SOAR: Simultaneous Or-of-And Rules for classification of positive and negative classes

Elena Khusainova | Emily Dodwell | Ritwik Mitra

Algorithmic decision making has proliferated and now impacts our daily lives in both mundane and consequential ways. Machine learning practitioners use a myriad of algorithms for predictive models in applications as diverse as movie recommendations, medical diagnoses, and parole recommendations without delving into the reasons driving specific predictive decisions. The algorithms in such applications are often chosen for their superior performance among a pool of competing algorithms; however, popular choices such as random forest and deep neural networks fail to provide an interpretable understanding of the model's predictions. In recent years, rule-based algorithms have provided a valuable alternative to address this issue. Previous work established an or-of-and (disjunctive normal form) based classification technique that allows for classification rule mining of a single class in a binary classification. In this work, we extend this idea to provide classification rules for both classes simultaneously. That is, we provide a distinct set of rules for each of the positive and negative classes. We also present a novel and complete taxonomy of classifications that clearly capture and quantify the inherent ambiguity of noisy binary classifications in the real world. We show that this approach leads to a more granular formulation of the likelihood model and a simulated annealing-based optimization achieves classification performance competitive with comparable techniques. We apply our method to synthetic and real-world data sets for comparison with other related methods to demonstrate the utility of our contribution.

KEYWORDS
interpretable machine learning, rule-based algorithms

1 | INTRODUCTION

The use of machine learning (ML) tools is ubiquitous in today's world, with applications ranging from the purely technical, for example, facial recognition or spam detection, to the biomedical (Esteva et al., 2017; Libbrecht & Noble, 2015; Shen et al., 2015) and social sciences (Berk, 2012). As researchers and practitioners turn to ML methods to perform increasingly complicated and highly impactful tasks, good model fit and high predictive accuracy of ML tools—while desirable—are proving insufficient. There is a need for transparency in large-scale automated decisions to enable proper assignment of accountability for applications with important implications to human lives; see Varshney and Alemzadeh (2017). This need has found further validation in the European Union’s (EU) adoption of General Data Protection Regulation (GDPR) (see Council of European Union, 2016), guidelines that address the collection, storage, processing, and use of personal data of EU residents. GDPR stipulates that in situations where personal data are processed for use in an automated decision mechanism, individuals should have
the right to obtain human intervention, to express his or her point of view, to obtain an explanation of the decision reached after such assessment and to challenge the decision.

This could potentially lead the way for wider adoption of and preference for interpretable, non-black-box models in certain domains. See also Goodman and Flaxman (2017) and Wachter et al. (2017) for further discussion of legal implications regarding interpretability and explainability as stated in GDPR.

This need for understanding has spurred the development of Interpretable machine learning (IML), a subdivision of ML that focuses on discovering and making explicit the relationships between predictors and a specific outcome in a form understandable by humans. Interpretability in ML is a rapidly growing field,1 and researchers have tried to achieve it in a variety of ways. Perhaps necessarily, it is an ambiguous term with ‘domain-specific’ implications (Doshi-Velez & Kim, 2017; Murdoch et al., 2019; Rudin, 2019). One approach to achieve interpretability has been to build black-box models and assign explainability to their predictions post-hoc through various mechanisms; we refer to Guidotti et al. (2018) for a detailed accounting and references. In this current work, we instead adopt IML to refer to that definition suggested by Murdoch et al. (2019):

The use of machine-learning models for the extraction of relevant knowledge about domain relationships contained in data.

The term relevant means that the insights obtained are useful for the chosen audience and problem domain. The interpretability that we are interested in is model-based, rather than post hoc, meaning that we do not seek new ways of deriving insights from existing methods but rather create a new algorithm that is inherently designed to be interpretable.

Given this increased need for transparency in situations where ML algorithms have the potential to significantly impact human subjects, and in light of the distinction between explainable and interpretable models, we focus our attention on the latter with the evolution of rule-based classifiers that are inherently interpretable.

A widely used class of IML tools is rule ensemble algorithms (Friedman & Popescu, 2008). Rule-based algorithms are inherently interpretable as they fit the model with a set of rules that can be understood by a human. For example, the following may define the outcome of a customer’s choice regarding whether or not to buy a piece of clothing based on its color, size, and price:

\[
\text{If color is blue and price is low then buy } = \text{ “yes”}
\]

\[
\text{If color is red and size is M and price is high then buy } = \text{ “no”}
\]

\[
\text{If size is XXXS then buy } = \text{ “yes”}
\]

Such rules enable us to see relationships between variables by expressing dependencies of the outcome variable on the predictors in a manner that can be easily understood.

The history of rule-based IML (especially rules of the above form) is rich, and the field is growing. Early instances of rule-based ML models may be found in Crama et al. (1998) and Boros et al. (2000) in the context of “logical analysis of data,” which aims to detect and group patterns that can correctly classify examples. Friedman and Fisher (1999) introduced the Patient Rule Induction Method (PRIM), which identifies simple rules to define rectangular subregions of the input variable space that correspond to above- or below-average values of the output variable. Further extensions of PRIM have been studied in Goh and Rudin (2014), where exact and approximate-yet-fast rule sets can be derived through mixed integer programming. Cohen (1995) proposed a fast algorithm RIPPERk, which creates a rule-based model by first growing a rule set and then repeatedly pruning it based on error-reducing criteria. Other attempts at classification rule mining such as that of Yildirim and Alatas (2021) were made. We refer to Molnar (2020) for a recent accounting of IML methods and further references because research in this field has evolved in various directions too numerous to note here in detail. A parallel thread of research in IML involves fuzzy rule based systems (FRBs). We refer to Ishibuchi et al. (2004) for a detailed review, and Gacto et al. (2011) for an overview of different interpretability measures in this context. See also Lughofer (2013) for a more recent overview of research in evolving fuzzy sets. In this approach (see Chi et al., 1996), a set of fuzzy rules with certain rule weights are obtained; the rules themselves are defined via linguistic labels modeled through triangular membership functions. A final classification is made via the so-called “winning rule” (see Cordón et al., 1999) that takes into account both matching degree and association degree. There are some parallels of our approach to the fuzzy rule-based classification systems; however, we focus on a very particular binarized predictor and corresponding and-of-or rule set and allow Bayesian priors to assign ‘weights’ to the rules.

More relevant to our current work, Wang et al. (2015, 2017) proposed a rule-based algorithm for binary classification called Bayesian Or’s of And’s (BOA), which represents a Bayesian framework to address the issue of model interpretability. As the name suggests, the algorithm requires a prior distribution on the set of possible rules that may serve as a proxy for professional opinion about the shape of the rule set. This algorithm

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1Google Scholar produces more than 5000 results for the search “Interpretable Machine Learning” for the period from January 2015 to April 2020 as opposed to less than 200 for all time before 2015.
results in one rule set that defines the positively classified observations, while the negative class is passively defined as its complement. The algorithm was created in the context of recommendation systems (Wang et al., 2015) for which the positive class is of primary interest.

However, in certain applications, obtaining a rule set for the negative class may be just as important as defining the positive class. Consider for example, a classification model that predicts whether a patient will have a drug-related adverse reaction (positive class) or not (negative class) given their medical history, including, for example, comorbidities, results of diagnostic tests, and prior prescribed medication. Such a model may enable safer administration of a newer drug when, for example, adverse effects of a treatment and its potential toxicity require further study and consideration. In this scenario, there is significant value for both the doctor and subject receiving the treatment to understand the combination of factors associated with non-occurrence of an adverse event (i.e., definition of the negative class) to inform safe treatment and motivate patient compliance. Furthermore, cases where rules associated with both an adverse event’s occurrence and non-occurrence are satisfied may indicate complicated interactions of multiple factors, which alerts both the doctor and patient to the potential for extenuating circumstances and enable closer monitoring. We address this important aspect of rule-based modeling directly in this work.

**Contribution:** In this paper, we propose SOAR, Simultaneous Or-of-And Rules, an algorithm to identify rule sets for each of the positive and negative classes in a binary classification problem. The SOAR algorithm is an extension of the BOA algorithm. It treats the positive and negative classes separately and produces a defined rule set for each, rather than creating rules for the positive class and assigning the complement to the negative class. We therefore take a direct approach through the Bayesian framework as proposed in Wang et al. (2015) and describe a complete likelihood for both classes. We calculate the posterior likelihood through annealing (Van Laarhoven & Aarts, 1987). A key advantage of this approach is that two rule sets allow for cases that may satisfy both or neither of them; we refer to such cases as “ambiguous”. We argue that for these ambiguous cases, insight into which of an observation’s traits impact its assignment to both the positive and negative classes (or neither) is important for interpretability. Recognizing this need for describing ambiguity, SOAR provides a complete taxonomy of classifications that identify conflicts when the same rules suggest different classes. This proposed taxonomy is useful and important for real world applications which tend to be noisy and do not lend themselves to neat categorizations. Finally, for interested practitioners, we have made available an R package ORAND \(^2\) that implements our proposed algorithm.

Given the objective of SOAR, some comparison to the literature on uncertainty quantification (UQ) is unavoidable. The objective of UQ is usually to model uncertainty in a probabilistic way, often through Bayesian modeling, taking into account two main sources of uncertainty in ML models: aleatoric and epistemic; see Der Kiureghian and Ditlevsen (2009) and Hüllermeier and Waegeman (2021). In broad terms, the goal of UQ is to assign a measure of plausibility to an outcome based on the model uncertainty (epistemic) and data noise (aleatoric). The objective of SOAR is not to assign a specific metric of uncertainty, but rather to clearly delineate the ambiguity in the outcomes through interpretable rule sets. It is conceivable that some measure of uncertainty can be assigned to the prediction outcomes from SOAR based on the posterior probabilities of the rule sets. We do not pursue this line of research in our current work, but rather leave it for future exploration.

Our work is organized as follows: In Section 2, we present an implementation of the SOAR algorithm and discuss terminology and key notation as they appear throughout the remaining sections. We present a detailed description of our proposal and introduce the complete taxonomy of classifications in Section 3, as well as explain the algorithm for creating simultaneous rules. In Section 4, we validate our algorithm with one simulated and two real-world data sets. By comparing SOAR to algorithms such as BOA and random forest, we find that SOAR’s performance is comparable in predictive accuracy; by offering deeper insights provided by a rule set that explicitly defines the negative class, our algorithm provides increased descriptive accuracy.

## 2 PROBLEM SET UP

In this section we define the problem and the terminology we use. Where possible we adopt notation and terminology from either Friedman and Popescu (2008) or Wang et al. (2015).

The algorithm is intended to address the standard binary classification problem. We assume that the data, denoted as \(X\), consists of \(p\) categorical predictors and \(n\) observations. That is \(X := [X_1, \ldots, X_p]\), with \(X_i \in \{0,1\}^p\) for \(1 \leq i \leq p\). Note, that \(X\) can also be expressed as \(X := [X_1, \ldots, X_n]^T\). When it does not cause confusion, we will abandon dots in the notation and use \(x_i = X_i\) to refer to observations in the data. For simplicity of notation, we also say that \(X = \{x_1, \ldots, x_n\}\). Additionally, each observation belongs to one of two classes, labeled as 0 and 1, with labels stored in the variable of interest \(Y = [y_1, \ldots, y_n] \in \{0,1\}^n\).

In order to define the form of the model to fit the data, we need to first define rules. Let function \(r = r(x)\) be a product of indicators:

\[
r(x) = \prod_{i=1}^{k} \mathbb{1}\{x[i] = x_i\},
\]

\(^2\)https://github.com/elenakhusainova/ORAND.
where $x \in X$, $1 \leq i \leq p$ and values $x_i$ belong to the range of corresponding predictors $X_{s_i}, i=1,\ldots,k$. We say that any function of the form (1) is a rule or pattern of length $k$. For a set of rules $R$, we say that

$$R(x) = \begin{cases} 1 & \text{if there exists } r \in R \text{ such that } r(x) = 1, \\ 0 & \text{otherwise} \end{cases}$$

and define $X_R := \{x \in X : R(x) = 1\}$ to be the set of all observations that satisfy the rule set $R$.

The model we fit then takes the following form:

$$f(x) = \sum_{m=1}^{M} r_m(x),$$

where $r_1,\ldots,r_m$ are rules. This form of the model can be seen as a disjunction of conjunctions, or simply, Or-of-Ands (hence the name of the algorithm). If sets $X^+$ and $X^-$ are such that

$$X^+ = \{x_i \in X : y_i = f(x_i) = 1\}, X^- = \{x_i \in X : y_i = f(x_i) = 0\},$$

that is, $X^+$ and $X^-$ consist of observations from positive and negative classes respectively, then the goal of the algorithm is to find rule sets $R^+$ and $R^-$ such that $X_{R^+}$ and $X_{R^-}$ are close (in terms of maximizing the posterior distribution, see Section 3.2) to $X^+$ and $X^-$, respectively.

## 3 | SOAR

In this section, we present the construction of the prior and log-likelihood model and also introduce the new taxonomy to be used with simultaneous classification.

The main contribution of the SOAR algorithm is that instead of finding trends and patterns among just the positive observations, we do so simultaneously for each of the positive and negative classes.

### 3.1 | Taxonomy of classifications

Consider two rule sets $R^+_R$ and $R^-_R$ and the corresponding sets of observations $X_{R^+_R}$ and $X_{R^-_R}$. Intuitively, $R^+_R$ and $R^-_R$ describe the characteristics of positive and negative sets, respectively. We call cases in $X_{R^+_R} \cap X_{R^-_R}$ *active ambiguous* and those in $X \setminus (X_{R^+_R} \cup X_{R^-_R})$ *passive ambiguous*. That is, active ambiguous refers to those cases that exhibit characteristics of both classes, whereas passive ambiguous are cases that do not exhibit characteristics of either class.

For cases in $X_{R^+_R} \cap X_{R^-_R}$ or $X_{R^+_R} \cap X_{R^-_R}$, where $X_{R^+_R} := X \setminus X_{R^-_R}$ and $X_{R^-_R} := X \setminus X_{R^+_R}$, we say that there is consensus. There represent cases that satisfy the positive class definition and not that of the negative class, or vice versa. The complete taxonomy is presented in Table 1. For an observation $x_i$, we can have one and only one of the eight possible scenarios. The first four cases are standard for classification problems, but the last four are slightly unusual. We allow the algorithm to give any prediction if there is uncertainty in the data, which in turn highlights the inherent ambiguity. We argue that allowing such cases makes our method more appropriate in circumstances where the user would prefer a second opinion model, as our expanded taxonomy provides for this detailed look.

**Table 1** Taxonomy.

| $\{y = 1 | R^+(x) = 1, R^-(x) = 0\}$ | Consensus - True Positive (CTP) |
| $\{y = 1 | R^+(x) = 0, R^-(x) = 1\}$ | Consensus - False Positive (CFP) |
| $\{y = 0 | R^+(x) = 1, R^-(x) = 0\}$ | Consensus - True Negative (CTN) |
| $\{y = 0 | R^+(x) = 0, R^-(x) = 1\}$ | Consensus - False Negative (CFN) |
| $\{y = 1 | R^+(x) = 1, R^-(x) = 1\}$ | Active Ambiguous - Positive (AAP) |
| $\{y = 0 | R^+(x) = 1, R^-(x) = 1\}$ | Active Ambiguous - Negative (AAN) |
| $\{y = 1 | R^+(x) = 0, R^-(x) = 0\}$ | Passive Ambiguous - Positive (PAP) |
| $\{y = 0 | R^+(x) = 0, R^-(x) = 0\}$ | Passive Ambiguous - Negative (PAN) |
It is worthwhile to point out the differences between our notations and more well-known measures such as positive predictive (PPR) and true positive rate (TPR). Recall that PPR = TP/(all discovered positives) and TPR = TP/(all positives in the data). Our definition states that it is true positive among all the positive decisions from “both rule sets.” Because we are focusing on ambiguous cases, the binarized language of TPR and PPR does not transfer directly to our setup.

3.2 Beta-binomial prior and log-likelihood model

We now describe the prior distribution for the model and the model itself. The first step of the algorithm (described in Section 3.3) results in two pattern sets $P^+$ and $P^-$ called pattern pools. The patterns in each of them satisfy three conditions:

- each pattern consists of no more than $L$ literals, with $L$ provided by the user;
- each pattern is frequent in the data. That is, there are more than a pre-specified threshold of observations that agree with the pattern;
- each pattern on its own has a strong relationship with the outcome variable (in terms of impurity score).

The prior is defined on the sets of all subsets of $P^+$ and $P^-$ in the following way:

1. For each $l^+, l^- \in \{1,2,...,L\}$ we simulate $p_l^+$ and $p_l^-$ such that

$$ p_l^+ \sim \text{Beta}(\alpha_l^+, \beta_l^+) \quad \text{and} \quad p_l^- \sim \text{Beta}(\alpha_l^-, \beta_l^-). $$

2. Each pattern of length $l^+$ (or $l^-$) is selected from $P^+$ (or $P^-$) with probability $p_l^+$ (or $p_l^-$).

Note, the parameters $\theta_{\text{prior}} = \{\alpha_1^+, \beta_1^+, \alpha_1^-, \beta_1^-, \cdots, \alpha_L^+, \beta_L^+, \alpha_L^-, \beta_L^-\}$ are user-specified to reflect the prior knowledge: For example, $\mathbb{E}[R^+_l] = \frac{\alpha_l^+}{\alpha_l^++\beta_l^+} |P^+_l|$, where $R^+_l$ is the subset of rules of length $l$ in the final rule set and $P^+_l$ are all mined rules of length $l$.

In subsequent discussions, we describe the prior on the positive and negative rules jointly as $x(R^+, R^- | \theta_{\text{prior}})$.

With full control over parameters of the prior, the user can influence the shape of the outcome by limiting the maximal pattern length, favoring longer or shorter patterns, and affecting the size of each of the rule sets.

We next explicitly write the likelihood of the data given a model. The following likelihood parameters govern the probability that an observation is of a true positive (or negative) class when it satisfies the corresponding pattern sets:

$$ \rho_A^+ = \mathbb{P}(y_n = 1 | R^+(x_n) = 1, R^-(x_n) = 0), \quad \rho_A^- = \mathbb{P}(y_n = 0 | R^+(x_n) = 0, R^-(x_n) = 0), $$
$$ \rho_C^+ = \mathbb{P}(y_n = 1 | R^+(x_n) = 1, R^-(x_n) = 0), \quad \rho_C^- = \mathbb{P}(y_n = 0 | R^+(x_n) = 0, R^-(x_n) = 1). $$

The prior for these four parameters are assigned as follows:

$$ \rho_A^+ \sim \text{Beta}(\alpha_A^+, \beta_A^+), \quad \rho_A^- \sim \text{Beta}(\alpha_A^-, \beta_A^-), \quad \rho_C^+ \sim \text{Beta}(\alpha_C^+, \beta_C^+), \quad \rho_C^- \sim \text{Beta}(\alpha_C^-, \beta_C^-). $$

As before, parameters $\theta_{\text{likelihood}} = \{\alpha_A^+, \beta_A^+, \alpha_A^-, \beta_A^-, \alpha_C^+, \beta_C^+, \alpha_C^-, \beta_C^-\}$ are provided by the user. Denote $\rho = \{\rho_A^+, \rho_A^-, \rho_C^+, \rho_C^-\}$; then the log-likelihood of the data is given by

$$ \log(\mathbb{P}(\{x, y\}_{i=1}^n | R^+, R^-, \rho)) $$

$$ = \sum_{i=1}^n \left[ y_i R^+(x_i) (1 - R^-(x_i)) \log \rho_A^+ + (1 - y_i) R^-(x_i) (1 - R^-(x_i)) \log (1 - \rho_A^+) + (1 - y_i) (1 - R^+(x_i)) R^-(x_i) \log (1 - \rho_A^-) + y_i (1 - R^+(x_i)) R^-(x_i) \log \rho_A^- \right] $$

$$ + \left[ y_i R^+(x_i) R^-(x_i) \log \rho_C^+ + (1 - y_i) R^+(x_i) R^-(x_i) \log (1 - \rho_C^+) + (1 - y_i) (1 - R^+(x_i)) R^-(x_i) \log \rho_C^- + y_i (1 - R^+(x_i)) (1 - R^-(x_i)) \log (1 - \rho_C^-) \right] $$

$$ = \text{CTP} \log(\rho_C^+) + \text{CFP} \log(1 - \rho_C^+) + \text{CTN} \log(\rho_C^-) + \text{CFN} \log(1 - \rho_C^-) + \text{AAP} \log(\rho_A^+) + \text{AAN} \log(1 - \rho_A^+) + \text{PAN} \log(\rho_A^-) + \text{PAP} \log(1 - \rho_A^-). $$
where CTP, CFP, CTN, CFN, AAP, AAN, PAN, PAP are the counts of the corresponding cases. Here, we have (with slight abuse of notation) used the empirical versions of the definitions defined in Table 1. Incorporating the prior structure for \( \rho \), we get

\[
\mathbb{P}(\mathbf{X}, \mathbf{Y}) = P(\{\mathbf{X}, \mathbf{Y}\}) \times \text{Beta}(\alpha_{\mathbf{A}}, \beta_{\mathbf{A}}) \times \text{Beta}(\alpha_{\mathbf{C}}, \beta_{\mathbf{C}}) \times \text{Beta}(\alpha_{\mathbf{P}}, \beta_{\mathbf{P}}) \times \text{Beta}(\alpha_{\mathbf{A}}, \beta_{\mathbf{A}}) \times \text{Beta}(\alpha_{\mathbf{C}}, \beta_{\mathbf{C}}) \times \text{Beta}(\alpha_{\mathbf{P}}, \beta_{\mathbf{P}}) \times \text{Beta}(\alpha_{\mathbf{A}}, \beta_{\mathbf{A}}) \times \text{Beta}(\alpha_{\mathbf{C}}, \beta_{\mathbf{C}}) \times \text{Beta}(\alpha_{\mathbf{P}}, \beta_{\mathbf{P}})
\]

where \( B(a, b) = \Gamma(a)\Gamma(b)/\Gamma(a + b) \). The final posterior distribution for the rules and data is then given by

\[
\mathbb{P}(\{\mathbf{X}, \mathbf{Y}\} | \mathbf{R}^{+}, \mathbf{R}^{-}, \theta_{\text{likelihood}}, \theta_{\text{prior}}) \propto \mathbb{P}(\{\mathbf{X}, \mathbf{Y}\}) \times \pi(\mathbf{R}^{+}, \mathbf{R}^{-} | \theta_{\text{prior}}).
\]

The MAP (maximum a posteriori) estimator for these rules is then given by

\[
(R^{+}, R^{-}) := \arg\max_{R^{+}, R^{-} \subset \mathbb{P}} \mathbb{P}(\{\mathbf{X}, \mathbf{Y}\} | \mathbf{R}^{+}, \mathbf{R}^{-}, \theta_{\text{likelihood}}, \theta_{\text{prior}}).
\]

### 3.3 Algorithm

The algorithm can be divided into three main steps:

1. **Frequent pattern mining.** The most frequent patterns are mined from the data using the scalable FPGrowth algorithm introduced by Han et al. (2000) and implemented by Borgelt (2005).
   
   We note that frequent pattern mining (FPM) is agnostic of the positive or negative class membership of the observation. As such, one could run a single FPM on the whole dataset to get a set of frequent rules for both positive and negative classes. That is, at this stage the positive and negative pattern pools are identical.

2. **Pattern screening.** The patterns mined in the previous step are ranked based on one of the following, user-chosen, impurity functions: Conditional entropy or Gini index. The best ones form the final pattern pools of the size limited by the user.

3. **Simulated annealing to find MAP (7).** For details, see Algorithm 1.
Next we define

$$\text{Score}(R^+, R^-) = -\log P(\{x_i, y_i\}_{i=1}^n \mid R^+, \theta_{\text{likelihood}}, \theta_{\text{prior}}).$$

and the cooling schedule: $T(t) := T_0 / \log(1 + t)$, where the initial temperature $T_0$ is user-defined. Then the simulated annealing algorithm to find MAP solution is as shown in Algorithm 1.

The procedures COVERMORE and COVERLESS used in the algorithm are the same as in Wang et al. (2015):

- COVERMORE $(R, p)$ With probability $p$, add a random pattern to $R$ from the corresponding pool. Else, evaluate the objective Score() for all neighboring solutions where a pattern is added to $R$ and choose the one with the best score.
- COVERLESS $(R, p)$ With probability $p$, remove a random pattern from $R$. Else, evaluate the objective Score() for all neighboring solutions where a pattern is removed from $R$ and choose the one with the best score.
In this section, we present the comparison of SOAR’s performance to that of BOA by Wang et al. (2015) and random forest (Breiman, 2001). We use three data sets to illustrate the benefits of our algorithms, as well as its limitations:

1. Synthetic data manually generated to enable complete control over actual positive and negative rule sets.
2. The Adult data set (Kohavi, 1996) extracted from the 1994 Census Bureau database, which contains socioeconomic information on ~32 K adults.
3. Car data from Bohanec and Rajkovic (1988) that represents evaluation of 1728 cars based on their characteristics.

### 4.1 Performance metric

For comparison of algorithm performance, we split the data randomly into training and test sets, train each model on the same training set, and compare model predictions on the same test set. By design, SOAR works to bring forth the ambiguity in classifications. As such, it is not straightforward to define a single metric to assess classifier performance. Nevertheless, we propose two variants of the misclassification error (ME) rate. Because SOAR allows for ambiguous classification (AAN, AAP, AAN, PAP), we differentiate such ambiguous cases from those that are truly misclassified, that is, predicted incorrectly, by our algorithm (CFP, CFN). This misclassification rate is given by \((\text{CFP} + \text{CFN})/N\), where \(N\) is the number of observations in the test set. For a more classical performance comparison, we also propose a “forced” prediction that forces a class on the ambiguous cases. In detail, in the event that SOAR predicts an observation to be actively ambiguous, it is assigned to the class that has the longest rule it agrees with (unless the lengths are the same, in which case it stays ambiguous). We refer to the ME rate obtained through such forced prediction as the “Forced ME.”

### 4.2 Synthetic data

We simulate a data set of 1000 observations with five binary predictors \((x_1, x_2, x_3, x_4, x_5)\) and a single binary outcome. Because there are \(2^5 = 32\) possible combinations of predictors under this scheme, this naturally results in duplicate rows in the data matrix, as we may expect in real-world applications when different observations share the same characteristics. The following rules determine the true classification of each observation:

\[
R_{\text{truth}}^+ = \{(x_1,0) \land (x_2,1) \land (x_3,0), (x_2,1) \land (x_3,0) \land (x_5,1)\},
\]

\[
R_{\text{truth}}^- = \{(x_1,1) \land (x_3,1), (x_1,0) \land (x_2,0) \land (x_4,0), (x_1,1) \land (x_2,0) \land (x_3,0)\}.
\]

Among the 1000 observations, 500 are classified as positive and 490 are classified as negative. The intersection between these two classes (i.e., observations that satisfy both positive and negative rules) is 59, and the remaining 69 observations are neither positive nor negative. We assign those that satisfy both positive and negative rules to a final positive class with probability 0.05, and those that satisfy neither to a final positive class with probability 0.5. Table 2 summarizes the data.

We randomly split the data into a training set of 800 observations and a test set of the remaining 200 observations. Regarding interpretability, the patterns produced by SOAR algorithm are as follows:

\[
R^+ = \{(x_2,1), (x_3,0) \land (x_5,1)\},
\]

\[
R^- = \{(x_1,1) \land (x_3,1), (x_2,0) \land (x_5,0), (x_1,1) \land (x_2,0) \land (x_4,1) \land (x_5,1), (x_1,1) \land (x_2,0) \land (x_4,0) \land (x_5,1)\}.
\]

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3All testing was done on a MacBook Pro 2017, 2 cores, 16Gb, using code provided at https://github.com/elenakhusainova/ORAND.
Table 3 illustrates that the positive and negative classes defined by these rules are close to those defined by $R_{\text{truth}}^{+}$ and $R_{\text{truth}}^{-}$; predictor combinations for which the two pairs of rule sets disagree are marked with (*). Because both positive and negative rule sets provide a determination as to whether or not they were satisfied, we capture the determination of each rule set for observation $x$ as a pair $(r^{+}, r^{-})$, where $r^{+}$ is the outcome of the positive rule set, and $r^{-}$ is the outcome of the negative rule set. For example, an observation $x = [0,0,1,0,1]$ with true class $(0,1)$ and predicted class $(0,0)$ can be interpreted as

$$R_{\text{truth}}^{+}(x) = 0, R_{\text{truth}}^{-}(x) = 1, R^{+}(x) = 0, R^{-}(x) = 0.$$ 

The comparison of all three algorithms is presented in Table 4. While the overall misclassification rate is high for unforced SOAR, no observations are truly misclassified; that is, observations for which the algorithm's prediction fails to match the true label ultimately represent “ambiguous” cases. Once we force our algorithm to make a prediction (SOAR-forced), the true misclassification rate stays remarkably low and the overall misclassification rate is competitive with random forest and BOA.

### Table 3  True class and predicted class for all $2^5$ possible predictor combinations.

| ×1 | ×2 | ×3 | ×4 | ×5 | Truth | Prediction |
|----|----|----|----|----|-------|------------|
| 0  | 0  | 0  | 0  | 0  | (0,1) | (0,1)      |
| 0  | 0  | 0  | 0  | 1  | (1,0) | (1,0)      |
| 0  | 0  | 0  | 1  | 0  | (0,0) | (0,1)*     |
| 0  | 0  | 0  | 1  | 1  | (1,0) | (1,0)      |
| 0  | 0  | 1  | 0  | 0  | (0,1) | (0,1)      |
| 0  | 0  | 1  | 0  | 1  | (0,1) | (0,0)*     |
| 0  | 0  | 1  | 1  | 1  | (0,0) | (0,0)      |
| 0  | 1  | 0  | 0  | 0  | (1,0) | (1,0)      |
| 0  | 1  | 0  | 0  | 1  | (1,0) | (1,0)      |
| 0  | 1  | 0  | 1  | 0  | (1,0) | (1,0)      |
| 0  | 1  | 0  | 1  | 1  | (1,0) | (1,0)      |
| 0  | 1  | 1  | 0  | 0  | (1,0) | (1,0)      |
| 0  | 1  | 1  | 0  | 1  | (1,0) | (1,0)      |
| 0  | 1  | 1  | 1  | 1  | (1,0) | (1,0)      |
| 0  | 1  | 1  | 1  | 0  | (1,0) | (1,0)      |
| 1  | 0  | 0  | 0  | 0  | (0,1) | (0,1)      |
| 1  | 0  | 0  | 0  | 1  | (1,1) | (1,1)      |
| 1  | 0  | 0  | 1  | 0  | (0,1) | (0,1)      |
| 1  | 0  | 0  | 1  | 1  | (1,1) | (1,1)      |
| 1  | 0  | 1  | 0  | 0  | (0,1) | (0,1)      |
| 1  | 0  | 1  | 0  | 1  | (0,1) | (0,1)      |
| 1  | 0  | 1  | 1  | 0  | (0,1) | (0,1)      |
| 1  | 0  | 1  | 1  | 1  | (0,1) | (0,1)      |
| 1  | 1  | 0  | 0  | 0  | (1,0) | (1,0)      |
| 1  | 1  | 0  | 0  | 1  | (1,0) | (1,0)      |
| 1  | 1  | 0  | 1  | 0  | (1,0) | (1,0)      |
| 1  | 1  | 0  | 1  | 1  | (1,0) | (1,0)      |
| 1  | 1  | 1  | 0  | 0  | (1,0) | (1,0)      |
| 1  | 1  | 1  | 0  | 1  | (1,0) | (1,0)      |
| 1  | 1  | 1  | 1  | 0  | (1,0) | (1,0)      |
| 1  | 1  | 1  | 1  | 1  | (1,0) | (1,0)      |

Note: Predictor combinations for which the two pairs of rule sets disagree are marked with (*).
4.3 | Adult data

The Adult data set (Kohavi, 1996) is a Census Bureau data on the income of ~32 k adults. The data have 14 categorical socioeconomic predictors and one binary outcome, indicating whether a person makes more than $50k a year. The rules for classification are not known. The positive support (that is, people who make more than $50k) is ~8 k observations, and the negative support is ~24 k observations. We split the data into a training set with 25 k observations and test set with ~7.5 k observations. The rules produced by SOAR are as follows:

\[
R^+ = \{ \text{(marital status, Married-civ-spouse), (education, Masters), (sex, Male) \land (capital loss, 0) \land (native country, United-States), (occupation, Exec-managerial) \land (education, Bachelors), (sex, Male) \land (capital loss, 0)} \}
\]

\[
R^- = \{ \text{(education, um, 9), (relationship, Own-child), (occupation, Other-service), (capital gain, 0) \land (capital loss, 0), (occupation, Adm-clerical) \land (sex, Female) \land (capital ********************************************************************************

SOAR predicts that people who are married, have achieved higher levels of education, and men who work in managerial positions make more money, while people with fewer years of education, and those who work in administrative or service jobs make less. These rules are intuitive based on what we know of income factors. The comparison between the three algorithms is presented in Table 5.

As before, SOAR's misclassification rate is very low, and the performance of SOAR-forced is superior to BOA. To illustrate the strength of the algorithm we show examples of ambiguous—both passive and active—cases in Table 6.

Upon the inspection of these examples, we can see what might cause the ambiguity in prediction: The first example is a White male with a graduate degree but the occupation is not clear; thus, the algorithm cannot provide a consensus prediction. We argue that this case would not be possible to classify even for a human, thus the ambiguity in prediction is an accurate reflection of reality. Moreover the produced rule sets indicate exactly where the ambiguity comes from thus providing valuable insights. The other examples follow similar patterns. For example, in the fourth example, we have a white unmarried female with a BA degree with a highly paid occupation. This does not fall into any rule set as a highly paid occupation only appears together with male gender (possibly due to the lower frequency of \( (occupation, Exec-managerial) \land (sex, Female) \) pattern in the data).

Note also that from these examples and the rules (8), we immediately see that rule-based algorithms in general and SOAR in particular can be used to assess bias inherent in this data set. The characteristic \( (sex, Male) \) is present in two patterns for positive classification, and the first example of passive ambiguous classification (a woman with a managerial position and college education) is not labeled as positive.

To illustrate our taxonomy, Table 7 presents the comparative results between BOA and SOAR. We see that both algorithms are better at detecting observations in the positive class. There are only 149 FN-cases for BOA and 158 CFN-cases for SOAR. Observations in the negative class are less frequent, which is why the algorithms perform better.

### Table 4: Comparison of misclassification error (ME) performance of SOAR, BOA, and random forest on synthetic data.

|               | SOAR (ME) | SOAR (forced ME) | BOA (ME) | RF (ME) |
|---------------|-----------|------------------|----------|---------|
| Truly misclassified | 0         | 0.005            | 0.05     | 0.05    |
| Ambiguous     | 0.25      | 0.07             | 0        | 0       |

### Table 5: Comparison of misclassification error (ME) performances of SOAR, BOA, and random forest using Adult data.

|               | SOAR (ME) | SOAR (forced ME) | BOA (ME) | RF (ME) |
|---------------|-----------|------------------|----------|---------|
| Truly misclassified | 0.034     | 0.174            | 0.297    | 0.159   |
| Ambiguous     | 0.432     | 0.044            | 0        | 0       |

### Table 6: Examples of cases from Adult data labeled as ambiguous by SOAR algorithm.

| Education | Ed_num | Marital_status | Occupation | Relationship | Race | Sex | Capital_loss | Capital_gain | >50K |
|-----------|--------|----------------|------------|--------------|------|-----|--------------|--------------|------|
| Active    | Masters | 14    | Married-civ-spouse | Other-service | Husband | White | Male | 0 | 0 | 0 |
| Bachelors | 13     | Never-married | Exec-managerial | Own-child | White | Male | 0 | 0 | 0 |
| Masters   | 14     | Never-married | Sales       | Own-child | Black | Male | 0 | 0 | 0 |
| Passive   | Bachelors | 13    | Never-married | Exec-managerial | Other-relative | White | Female | 0 | 1 | 0 |
| 10th      | 6      | Never-married | Adm-clerical | Not-in-family | White | Female | 1 | 0 | 0 |
| Masters   | 14     | Divorced | Exec-managerial | Not-in-family | White | Male | 0 | 1 | 1 |
class prove more problematic for BOA, which has more than 2000 FP-cases; comparatively, SOAR classifies the majority of those same cases as ambiguous.

Table 8 presents the most common patterns that appear in final positive and negative rule sets in 100 runs of the algorithm. These common patterns are consistent with those observed in the rules (8).

### 4.4 Car evaluation data

Car data from Bohanec and Rajkovic (1988) represents evaluation of 1728 cars according to six categorical variables:

- **buyingPrice**: buying price of a car
- **maintainPrice**: maintenance price
- **doors**: number of doors
- **persons**: number of passengers
- **lugBoot**: size of a trunk
- **safety**: safety level

The outcome variable indicates whether the car was assessed as not acceptable, acceptable, good, or very good. For the purpose of binary classification, we encode the unacceptable category as 0 and the three remaining categories as 1. The positive support is 518 observations and negative support is 1210 observations. We randomly split the data into a training set of 1200 observations and a test set of 528 observations. SOAR produces the following rules:

\[
R^+ = \{ (\text{buyingPrice}, \text{low}) \land (\text{persons}, 4) \land (\text{safety}, \text{high}), (\text{buyingPrice}, \text{med}) \land (\text{persons}, 4) \land (\text{safety}, \text{high}), \\
(\text{maintainPrice}, \text{low}) \land (\text{persons}, 4) \land (\text{safety}, \text{high}), (\text{maintainPrice}, \text{med}) \land (\text{persons}, 4) \land (\text{safety}, \text{high}), \\
(\text{maintainPrice}, \text{low}) \land (\text{persons}, \text{more}) \land (\text{safety}, \text{high})\}
\]

\[
R^- = \{ (\text{persons}, 2), (\text{safety}, \text{low}), (\text{buyingPrice}, \text{high}) \land (\text{maintainPrice}, \text{vhigh}), (\text{doors}, 2) \land (\text{lugBoot}, \text{small}), \\
(\text{buyingPrice}, \text{vhigh}) \land (\text{maintainPrice}, \text{vhigh}), (\text{buyingPrice}, \text{vhigh}) \land (\text{maintainPrice}, \text{high})\}
\]

Based on these rules, cars that are safe, spacious, and inexpensive (either in terms of buying or maintaining) are classified as acceptable, while small or expensive cars are classified as unacceptable. The comparison of all three algorithms is presented in Table 9.

Again, we see that observations truly misclassified by SOAR and SOAR-forced are few, while ambiguous cases account for most instances of overall misclassification. We present examples in Table 10 to illustrate how our algorithm manages to provide useful insights even when it is uncertain.

### Table 7 Comparison between traditional prediction classification for BOA and the newly proposed SOAR taxonomy using Adult data.

|     | CTP | CTN | CFN | CFP | AAN | AAP | PAN | PAP |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| TP  | 433 | 0   | 21  | 0   | 0   | 1234| 0   | 39  |
| TN  | 0   | 3525| 0   | 0   | 16  | 0   | 45  | 0   |
| FN  | 0   | 0   | 137 | 0   | 0   | 1   | 0   | 11  |
| FP  | 0   | 68  | 0   | 118 | 1864| 0   | 49  | 0   |

### Table 8 Most common rules for Adult data.

| Classification | Rule                                      | Frequency |
|---------------|-------------------------------------------|-----------|
| Positive      | (marital_status, Married-civ-spouse)      | 42        |
|               | (education_num, 15)                       | 38        |
|               | (education, Prof-school)                  | 37        |
| Negative      | (relationship, Own-child)                | 54        |
|               | (occupation, Other-service)               | 42        |
|               | (capital_gain, 0) \land (capital_loss, 0)| 41        |
We see that active ambiguous cases are those cars that appear small (two doors, small trunk), but are able to fit four or more people. Meanwhile, passive ambiguous cases are cars with medium safety (note that all rules for positive classification include literal [safety, high]), but they otherwise have low buying and maintenance prices and enough space, all of which we previously observed as associated with positive classification.

| SOAR          | BuyingPrice | MaintainPrice | Doors | Persons | lugBoot | Safety | Class |
|---------------|-------------|---------------|-------|---------|---------|--------|-------|
| Active ambiguous | Vhigh       | Low           | 2     | 4       | Small   | High   | 1     |
|               | Vhigh       | Low           | 2     | More    | Small   | High   | 0     |
|               | High        | Low           | 2     | More    | Small   | High   | 0     |
|               | Low         | Low           | 2     | 4       | Small   | High   | 1     |
| Passive ambiguous | Vhigh      | Med           | 2     | 4       | Big     | Med    | 1     |
|               | Low         | Med           | 3     | More    | Med     | Med    | 1     |
|               | Low         | Med           | More  | Big     | High    | 1     |
|               | High        | Low           | 4     | More    | Small   | Med    | 0     |

We are aware of a few limitations of our current work, each of which provides a valuable opportunity for continued exploration and future research. We focus our attention on a binary design matrix, and there may be instances where extending this framework to categorical or even continuous predictors may be warranted. The former seems straightforward, while using a preliminary binning of predictors (e.g., defined by quantiles) for continuous predictors could prove useful. Future research would be required to validate these ideas. Furthermore, we have not fully addressed the computational challenges of our framework for larger datasets, nor have we addressed the more general case of multiclass classification. A proper extension of our taxonomy of ambiguity to such a setting is not straightforward, as it would influence the log-likelihood and MAP estimator. Future research to address these known limitations may extend the use of the SOAR algorithm to a broader set of applications where IML algorithms are warranted.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available in UCI Machine Learning Repository at https://archive.ics.uci.edu/ml/. These data were derived from the following resources available in the public domain: - Car Evaluation Data Set, https://archive.ics.uci.edu/ml/datasets/car+evaluation - Adult Sata Set, https://archive.ics.uci.edu/ml/datasets/adult

ORCID

Elena Khusainova (https://orcid.org/0000-0001-9370-3597

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