracy.

Note that rules used to the final classifier are only a very small portion of a class association rule set. I strongly argue that the optimal class association rule set [13] should be a proper base to build rule based classifiers. In this paper, we start with the complete class association rule set and then move to the optimal class association rule set to make the connection and distinction between our work and other works clear.

We use association rule concepts [1] to define class association rules. Given a relational data set D with n attributes, a record of D is a set of attribute-value pairs, denoted by T. An attribute is dedicated to class labels. Or every tuple has one class. A *pattern* is a set of attribute-value pairs. The *support* of a pattern P is the ratio of the number of records containing P to the number of records in the data set, denoted by $\supp(P)$. An *implication* is a formula $P \to c$, where P is a pattern and c is a class. The support of the implication $P \to c$ is $\supp(P \cup c)$. The confidence of the implication is $\supp(P \cup c) / \operatorname{supp}(P)$, denoted by $\operatorname{conf}(P \to c)$. The covered set of the rule is the set of all records containing the antecedent of the rule, denoted by $\operatorname{cov}(P \to c)$. We say $A \to c$ is a *class association rule* if $\operatorname{supp}(A \to c) \ge \sigma$ and $\operatorname{conf}(A \to c) \ge \phi$, where σ and ϕ are the minimum support and confidence respectively.

Definition 1 The complete class association rule set is the set of all class association rules that satisfies the minimum support and the minimum confidence.

Given a data set D, the minimum support σ and the minimum confidence ϕ , the complete class association rule set is denoted by $R_c(\sigma, \phi)$, or simply R_c .

Notations	Meanings	Defined in
R_c	the complete class association rule set	Section 2
R_{opt}	the optimal class association rule set	Section 3.1
R_k	a k-optimal class association rule set	Section 4
R_{min}	when $k = 0$	Section 4
cond(r) and $cons(r)$	the antecedent (conditions) and the consequence of rule r	Section 3.1
$\operatorname{supp}(A \to c)$	the support of rule $A \rightarrow c$	Section 2
$\operatorname{conf}(A \to c)$	the confidence of rule $A \rightarrow c$	Section 2
$\operatorname{acc}(A \to c)$	an estimated accuracy of rule $A \rightarrow c$	Section 2
$\operatorname{cov}(A \to c)$	the cover set of rule $A \rightarrow c$	Section 3.1

Table 2: Some frequently used notations in the paper

We list some frequently used notations of this paper in Table 2 for the fast referral.

In classification study, the basic requirements of a rule are accuracy and coverage. More specifically, a rule covers few negative records in the training data set and identifies certain number of records that have not been identified by other rules. The formal definition of "identify" will appear in the next section. A classification rule generation algorithm usually uses implicit minimum accuracy and support requirements. For example, the accuracy of a classification rule is generally very high, and those small coverage rules are more likely to be removed in the post pruning. Hence the minimum thresholds in the above definition should not cause problems in practice.

In practice, predictions are made by a classifier. A classifier is a sequence of rules sorted by decreasing accuracy and tailed by a default prediction. In classifying an unseen record without class information, the first rule that matches the case classifies it. If no rule matches the record, the default prediction classifies it.

An estimation of rule accuracy is important since it directly affects how rules are used in the prediction. There are a few ways to estimate rule accuracy. Laplace accuracy is a widely used estimation [6]. We rewrite the Laplace accuracy in terms of support and cover set as follows.

$$\operatorname{Laplace}(A \to c) = \frac{\operatorname{supp}(A \to c) \times |D| + 1}{|\operatorname{cov}(A \to c)| + |C|}$$

where |C| is the number of all classes, $\operatorname{supp}(A \to c) \times |D|$ is the number of correct predictions made by the rule on the training data and $|\operatorname{cov}(A \to c)|$ is the number of reords containing the antecedent of the rule in the training data.

Quinlan used the pessimistic error rate in rule pruning [20]. We present the pessimistic error as the pessimistic accuracy in the following.

Pessimistic
$$(A \to c) = 1 - \frac{f + \frac{z^2}{2N} + z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}}}{1 + \frac{z^2}{N}}$$

where $f = 1 - conf(A \rightarrow c)$, $N = |cov(A \rightarrow c)|$, and z is the standard deviation corresponding to a statistical confidence c, which for c = 25% is z = 0.69.

Other interestingness metrics [21], such as, Chi-square test, can be used to compare predictive power of association rules. Our intention is not to discuss which estimation is the best in this paper. The accuracy of a rule can be estimated by a means. We represent the accuracy of rule $A \rightarrow c$ as $acc(A \rightarrow c)$. We used Laplace accuracy in our experiments.

Usually, the minimum confidence of a class association rule is high so it naturally excludes conflicting rules, such as $A \rightarrow y$ and $A \rightarrow z$, in a complete class association rule set.

We will consistently discuss class association rules in the rest of the paper. For the sake of brevity, we omit class association in the following discussions.

3 The optimal rule set and its robustness

3.1 Ordered rule-based prediction model and the optimal rule set

In this section, we first formalise the procedure of rule-based classification and then define the optimal classification rule set.

We start with some notations. For a rule r, we use cond(r) to represent its antecedent (conditions), and cons(r) to denote its consequence. Given a test record T, we say rule r covers T if $cond(r) \subseteq T$. The set of records that are covered by a rule r is called the cover set of the rule, denoted by cov(r). A rule can make a prediction on a covered record. If cons(r) is the class of T, then the rule makes a correct prediction. Otherwise, it makes a wrong prediction. Let the *accuracy* of a prediction equal the estimated accuracy of the rule making the prediction. If a rule makes the correct prediction on a record, then we say the rule *identifies* the record.

There are two types of rule-based classification models.

- Ordered rule-based classifiers: rules are organised as a sequence, e.g. in the descending accuracy order. When classifying a test record, the first rule covering the record in the sequence makes the prediction. This sequence is usually tailed by a default class (prediction). When there is no rules in the sequence covering the test record, the record is predicted to belong to the default class. C4.5rules [20] and CBA [16] employ this model.
- 2. Unordered rule-based classifiers: rules are not organised in a sequence and all (or some) rules covering a test record participate in the determination of the class of the record. A straightforward way is to adopt the majority vote of rules like in CPAR [23]. A more complex way is to build a model to compute the combined accuracy of multiple rules. Improved CN2 [6] and CMAR [15] employ this method.

We do not consider committee prediction, e.g. Bagging [5] which use multiple classifiers.

The first model is simple and effective. It makes a prediction based on the maximum likelihood. This is because that rules with higher accuracy usually precede rules with lower accuracy and the accuracy approximates the conditional probability when the data set is large.

There is no uniform form for the second model. Methods of voting vary in different proposals. An important condition for using the second model, independence of rules, is normally not satisfied. For example, in a complete class association rule set, the conditions of most rules are correlated. Further, voting may be bias against small distributed classes.

In this paper, we employ the ordered rule-based classification model. We formalise rule order as follows.

Definition 2 Rule r_1 precedes rule r_2 if 1) $\operatorname{acc}(r_1) > \operatorname{acc}(r_2)$, 2) $\operatorname{acc}(r_1) = \operatorname{acc}(r_2)$ and $\operatorname{supp}(r_1) > \operatorname{supp}(r_2)$, or 3) $\operatorname{acc}(r_1) = \operatorname{acc}(r_2)$, $\operatorname{supp}(r_1) = \operatorname{supp}(r_2)$ and $|\operatorname{cond}(r_1)| < |\operatorname{conf}(r_2)|$.

In the above definition, we take the support and the length of a rule into consideration because they have been minor criteria for sorting rules in practice, such as in [16]. Building a classifier is more complicated than this. We use this simple model to draw some theoretical conclusions, and then verify the conclusions by experiments.

A predictive rule is defined as follows.

Definition 3 Let T be a record and R be a rule set. Rule r in R is the predictive rule for T if r covers T and is the most preceding rule among all rules covering T.

For example, both rule $ab \to z$ (acc = 0.9) and rule $d \to y$ (acc = 0.6) cover record {abcde}. Rule $ab \to z$ is the predictive rule for the record but rule $d \to y$ is not. As both the accuracy and the support are real numbers, in a large data set it is very unlikely that a record is covered by two rules with the same accuracy, support, and length. Therefore, it is a reasonable assumption that each record has a unique predictive rule for a given data set and a rule set, and we use this assumption in the rest of paper.

In the ordered rule-based classification model, only one rule makes prediction on a record, and hence we have the following definition.

Definition 4 *Let the prediction of rule set R on record T be the same as the prediction of the predictive rule in R on T.*

For example, rule $ab \rightarrow z$ (acc = 0.9) predicts record $\{abcdef\}$ to belong to class z with the accuracy of 90%. Rule set $\{ab \rightarrow z \text{ (acc = 0.9)}, d \rightarrow y \text{ (acc = 0.6)}\}$ predicts record $\{abcdef\}$ to belong to class z with the accuracy of 90% since rule $ab \rightarrow z \text{ (acc = 0.9)}$ is the predictive rule.

Some rules in the complete rule set never make predictions on any records, and we exclude them in the following.

Firstly we discuss how to compare predictive power of rules. We use $r_2 \subset r_1$ to represent $\operatorname{cond}(r_2) \subset \operatorname{cond}(r_1)$ and $\operatorname{cons}(r_2) = \operatorname{cons}(r_1)$. We call r_2 is *more general* than r_1 , or r_1 is *more specific* than r_2 . A rule covers a subset of records covered by one of its more general rules.

Definition 5 Rule r_2 is stronger than rule r_1 if $r_2 \subset r_1$ and $\operatorname{acc}(r_2) \geq \operatorname{acc}(r_1)$. In a complete rule set R_c , a rule is (maximally) strong if there is not another rule in R_c that is stronger than it. Otherwise, the rule is weak.

Only strong rules make predictions in the complete rule set. For example, rule $ab \rightarrow z$ is weak because $acc(ab \rightarrow z) < acc(a \rightarrow z)$. Whenever rule $ab \rightarrow z$ covers a record, rule $a \rightarrow z$ does. Since rule $a \rightarrow z$ precedes rule $ab \rightarrow z$, rule $ab \rightarrow z$ never

has a chance to be a predictive rule. Therefore, we have the following definition to exclude weak rules like $ab \rightarrow z$.

Definition 6 The set of all strong rules in the complete rule set is the optimal rule set, denoted by R_{opt} .

A related concept of optimal rule set is non-redundant rule set. A definition of non-redundant association rule sets is presented by Zaki [24] and a non-redundant classification rule set is called an essential classification rule set [2]. The definition of essential classification rule sets is more restrictive than the definition of optimal rule sets. A more specific rule is excluded from an essential rule set only when both its support and its confidence are the identical to those of one of its more general rules. The definition of the optimal rule definition follows the observation that a more specific rule with accuracy lower than that of one of its more general rule does not participate in building an ordered rule based classifier. An optimal rule set is a subset of essential rule set. More detailed discussions on the relationships between optimal rule sets and non-redundant rule sets is characterised in my other work [12].

3.2 Robustness of the optimal rule set

In this section, we first define robustness of rule sets and then discuss the robustness of the optimal rule set.

We use a concept of robustness to characterise the capability of rule set making predictions on incomplete data sets. We say that a rule set gives any prediction on a record with the accuracy of zero when it cannot provide a prediction on the record.

Definition 7 Let D be a data set, and R_1 and R_2 be two rule sets for D. R_2 is at least as robust as R_1 if, for all $T' \subseteq T$ and $T \in D$, predictions made by R_2 are at least as accurate as those by R_1 . For example, let $R_1 = \{ab \rightarrow z \text{ (acc} = 0.9)\}$ and $R_2 = \{ab \rightarrow z \text{ (acc} = 0.9), d \rightarrow z \text{ (acc} = 0.8)\}$. For record $\{abcde\}$, both rule sets predict it to belong to class z with the same accuracy of 90%. When b is missed from the record, R_2 predicts it to belong to class z with the accuracy of 80% whereas R_1 predicts it to belong to class z with the accuracy of 0%. Thus, R_2 is more robust than R_1 .

For a large data set, estimated accuracies of rules approach true accuracies of rules. Consider that rule set R_2 is more robust than rule set R_1 . For a complete test data set both rule sets make predictions with the same accuracy. For an incomplete test data set, rule set R_2 makes predictions at least as accurately as rule set R_1 .

Ideally, we would like to have a rule set to make predictions on any incomplete record, but it is impossible since there may not be a rule in R_c covering every incomplete record. The robustness of a rule set is limited by rules in R_c . On the other hand, this rule set is unnecessarily large. The optimal rule set is a smaller equivalence.

Theorem 1 For any complete class association rule set R_c , the optimal classification rule set R_{opt} is the smallest rule set in size that is as robust as R_c .

Proof All weak rules excluded by the optimal rule set cannot be predictive rules in any cases because they are ordered lower and more specific than their corresponding strong rules that exclude them. On the other hand, every strong rule is a potentially predictive rule. When an incomplete record contains only the antecedent of a strong rule, the strong rule is the predictive rule for the record. Therefore, both the complete rule set and the optimal rule set have the same set of predictive rules, and hence the optimal rule set is as robust as the complete rule set.

Now we prove the minimum property. Suppose that we may omit a rule r from the optimal rule set R_{opt} and the new rule set $R'_o = R_{opt} \setminus r$ is still as robust as the complete rule set R_c . Consider a test record that is covered only by rule r. By the definition of the optimal rule set, there is no rule in R'_o covering the record or at most there are some covering rules with a lower accuracy than r. Hence, the prediction made by R'_o cannot be as accurate as that from R_{opt} . As a result, R'_o is not as robust as R_c , and this contradicts the assumption.

The theorem is proved. \Box

This theorem means that no matter what an input record is (complete or incomplete) the optimal rule set gives the same prediction on the record as the complete rule set with the same accuracy.

Let us look at differences between the complete rule set and the optimal rule set through an example.

Example 2 For the data set in Example 1, there are 21 rules in the complete rule set when the minimum support is 2/14 and the minimum confidence as 80%. However, there are only 10 rules in the optimal rule set, and they are listed as follows. We take confidence as accuracy in this example for easy illustration since otherwise an accuracy estimation method requires a calculator. (Numbers in parentheses are support and accuracy, respectively.)

- 1. If outlook is sunny and humidity is high, then do not play tennis. (3/14, 100%)
- 2. If outlook is sunny and humidity is normal, then play tennis. (2/14, 100%)
- 3. If outlook is overcast, then play tennis. (4/14, 100%)
- 4. If outlook is rain and wind is strong, then do not play tennis. (2/14, 100%)
- 5. If outlook is rain and wind is weak, then play tennis. (3/14, 100%)
- 6. If humidity is normal and wind is weak, then play tennis. (3/14, 100%)
- 7. If temperature is cool and wind is weak, then play tennis. (2/14, 100%)
- 8. If temperature is mild and humidity is normal, then play tennis. (2/14, 100%)
- 9. If outlook is sunny and temperature is hot, then do not play tennis. (2/14, 100%)
- 10. If humidity is normal, then play tennis. (6/14, 87%).

Since the complete rule set is larger, we do not show it here. However, to demon-

strate why some rules in the complete rule set are not predictive rules, we list 7 rules including attribute value overcast as follows:

3. *if outlook is overcast, then play tennis.* (4/14, 100%)

11. if outlook is overcast and temperature is hot, then play tennis. (2/14, 100%)

12. if outlook is overcast and humidity is high, then play tennis. (2/14, 100%)

13. if outlook is overcast and humidity is normal, then play tennis. (2/14, 100%)

14. if outlook is overcast and wind is strong, then play tennis. (2/14, 100%)

15. *if outlook is overcast and wind is weak, then play tennis.* (2/14, 100%)

16. *if outlook is overcast and temperature is hot and wind is weak, then play tennis.* (2/14, 100%)

Only rule 3 is included in the optimal rule set out of the above 7 rules. The other 6 rules are not predictive rules since they follow rule 3 in the rule sequence defined by Definition 2 and are more specific than rule 3. Therefore, they cannot be predictive rules.

In the above example, the size difference between the complete rule set and the optimal rule set is not very significant because the underlying data set is very small. In some data sets, however, the optimal rule set can be less than 1% of the complete rule set.

Even though the optimal rule set is significantly smaller than the complete rule set, it is still much larger than a traditional classification rule set. Some rules in the optimal rule set are unnecessary when the number of missing attribute values is limited. Therefore, we show how to reduce the optimal rule set for a limited number of missing values in the following section.

4 *k*-optimal rule sets and their robustness

In this section, we further simplify the optimal rule set to k-optimal rule sets for test data sets with up to k missing attribute values. We then discuss properties of k-optimal rule sets.

We first define the k-incomplete data set to be a new data set with exactly k missing values from every record of the data set. We use k-incomplete data sets as test data sets.

Definition 8 Let D be a data set with n attributes, and $k \ge 0$. The k-incomplete data set of D is $D_k = \{T' \mid T' \subset T, T \in D, |T| - |T'| = k\}$. Conveniently, D_k consists of a set of $\binom{n}{k}$ data sets where each omits exactly k attributes (columns) from D.

For example, the 1-incomplete data set contains a set of n data sets where each omits one attribute (column) from D. Note that the 0-incomplete data set of D is D itself.

Let us represent the optimal rule set in terms of incomplete data sets.

Lemma 1 The optimal rule set is the set of predictive rules for records in the union of k-incomplete data sets for $0 \le k < n$.

Proof Firstly, a weak rule, excluded by the optimal rule set, cannot be a predictive rule for the k-incomplete record. When a weak rule and one of its corresponding strong rules cover the k-incomplete record, the strong rule will be the predictive rule. The weak rule is more specific than the strong rule and hence there is no chance for the weak rule to cover a record that is not covered by the strong rule.

Secondly, a strong rule, included by the optimal rule set, will be the predictive rule for an incomplete record. Let an incomplete record contain only the antecedent of the strong rule. The strong rule is the predictive rule of the record because other more general rules covering the record have lower accuracy than the strong rule. Consequently, the lemma is proved. \Box

In other words, if the optimal rule set could not make a prediction on an incomplete record, another rule set, e.g. the complete rule set, could not neither; a rule in an optimal rule set is a predictive rule for some incomplete records. For example, given an optimal rule set $\{a \rightarrow z \ (acc = 0.9), b \rightarrow z \ (acc = 0.8), c \rightarrow z \ (acc = 0.7)\}$. For record $\{abcdefg\}$, rule $c \rightarrow z$ becomes the predictive rule when both a and b are missing.

The optimal rule set preserves all potential predictive rules for k-incomplete data sets with k up to n - 1. However, it is too big in many applications. Now we consider how to preserve a small number of predictive rules for limited number of missing values in incomplete data sets.

Definition 9 A k-optimal rule set contains the set of all predictive rules on the kincomplete data set.

For example, rule set $\{a \rightarrow z \text{ (acc} = 0.9), b \rightarrow z \text{ (acc} = 0.8)\}\$ is 1-optimal for record $\{abcdefg\}$. When a is missing, rule $b \rightarrow z$ is the predictive rule. When b, c, d, e, f or g is missing, rule $a \rightarrow z$ is the predictive rule.

We have used the name of k-optimal rule sets in one of our previous work [14]. Recently, another rule mining algorithm [22] also generates k-optimal rule sets, which contain k rules with the largest leverage. k in our k-optimal rule sets stands for kmissing values per record, and is usually a small number. k in the other k-optimal rule sets indicates the number of rules, and is a reasonable big number.

We have the following property for k-optimal rule sets.

Lemma 2 The k-optimal rule set makes the same predictions as the optimal rule set on all p-incomplete data sets for $0 \le p \le k$. **Proof** The k-optimal rule set contains predictive rules for all p-incomplete data sets with $0 \le p \le k$ according to Definition 9, and hence this lemma holds immediately.

For example, given an optimal rule set $\{a \rightarrow z \text{ (acc} = 0.9), b \rightarrow z \text{ (acc} = 0.8), c \rightarrow z \text{ (acc} = 0.7), d \rightarrow z \text{ (acc} = 0.6)\}$. Rule set $\{a \rightarrow z \text{ (acc} = 0.9), b \rightarrow z \text{ (acc} = 0.8), c \rightarrow z \text{ (acc} = 0.7)\}$ is 2-optimal for record $\{abcdefg\}$. It makes the same prediction as the optimal rule set on record $\{abcdefg\}$ with up to two missing values, e.g. $\{bcdefg\}$ and $\{cdefg\}$.

The k-optimal rule set is a subset of the optimal rule set that makes the same predictions as the optimal rule set on a test data set with k missing attribute values per record. As a special case, a 0-optimal rule set¹ makes the same predictions as the optimal rule set on the complete test data set.

Theorem 2 The (k+1)-optimal rule set is at least as robust as the k-optimal rule set.

Proof For those records in *p*-incomplete data sets for $p \le k$, both rule sets make the same predictions because both make the same predictions as the optimal rule set according to Lemma 2.

For those records in the (k + 1)-incomplete data set, the (k + 1)-optimal rule set makes the same predictions as the optimal rule set and the k-optimal rule set does not. Hence, there may be some records that are identified by the (k + 1)-optimal rule set but not by the k-optimal rule set.

Consequently, the (k+1)-optimal rule set is at least as robust as the k-optimal rule set. \Box

For example, 2-optimal rule set $\{a \rightarrow z \text{ (acc} = 0.9), b \rightarrow z \text{ (acc} = 0.8), c \rightarrow z \text{ (acc} = 0.7)\}$ is more robust than 1-optimal rule set $\{a \rightarrow z \text{ (acc} = 0.9), b \rightarrow z \text{ (acc}$

¹To avoid possible confusion, we call a 0-optimal rule set as a min-optimal rule set.

z (acc = 0.8)}. When values a and b are missed from the record $\{abcdefg\}$, the first rule set predicts it to belong to class z with the accuracy of 70% whereas the second rule set makes any prediction with the accuracy of 0%.

We give an example to show k-optimal rule sets and their predictive capabilities.

Example 3 In the data set of Example 1, with the minimum support of 2/14 and the minimum confidence of 80%, we have the optimal rule set with 10 rules as shown in Example 2. These 10 rules can identify all records in the data set. We take confidence as accuracy in this example for easy illustration since otherwise an accuracy estimation method requires a calculator. We have a min-optimal rule set as follows, where two numbers in the parentheses are support and accuracy respectively.

- 1. If outlook is sunny and humidity is high, then do not play tennis. (3/14, 100%)
- 2. If outlook is sunny and humidity is normal, then play tennis. (2/14, 100%)
- 3. If outlook is overcast, then play tennis. (4/14, 100%)
- 4. If outlook is rain and wind is strong, then do not play tennis. (2/14, 100%)
- 5. If outlook is rain and wind is weak, then play tennis. (3/14, 100%)
- 6. If humidity is normal and wind is weak, then play tennis. (3/14, 100%)

Rules 1, 2, 3, 4 and 5 identify different records in the data set, so they are included in the min-optimal rule set. As to rule 6, it is the predictive rule for record 9. When identifying record 9, rule 6 has higher support than rule 2 and hence is the predictive rule for the record. This consideration results in that the min-optimal rule set is more robust than the rule set from the decision tree. When Outlook information is missing, the rule set from the decision tree identifies nothing while the min-optimal rule set identifies 3 records. The min-optimal rule set provides exactly the same predictions as the optimal rule set on the complete test data set.

With the following 4 additional rules, the rule set becomes 1-optimal.

- 7. If temperature is cool and wind is weak, then play tennis. (2/14, 100%)
- 8. If temperature is mild and humidity is normal, then play tennis. (2/14, 100%)

9. If outlook is sunny and temperature is hot, then do not play tennis. (2/14, 100%)
10. If humidity is normal, then play tennis (6/14, 87%).

This rule set gives more correct predictions on incomplete test data than the minoptimal rule set. For example, when Outlook information is missing, the 1-complete rule set identifies 6 records, which are 3 records more than the min-optimal rule set; when Temperature, 14, equal; when Humidity, 11, 2 more; and when Wind, 11, 2 more. The improvement is clear and positive. In this example, the 1-optimal rule set equals the optimal rule set. This is because that the data set contains only four attributes. In most data sets, a 1-optimal rule set is significantly smaller than an optimal rule set.

The *k*-optimal rule sets form a hierarchy.

Lemma 3 Let R_k and R_{k+1} be the k-optimal and the (k + 1)-optimal rule sets for D. Then $R_k \subseteq R_{k+1}$.

Proof R_k contains the set of all predictive rules over all *p*-incomplete data sets for $p \le k$. R_{k+1} contains the set of all predictive rules over all *p*-incomplete data sets for $p \le k$ and all predictive rules for (k + 1)-incomplete data sets. The predictive rule for a record is unique as assumed following Definition 3. So, $R_k \subseteq R_{k+1}$. \Box

In Example 2 and 3, $R_{opt} = R_4 = R_3 = R_2 = R_1 \supset R_{min}$. Theoretically, k is up to n, the number of attributes, but practically, only a small $k \ll n$ is meaningful.

Till now, we have introduced the set of optimal rule sets, and we observe that the following hierarchy holds these optimal rule sets.

$$R_{opt} \supseteq \cdots \supseteq R_{k+1} \supseteq R_k \supseteq \cdots \supseteq R_{min}$$

The robustness of a k-optimal rule set for k > 0 is due to that it preserves more potentially predictive rules in case that some rules are paralysed by missing values in a data set. Usually, a traditional classification rule set is smaller than a min-optimal rule set, since most traditional classification systems post prune the final rule set to a small size. From our observations, most traditional classification rule sets are subsets of min-optimal rule sets. For example, the rule set from c4.5 in Example 1 is a subset of the min-optimal rule set in Example 3 and is less robust than the min-optimal rule set. Experimental results will show this.

Finally, we consider a property that will help us to find k-optimal rule sets. We can interpret the k-optimal rule set through a set of min-optimal rule sets.

Lemma 4 Consider that a k-incomplete sub data set omits exactly k attributes from data set D. The union of min-optimal rule sets over all k-incomplete sub data sets is k-optimal.

Proof For each of every k-incomplete sub data set, we obtain a min-optimal rule set that contains all predictive rules for the incomplete data set. The union of these min-optimal rule sets contains all predictive rules on the k-incomplete data set, and hence is k-optimal. \Box

We give an example to show this lemma.

Example 4 Follow Example 3. When Outlook information is omitted, a min-optimal rule set consists of rule 6, 7, 8 and 10; when Temperature, rule 1, 2, 3, 4, 5 and 6; when Humidity, rule 3, 4, 5, 7 and 9; when Wind, rule 1, 2, 3, 8, 9 and 10. The union of the above four min-optimal rule sets on four 1-incomplete data sub sets is 1-optimal.

This lemma suggests that we can generate the k-optimal rule set by generating min-optimal rule sets on a set of incomplete data sets.

5 Constructing *k*-optimal rule sets

We now consider two different methods for constructing robust rule sets. The first method extends a traditional classification rule generation technique and the second one extends an optimal classification rule mining technique.

5.1 A multiple decision tree approach

Heuristic methods have been playing an important role in classification problems, so here we first discuss how to generate k-optimal rule sets by a heuristic method.

In order to use a rule set on incomplete data sets, we may generate a rule set from a incomplete data set. For a set of k-incomplete sub data sets of the training data set, we can construct a set of rule sets on them. Intuitively, the union rule set will withstand up to k missing values to some extent.

We use C4.5rules [20] as the base rule generator in this algorithm. Although constructing multiple classifiers has been discussed before, such as Bagging [5] and Boosting [9, 10]. This algorithm differs from others in that it samples attributes systematically rather than records randomly, and that it uses the union of all rule sets instead of individual classifiers.

The *k*-incomplete data set consists of a set of $\binom{n}{k}$ (*n* is the number of attributes for *D*) sub data sets in which each omits exactly *k* attribute (column) information from *D*.

Algorithm 1 Multiple tree algorithm

Input: data set D, integer $k \ge 1$ Output: Rule set R

(1) set $R = \emptyset$

(2) for each k-incomplete sub data set D' of D

(3) build a decision tree T from D' by C4.5

(4) call C4.5 rules to generate a rule set R' from T

- (5) $let R = R \cup R'$
- (6) return R

We now study the robustness of the output rule set of the algorithm. Suppose that each R' is the min-optimal rule set for the corresponding k-incomplete sub data set. The final rule set is the k-optimal rule set by Lemma 4. A traditional classification rule set is usually less robust than a min-optimal as shown in the experiments. Therefore, the output rule set is at most as robust as the k-optimal rule set.

This algorithm may be inefficient when k is large. This is because $\binom{n}{k}$ rule sets have to be generated where significant repeating computation is involved. It is possible to modify codes of the C4.5 and C4.5rules to avoid the repeating computation. However, this modification may not be necessary when precise k-optimal rule sets can be generated.

5.2 An optimal class association rule set approach

In this section, we present a precise method to compute k-optimal rule sets. A naive method would perform the following three steps:

- generate the complete rule set by an association rule approach, such as Apriori [1] or FP-growth [11].
- 2. find the min-optimal rule set for every k-incomplete data set,
- 3. union all min-optimal rule sets.

This method would be inefficient. Firstly, the complete rule set is usually very large, and is too expensive to compute for some data sets when the minimum support is low. Secondly, the process of finding the min-optimal rule set from a large complete rule set is expensive too.

An efficient algorithm [22] generating k-optimal rule sets actually serves different purposes since that k-optimal is different from this k-optimal as discussions following Definition 9.

In our proposed algorithm, we directly find a smaller optimal rule set and compute the k-optimal rule set from the optimal class rule set in a single pass over the data set.

An efficient algorithm for generating the optimal rule set is presented in [13, 12]. Here, we only present an algorithm to compute the k-optimal rule set from the optimal rule set.

Given a rule r, let Attr(r) be the set of attributes whose values appear in the antecedent of r. A p-attribute pattern is an attribute set containing p attributes. Given a record T and an attribute set X, let Omit(T, X) be a new partial record projected from T without attribute values from X.

Algorithm 2 k-optimal rule set generator

Input: data set D, optimal rule set R_{opt} and $k \ge 0$ Output: k-optimal rule set R

- (1) set $R = \emptyset$
- (2) for each record T_i in D

(3) let
$$R'_i$$
 contain the set of rules that cover T_i

(4) for each
$$r \in R'_i$$
 let UsedAttr = UsedAttr \cup Attr (r)

(5) for each
$$k$$
-attribute set X in UsedAttr

(6)
$$let T = Omit(T_i, X)$$

(7) if there is no predictive rule for
$$T$$
 in R_i

(8) then select a predictive rule
$$r'$$
 for T and move it from R'_i into R_i

$$(9) \qquad let R = R \bigcup R_i$$

(10) return R

We first illustrate the algorithm by the following example.

Example 5 Consider data set in Table 1 and the optimal rule set in Example 2. We use the above algorithm to generate the 1-optimal rule set. Let T_1 be the first row in Table 1. Initially, $R = \emptyset$ and $R'_1 = \{r_1, r_9\}$ where r_1 and r_9 represent the first rule and the ninth rule in the optimal rule set in Example 2. In line 4, UsedAttr ={Outlook, Temperature, Humidity}. From line 5 to line 8, firstly, value in Outlook column is omitted and no rule is selected. Secondly, value in Temperature column is omitted and the first rule r_1 is selected. Thirdly, value in Humidity column is omitted and the rule set for T_1 . As a comparison, rule set $\{r_1, r_9\}$. Rule set $\{r_1, r_9\}$ is the 1-optimal rule set for T_1 . As a comparison, rule set $\{r_1\}$ is the min-optimal rule set for T_1 . For any one missing value in T_1 , the min-optimal rule set has 50% of probability of being paralysed by the missing value, either in Outlook column or in Humidity column, whereas the 1-optimal rule set has 25% of probability of being paralysed by missing values.

Now we consider its correctness. In lines (4) and (5), we only consider attributes used in rules since missing values in other attributes do not affect the performance of rules. This algorithm selects predictive rules for all k-missing patterns on each of every record in the training data set in lines (5) to (7). The algorithm generates a k-optimal rule set correctly according to Lemma 4.

6 Experiments

In the previous sections, we build a theoretical model for selecting classification rule sets that are less sensitive to missing values in test data. In this section, we will experimentally prove that these rule sets do tolerate certain missing values in test data by showing their classification accuracies on incomplete test data. Missing values have not been handled, and we intend to show the ability of tolerating missing values of k-optimal rule sets and k-optimal classifiers.

In the first part of the experiments, we evaluate the robustness of k-optimal rule sets by following the definitions in the previous sections except that a record in a kincomplete data set does not contain k missing values exactly but on average.

In the second part of the experiments, we build classifiers based on *k*-optimal rule sets following a common practice in building rule-based classifiers. We compare our classifiers against other two benchmark rule-based classifiers on their classification performances on incomplete test data sets by using ten-fold cross validation. We also compare the proposed classifier with C4.5rules plus two well known missing value handling methods.

6.1 **Proof-of-concept experiment**

In this section, we conduct an experiment to show the practical implication of definitions and theorems. k-optimal rule sets are tested on randomly generated l-incomplete test data sets where $0 \le l \le 6$. The l-incomplete data sets are different from Definition 8 since they contain l-missing values on average rather than exactly.

Two data sets are selected from UCI ML repository [4] and a brief description of them are in the Appendix. They contain two classes each and their class distributions are relatively even. They are very easy to be classified by any classification method. We use them because they illustrate the main points of this paper very well.

k-optimal rule sets are generated by following algorithms 1 and 2. As a comparison, a traditional classification rule set is generated by C4.5rules [20]. k-incomplete test data sets are generated by omitting on average k values in each record. We control the total number of missing values, and let each record contain different number of missing values. To make the results reliable, we test every rule set on ten randomly generated incomplete test data sets and report the average accuracy.

In the experiment, all rule sets are tested without the default predictions, since here we test robustness of rule sets rather than classifiers. Predictive rules are defined by Definition 3 using Laplace estimated accuracy. We set the minimum support as 0.1 in each class, called local support, minimum confidence as 0.5, and maximum rule length as 6 for k-optimal rule sets.

			1-	multi (k=1)	min-	single
Rule set	complete	optimal	optimal	C4.5rules	optimal	C4.5rules
Mushrooms	99126	1118	78	46	32	16
Congressional Voting	57384	1472	92	32	35	7

Table 3: Sizes of different rule sets. A complete rule set is very large, an optimal rule set is large, and a rule set from C4.5rules is very small. A 1-optimal rule set is larger than a min-optimal rule set. A rule set from multiple C4.5rules is closer to a min-optimal rule set than to a 1-optimal rule set.

Table 2 shows that complete rule sets are significantly larger than optimal rule sets which are significantly larger than 1- and min-optimal rule sets. We observe the hierarchy of k optimal rule sets discussed in Section 4. Min-optimal rule sets are larger than rule sets from the C4.5rules [20]. Rule sets generated by multiple decision trees (k=1) are smaller than precise 1-optimal rule sets. This is because the C4.5rules prefers simple rule sets.

Figure 2 show that optimal rule sets perform the most accurately on incomplete test data, 1-optimal rule sets the second best, min-optimal rule sets the third, and rule sets from C4.5rules the worst. These results are consistent with Theorem 2. Rule sets from multiple C4.5rules (k=1) perform better than rule sets from single C4.5rules but worse than 1-optimal rule sets.

These results illustrate the main ideas in this paper very well. No rule set can be absolutely robust, but some rule sets are more robust than others. The robustness of k-optimal rule sets follows Theorem 2. The reason for the robustness is that some



Figure 2: The robustness of different rule sets. Optimal rule sets are the more robust, 1optimal rule sets the second, min-optimal rule set the third, and rule sets from C4.5rules the least robust. Rule sets from multiple C4.5rules are more robust than rule sets from single C4.5rules but less robust than 1-optimal rule sets.

additional rules are preserved in case other rules are paralysed by missing values in the test data set.

We note that there is not big room for accuracy improvement between 1-optimal rule sets and optimal rule sets. Therefore, k-optimal rule sets for k > 1 are unnecessary. We also note that 1-optimal rule sets from the multiple decision tree approach are not as robust as precise 1-optimal rule sets. This is consistent with our analysis in Section 5.

6.2 Comparative experiments

In this section, we conduct experiments to demonstrate the practical implication of the theoretical results in constructing robust rule-based classifiers. Different rule-based classifiers are tested on randomly generated incomplete test data sets where missing values have not been handled. The ten-fold cross validation method and 28 data sets have been employed in the experiments. A rule-based classifier that classifies incomplete test data with a higher accuracy is more robust than a rule-based classifier with a lower accuracy.

We construct k-optimal rule set based classifiers by following a common practice for building rule-based classifiers. All rules in a k-optimal rule set are sorted by their Laplace accuracy first. We then initiate an empty output rule sequence. We choose a rule with the minimum misclassification rate in the k-optimal rule set, and move this rule to the head of the output rule sequence. We remove the records covered by this rule, and compute the misclassification rate of remaining rules in the k-optimal rule set. Then we recursively move the rule with the minimum misclassification rate to the tail of output rule sequence until there is no record left. When there are two rules with the same misclassification rate, the preceding rule in the k-optimal rule set is removed. After the above procedure is finished, remaining rules in the k-optimal rule set are appended to the output rule sequence in the order of Laplace accuracy. The majority class in the data set is set as the default class.

All *k*-optimal classifiers are compared against two benchmark rule-based classifiers, C4.5rules [20] and CBA [16]. The former is a typical decision tree based classifier, and the latter is an association based classifier. We do not include the multiple decision tree approach since a 1-optimal rule set from the multiple decision tree approach is not as robust as a precise 1-optimal rule set as shown by our analysis and experiment. Further, the multiple decision tree approach is too time consuming when k > 1.

Twenty-eight data sets from UCI ML Repository [4] are used to evaluate the robustness of different classifiers. A summary of these data sets is given in the Appendix. The ten-fold cross validation method is used the experiment. k-incomplete test data sets are generated by randomly omitting values in test data sets so that each record has on average k-missing values. Because the k-incomplete test data sets are generated randomly, the accuracy of each fold of ten-fold cross validation is the average of accuracies obtained from 10 tests.

The parameters for the optimal rule set generation are listed as follows. Local



Figure 3: The average sizes of different classifiers on 28 data sets. An optimal classifier is large whereas a C4.5rules classifier is very small. A CBA classifier is close to a min-optimal classifier, and both are smaller than a 1-optimal classifier.

minimum support (support in a class), 0.01, minimum confidence, 0.5, and maximum length of rules, 6. For both C4.5rules and CBA, we used their default settings.

Figure 3 shows that an optimal classifier is significantly larger than both CBA and C4.5rules classifiers. A CBA classifier approaches a min-optimal classifier in size. A C4.5rules classifier is the smallest. A 1-optimal classifier is nearly twice as large as a min-optimal classifier.

Figure 4 shows that optimal, 1-optimal and min-optimal classifiers are more accurate than both CBA and C4.5rules classifiers on incomplete test data sets. Therefore, all optimal classifiers are more robust than CBA and C4.5rules classifiers.

The accuracy differences in Figure 4 is not so significant because the accuracies have been floated by the default predictions. A test record covered by no rule in a classifier is predicted to belong to the default class. The default prediction makes a classifier simple but may disguise the true accuracy. For example, in data set Hypothyroid, 95.2% records belong to class Negative and only 4.8% records belong to class Hypothyroid. So, if we set the default prediction as Negative, then this classifier will give 95.2% accuracy on a test data set that misses all values. The true accuracy for this "empty" data set should be zero rather than 95.2%. We see that how the accuracy is



Figure 4: The average accuracies of five classifiers with the default predictions on 28 data sets. Optimal, 1-optimal and min-optimal classifiers (top three lines) are more robust than CBA classifiers and C4.5rules classifiers.

floated by the default prediction. Further, this distribution knowledge is too general to be useful. For example, a doctor uses his patient data to build a rule-based diagnosis system. 80% patients coming to see him are healthy, and hence the system sets the default as healthy. Though the default easily picks up 80% accuracy, this accuracy is meaningless for the doctor.

In the following experiment, we remove the default prediction from each classifier. We repeat the same experiment for all classifiers without the default predictions and report the average accuracies on Figure 5. CBA has not been included because we could not remove its default prediction.

Figure 5 shows that all optimal classifiers are more accurate than C4.5rules classifiers on incomplete data, and hence are more robust. Optimal classifiers are more robust than 1-optimal classifiers, which are more robust than min-optimal classifiers on average. Optimal classifiers improve classification accuracies on incomplete test data by up to 28.2% over C4.5rules classifiers without the default predictions. This is a significant improvement.

By comparing size differences of optimal, 1-optimal and min-optimal classifiers with their classification accuracy differences on incomplete test data. 1-optimal clas-



Figure 5: The average accuracies of four classifiers without the default predictions on 28 data sets. Optimal rule classifiers are the most robust, 1-optimal classifiers the second, min-optimal classifiers the third and C4.5rules classifiers the least robust.

sifiers make use of rules effectively.

To show the advantages of building robust classifiers over imputing missing values, we compare the robust rule based classifiers to C4.5rules plus two different missing value imputing methods. Most common attribute value substitution is a simple but effective approach for imputing missing categorical values [7]. *k*-nearest neighbor substitution is the most accurate approach for imputing missing values as shown in the recent work [3]. In the former approach, a missing value is replaced by a value that occurs most frequently in an attribute. In the later approach, a missing value is replaced by a value that occurs most frequently in its k-nearest neighborhood.

We compare the proposed robust classifier, e.g. 1-optimal classifier without handling missing values, to C4.5rules with test values being imputed by both approaches. In the k-nearest neighbor substitution, k is set as 10 as in [3]. When the size of a test data set is smaller than 100 but greater than 30, k is set as 5. When the size of a test data set is smaller than 30, k is set as 3.

Figure 6 shows that 1-optimal classifier alone is more accurate than C4.5rules plus most common attribute substitution and k nearest neighbour substitution, respectively. This demonstrates that building robust rule based classifiers is better than treating



Figure 6: The comparison of 1-optimal classifier with two missing value imputation methods on 28 data sets. The 1-optimal classifier is more accurate than C4.5rules plus two imputation methods respectively in the presence of missing values.

missing values. In addition, 1-optimal classifier also benefits from a good imputation method. When the average missing values in each record exceeds two in our experiments, k-nearest neighbour substitution method improves the accuracy of 1-optimal classifier.

7 Conclusions

In this paper, we discussed a problem of selecting rules to build robust classifiers that tolerate certain missing values in test data. It differs from a missing value handling problem since our discussion is about "immunising" from the missing values rather than "treating" missing values. We defined a hierarchy of optimal rule sets, *k*-optimal rule sets, and concluded that the robustness of *k*-optimal rule sets decreases with the decreasing size of rule sets. We proposed two methods to find *k*-optimal sets. We demonstrated the practical implication of the theoretical results by extensive experiments. All optimal rule set based classifiers are more robust than two benchmark rule-based classification systems, C4.5rules and CBA. We further show that the proposed method is better than two well known missing value handling method for missing value

ues in test data.

Given the frequent missing values in real world data, *k*-optimal rule sets have great potential in building robust classifiers in the future applications. The theoretical results also provide a guideline for pruning rules in a large rule set.

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Data set	Size	#Attr	#Class
Anneal	898	38	5
Australian	690	14	2
Auto	205	25	7
Breast	699	10	2
Cleve	303	13	2
Crx	690	15	2
Diabetes	768	8	2
German	1000	20	2
Glass	214	9	7
Heart	270	13	2
Hepatitis	155	19	2
Horse-colic	368	22	2
House-vote	435	16	2
Нуро	3163	25	2
Ionosphere	351	34	2
Iris	150	4	3
Labor	57	16	2
Led7	3200	7	10
Lymph	148	18	4
Mushrooms	8124	22	2
Pima	768	8	2
Sick	2800	29	2
Sonar	208	60	2
Tic-tac	958	9	2
Vehicle	846	18	4
Waveform	5000	21	3
Wine	178	13	3
Zoo	101	16	7

Appendix: Data Set Description