Abstract

The overarching goal of Explainable AI is to develop systems that not only exhibit intelligent behaviours, but also are able to explain their rationale and reveal insights. In explainable machine learning, methods that produce a high level of prediction accuracy as well as transparent explanations are valuable. In this work, we present an explainable classification method. Our method works by first constructing a symbolic Knowledge Base from the training data, and then performing probabilistic inferences on such Knowledge Base with linear programming. Our approach achieves a level of learning performance comparable to that of traditional classifiers such as random forests, support vector machines and neural networks. It identifies decisive features that are responsible for a classification as explanations and produces results similar to the ones found by SHAP, a state of the art Shapley Value based method. Our algorithms perform well on a range of synthetic and non-synthetic data sets.

Introduction

The need for building AI systems that are explainable has been raised, see e.g., (Doran et al. 2017). The ability to make machine-led decision making transparent, explainable, and therefore accountable is critical in building trustworthy systems. Producing explanations is at the core of realising explainable AI. Two main approaches for explainable machine learning have been explored in the literature: (1) intrinsically interpretable methods (Rudin 2019), in which prediction and explanation are both produced by the same underlying mechanism, and (2) model-agnostic methods (Molnar 2019), in which explanations are treated as a post hoc exercise and are separated from the prediction model. In the case for methods (1), while many intrinsically interpretable models, such as short decision trees, linear regression, Naïve Bayes, k-nearest neighbours and decision rules (Yang et al. 2017) are easy to understand, they can be weak for prediction and suffer from performance loss in complex tasks. As for methods (2), model agnostic approaches such as local surrogate (Ribeiro et al. 2016), global surrogate (Alonso et al. 2018), feature importance (Fisher et al. 2018) and symbolic Bayesian network transformation (Shih et al. 2018) leave the prediction model intact and use interpretable but presumably weak models to “approximate” the more sophisticated prediction model. However, it has been argued that since model agnostic approaches separate explanation from prediction, explanation modules cannot be faithful representations of their prediction counterpart (Rudin 2019). In this context, we present a classification approach that produces accurate predictions and explanations as well as supports domain knowledge incorporation.

Given a set of data instances, whose class membership is known, classification is the problem of identifying to which of a set of classes a new instance belongs. Each instance is characterised by a set of features $F$. For some data $D$, there exists a labelling function $L : D \mapsto \{POS, -POS\}$.

Let $D \subseteq D$ be the training set s.t. for each $d \in D$, $L(d)$ is known. For $x \in D$, we would like to know:

- Q1: whether $L(x) = POS$.
- Q2: if so, which features $f \subseteq F$ make $L(x) = POS$.

Standard supervised learning techniques answer Q1 but not Q2, which asks for decisive features. Understanding “what causes a query instance $x$ to be classified as in some class $C$?” is as important as “does $x$ belong to $C$?” For instance, for a diagnostic system taking patients’ medical records as the input and producing disease classifications as the output, pinpointing symptoms that lead to the diagnosis is as important as the diagnosis itself. In this paper, we propose algorithms answering both questions. In a nutshell, we solve classification as inference on probabilistic Knowledge Bases (KBs) learned from data. Specifically, given training data $D$ with features $F$, we define a function $M$ that maps $D$ to a probabilistic KB. Then, for a query $x$, we check whether $M(D)$ and $x$ together entail $POS$. Very roughly, we take classification as evaluating

$$\mathcal{M}(D), x \models POS. \quad (1)$$

In this way, computing explanations for $L(x) = POS$ in our setting can be formulated as:

Given $\mathcal{M}(D), x \models POS$, identify some $x' \subseteq x$ s.t.

$$\mathcal{M}(D), x' \models POS.$$  

We present two algorithms for probabilistic KB construction. The first one constructs KBs from decision trees and.

$^1$POS stands for positive. For presentation simplicity, we only consider binary classification problems in this paper. Our approach generalises to multi-category classification by replacing POS with class labels for each candidate class accordingly.
the second constructs KBs directly from data. Query classification is modelled with probabilistic logic inference carried out with linear programming. The main contributions are: (i) a method of performing classification with probabilistic logic inference; (ii) a polynomial time inference algorithm on KBs; and (iii) algorithms for identifying decisive features as explanations and incorporating domain knowledge in classification and explanation.

Training as Knowledge Base Construction

KB construction is at the core of our approach. Specifically, a KB contains a set of disjunction clauses and each clause has a probability, defined formally as follows.

**Definition 1.** A Knowledge Base (KB) \( \{\langle p_1, c_1\rangle, \ldots, \langle p_m, c_m\rangle\} \) is a set of pairs of clauses \( c_i \) and probability of clauses \( p_i = P(c_i), 1 \leq i \leq m \). Each clause is a disjunction of literals and each literal is a propositional variable or its negation.

**Example 1.** With two propositional variables \( \alpha \) and \( \beta \), \( \{(0.6, \neg \alpha \lor \beta), (0.8, \alpha)\} \) is a simple KB containing two clauses with probabilities 0.6 and 0.8, respectively.

Generating logic clauses from data has been studied in the literature, see e.g., (Chiang et al. 2001; Quinlan 1987) for extracting rules from decision trees, and more recently, (Mashayekhi and Gras 2017) for extracting rules from random forests. Unlike these approaches where, due to their use of strict inference methods, non-probabilistic rules are generated, our KBs consist of probabilistic rules. Specifically, from a decision tree constructed from the training data, we create a clause \( c \) from each path from the root to the leaf of the tree. The probability of \( c \) is the ratio between the positive samples and all samples at the leaf. Formally, we define the KB \( K_T \) drawn from a decision tree \( T \) as follows.

**Definition 2.** Let \( T \) be a decision tree, each non-root node in \( T \) labelled by a feature-value pair \( a_i \), read as feature \( a \) having value \( v \). Let \( \{p_1, \ldots, p_k\} \) be the set of root-to-leaf paths in \( T \), where each \( p_i \) is of the form \( \langle \text{root}, a_1, v_1, \ldots, a_n, v_m\rangle \) and \( a_n, v_m \) labels a leaf node in \( T \). Then, the KB drawn from \( T \) is \( K_T = \{\langle p_1, c_1\rangle, \ldots, \langle p_k, c_k\rangle\} \) s.t. for each \( p_i \), \( \langle p_i, c_i\rangle \in K_T \), where \( c_i = \text{POS} \lor \neg a_1, v_1, \ldots, \lor \neg a_n, v_m \), and \( p_i \) is the ratio between positive and the total samples in \( n \cdot v_m \).

Algorithms 1 and 2 construct \( K_T \) from data \( D \). Specifically, Algorithm 1 takes a root-to-leaf path from a decision tree to generate a clause. The path with features \( a_1, \ldots, a_n \), s.t. each feature has a value in \( \{v_1, \ldots, v_m\} \), is interpreted as \( a_1, v_1 \land \ldots \land a_n, v_m \rightarrow \text{POS} \), and read as, a sample is positive if its feature \( a_1 \) has value \( v_1 \), . . . , feature \( a_n \) has value \( v_m \). As a disjunction, the clause is then written as \( \text{POS} \lor \neg a_1, v_1 \lor \ldots \lor \neg a_n, v_m \). Algorithm 2 builds a tree and then constructs clauses from paths in the tree. Example 2 illustrates how to build a KB from a decision tree.

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**Algorithm 1: Clause from Tree Path**

1: \( \text{procedure} \) ClauseFromPath(path)
2: \( \text{clause} \leftarrow \text{POS} \)
3: \( \text{for each edge } e \text{ in } \text{path do} \)
4: \( \text{a} \leftarrow \text{feature of } e \)
5: \( \text{v} \leftarrow \text{value of } e \)
6: \( \text{clause} \leftarrow \text{clause} \lor \neg \text{a}_{i,v} \)
7: \( \text{return clause} \)

**Algorithm 2: Construct KB with Decision Tree**

1: \( \text{procedure} \) DecisionTreeKB(D)
2: \( K_T \leftarrow \{} \); Use ID3 to compute a tree \( T \) from \( D \)
3: \( \text{allPaths} \leftarrow \text{all paths from the root to leaves in } T \)
4: \( \text{for each path in allPaths do} \)
5: \( n \leftarrow \text{end node in path} \)
6: \( r \leftarrow \text{ratio between positive and total samples in } n \)
7: \( \text{add } [r] \text{ ClauseFromPath(path)} \text{ to } K_T \)
8: \( \text{return } K_T \)

**Example 2.** Given a data set with four strings, 0000, 1111, 1100, 0011, 1011, 1000, labelled positive, and four strings, 0101, 0100, 1110, 1000, labelled negative. There are four features, bits 1–4, each feature takes its value from \( \{0, 1\} \). The decision tree constructed is shown in Figure 1. There are eight leaves, thus eight root-to-leaf paths and clauses. E.g., \( \text{root} \rightarrow a_3, 0 \rightarrow a_2, 0 \rightarrow a_3, 0 \) gives the clause \( \text{POS} \lor \neg a_1, 0 \lor \neg a_1, 0 \lor \neg a_1, 0 \). The probability of the clause is the number of positive samples over the total samples at the leaf. There is only one sample, 0000, at this leaf, since it is positive, the clause probability is 1. The KB \( K_T \) is shown in Table 1.

![Decision tree](image)

Figure 1: Decision tree learned from data in Example 2. A node \( a_i \rightarrow Y \) is read as “bit \( X \) has value \( Y \)”.

| Table 1: \( K_T \) from the tree in Figure 1. |
|-------------------------------------------|
| [0.0] POS \lor \neg a_3, 0 \lor \neg a_3, 0 \lor \neg a_3, 0 |
| [1.0] POS \lor \neg a_3, 0 \lor \neg a_3, 0 \lor \neg a_3, 0 |
| [0.0] POS \lor \neg a_3, 0 \lor \neg a_3, 0 \lor \neg a_3, 0 |
| [1.0] POS \lor \neg a_3, 0 \lor \neg a_3, 0 \lor \neg a_3, 0 |
| [0.0] POS \lor \neg a_3, 0 \lor \neg a_3, 0 \lor \neg a_3, 0 |
| [1.0] POS \lor \neg a_3, 0 \lor \neg a_3, 0 \lor \neg a_3, 0 |
| [0.0] POS \lor \neg a_3, 0 \lor \neg a_3, 0 \lor \neg a_3, 0 |

Algorithm 2 constructs clauses from root-to-leaf paths in a decision tree. We can also use paths from the root to all nodes, not just the leaves, to construct clauses, i.e., replacing \( [p] \) by \( z_1 \lor \ldots \lor z_l \) denotes an \( l \)-literal clause in a KB with probability \( p \).
line 3 in Algorithm 2 with
\[ \text{allPaths} \leftarrow \text{all paths from the root to all nodes} \text{ in } T. \]
As random forests have been introduced to improve the stability of decision trees, we can apply the same idea to obtain more clauses from a forest, i.e., repeatedly generated different decision trees, and for each tree, we construct clauses for each path originated at its root, in the spirit of (Mashayekhi and Gras 2017). If we further take the above idea of "generating as many clauses as possible" to its limit, we realise that constructing KBs from trees is a special case of selecting clauses constructed from all \( k \)-combinations of feature-value pairs, for \( k = 1 \ldots n \), where \( n \) is the total number of features in the data. Formally, we define the KB \( K_0 \) drawn directly from data \( D \) as follows.

**Definition 3.** Given data \( D \) with features \( F = \{a_1, \ldots, a_n\} \) taking values from \( V = \{v_1, \ldots, v_m\} \), for each \( F_k = \{a_1', \ldots, a_k'\} \in 2^F \setminus \{\} \), let \( C_k = \{a_i'v_i \mid v_i \in V\}, \ldots, C_{k}^{(v)} = \{a_i'v_i \mid v_i \in V\}. \) For each \( c = \{a_1'v_1, \ldots, a_k'v_k\} \in C_k, S_i \subseteq D \) is the set of samples s.t. feature \( a_i \) having value \( v_i \) for all \( i \in \{1, \ldots, k\} \). If \( |S_i| \neq 0 \), then let \( p_i \) be the ratio between positive samples in \( S_i \) and \( |S_i| \). \( (p_1, \ldots, p_k) \in \mathbb{R}^k \) is in the KB \( K_0 \) drawn directly from data. There is no other clause in \( K_0 \) except those constructed as above.

Definition 3 can be illustrated with the following example.

**Example 3.** Let \( F = \{a_1, a_2\} \) and \( V = \{0, 1\} \). Then \( 2^F \setminus \{\} = \{\{a_1\}, \{a_2\}, \{a_1, a_2\}\} \). For illustration, let us choose \( F_k = \{a_1, a_2\} \). Then \( C_k = \{a_1, a_2, 1\}, C_{k}^{(0)} = \{a_2\} \). Then \( (p_1, \ldots, p_k) \in \mathbb{R}^k \) is in the KB \( K_0 \) drawn directly from data. There is no other clause in \( K_0 \) except those constructed as above.

**Algorithm 3 Construct KB Directly**

```
1: procedure DIRECTKB(data)
2:  counts ← \{\}, \( K_0 \) ← \{\}
3:  for each entry in data do
4:  feaVals ← \{a_i \mid a_i \text{ has value } v \text{ in entry}\}
5:  label ← binary label of entry as integer
6:  \( S \leftarrow \text{POWerset(feaVals)} \setminus \{\} \)
7:  for each key as an element of \( S \) do
8:    if key is in counts then
9:      counts[key] ← counts[key] + [1, label]
10:  else
11:    counts[key] ← [1, label]
12:  for each key in counts do
13:    \( r \leftarrow \text{counts[key]}[1]/\text{counts[key]}[0] \)
14:    Insert \( \langle r \rangle \text{ POS } \wedge \neg \text{key} \rangle \text{ to } K_0\)
15: return \( K_0 \)
```

Algorithm 3 gives a procedural construction for \( K_0 \).\(^3\) The following propositions describe the relation between the two KB construction approaches. Proposition 1 and 2 sanction that all clauses extracted from decision trees can be constructed directly in \( K_0 \) and all clauses built in \( K_D \) can be extracted from some trees, respectively.

**Proposition 1.** Given a data set \( D \), \( K_T \subseteq K_0 \).

**Proof.** (Sketch.) \( S \) constructed in Line 6, Algorithm 3 is the powerset of all possible feature-value pairs in \( D \) and a path in a decision tree represents some feature-value pairs in \( D \). Thus, any clause produced by a tree is produced by Algorithm 3.

**Proposition 2.** Given a data set \( D \), for each clause \( c \in K_0 \), there exists a decision tree \( T \) constructed from \( D \) s.t. there is a path \( p \in T \) and the clause drawn from \( p \) is \( c \).

**Proof.** (Sketch.) All clauses in \( K_0 \) are of the form \( \text{POS } \vee \neg a_1 \text{v}_1 \vee \cdots \vee \neg a_n \text{v}_n \) where \( a_i \text{v}_j \) are feature-value pairs and for any \( a_i, a_j \in \{a_1, \ldots, a_n\} \), if \( i \neq j \), then \( a_i \neq a_j \). Thus, one can construct a tree \( T \) containing the path \( \text{root } \rightarrow a_1 \text{v}_1 \rightarrow \cdots \rightarrow a_n \text{v}_m \).

**Querying as Probabilistic Inference**

Our KB construction methods produce clauses with probabilities. Intuitively, for a query that asserting some feature-value pairs, we want to compute the probability of \( \text{POS} \) under these feature-value pairs and predicting the query being positive when the probability is greater than 0.5. To introduce our inference method for computing such probabilities, we first review a few concepts in probabilistic logic (Nilsson 1986), which pave the way for discussion.

Given a KB \( K^3 \) with clauses \( c_1, \ldots, c_m \) composed from \( n \) propositional variables, the complete conjunction set, as \( W \), over \( K \) is the set of \( 2^n \) conjunctions s.t. each conjunction contains \( n \) distinct propositional variables. A **probability distribution** \( \pi \) (w.r.t. \( K \)) is the set of \( 2^n \) probabilities \( \pi(w) \geq 0, (w \in W) \) s.t. \( \sum_{w \in W} \pi(w) = 1 \). \( \pi \) satisfies \( K \) iff for each \( i = 1, \ldots, m \), the sum of \( \pi(w) \) equals \( P(c_i) \) for all \( w \) s.t. the truth assignment satisfying \( w \) satisfies \( c_i \). A KB \( K \) is **consistent** iff there exists a \( \pi \) satisfying \( K \).

With a consistent KB, Nilsson suggested that one can derive **literal probabilities** from \( \pi \), i.e., for all literals \( z \) in the KB, \( P(z) \) is the sum of \( \pi(w) \) for all \( w \in W \) containing \( z \), e.g., for a consistent KB with two literals \( \alpha \) and \( \beta \), \( P(\alpha) = P(\alpha \land \beta) + P(\alpha \land \neg \beta) \) (Nilsson 1986). In short, to compute literal probabilities, one first computes probability assignments over the complete conjunction set, and then adds up all relevant probabilities for the literal.

At first glance, since \( \text{POS} \) is an literal in our knowledge base, it might be possible to perform our inference with the above approach for computing \( P(\text{POS}) \): all clauses in a KB are of the form \( \text{POS } \vee \neg a_1 \text{v}_1 \vee \cdots \vee \neg a_n \text{v}_m \) each with an associated probability; a query is a set of

\[ \text{and values being two-element arrays. label} \text{ is either 0 or 1. Line 9 is an element-wise addition, e.g., } [1,0]+[1,1]=[2,1]. \text{ At the end of the first loop, } counts[\text{key}][0] \text{ is the number of samples containing key and } counts[\text{key}][1] \text{ is the number of positive ones.} \]

\(^3\)From this point on, we use \( K \) to denote a KB constructed using either of the two approaches (\( K_T \) or \( K_D \)).
feature-value pairs, e.g., \(a_1^{v_1}, \ldots, a_m^{v_m}\), each with an assigned probability 1: \(P(\text{POS})\) computed as the sum of \(P(\text{POS} \land a_1^{v_1} \land \ldots \land a_m^{v_m})\), \(P(\text{POS} \land a_1^{0} \land \ldots \land a_m^{0})\), \(\ldots, P(\text{POS} \land a_1^{0} \land \ldots \land a_m^{0})\) estimates the likelihood of POS. However, this idea fails for the following two reasons. Firstly, this approach requires solving the probability distribution \(\pi\), which has been shown to be NP-hard wrt. the number of literals in the KB (Georgakopoulos et al., 1988), thus the state-of-the-art approaches only work for KB with a few hundred of variables (Finger and Bona, 2011).

Secondly, putting a KB and a query together introduces inconsistency, so there is no solution for \(\pi\). For instance, for the KB in Example 2, let the query be 0000, which translates to four clauses, \(a_1^{0}, a_2^{0}, a_3^{0}\) and \(a_4^{0}\), each with \(P(a_i^{0}) = 1\). Consequently, \(P(\neg a_i^{0}) = 0\). Together with \(P(\text{POS} \lor \neg a_1^{0} \lor \neg a_2^{0} \lor \neg a_3^{0} \lor \neg a_4^{0}) = 1\), we infer \(P(\text{POS}) = 1\). However, \(P(\text{POS}) = 1\) is inconsistent with \(P(\text{POS} \lor a_1^{0} \lor a_2^{0} \lor a_3^{0} \lor a_4^{0}) = 0\), as for any \(\alpha, \beta\), we must have \(P(\alpha) \leq P(\alpha \lor \beta)\). In this case, \(K\) is inconsistent with the query thus there is no solution for \(\pi\).

One might suspect the inconsistency illustrate above is an artefact of our KB construction, i.e., there could exist ways later in this paper, it becomes clear that being able to tolerate some of the constraints cannot be met, we allow clause probabilities to be relaxed by not forcing \(\omega(c_i) = P(c_i)\) as constraints. We still want the estimated clause probabilities \(\omega(c_i)\) to be as close to their specified values \(P(c_i)\) as possible, so Eqn. (2) minimises their difference. A linear difference is chosen to ensure a low computational complexity.

Note that, for all literals in a clause, their estimated probabilities are constrained by inequalities local to the clause (e.g., \(\omega(c_i) \leq \omega(z_1) + \ldots + \omega(z_l)\)). We avoid the exponential growth of constraints, which causes the NP computational difficulties, by forgoing not only explicit probability computation for the complete conjunction set but also global constraints on estimated clause probabilities, e.g., for two clauses \(c_1 = \alpha \land \beta\) and \(c_2 = \alpha \lor \beta \lor \gamma\), we do not enforce \(\omega(c_1) \leq \omega(c_2)\). We illustrate probability computation with the following example.

**Example 4. (Example 1 cont.)** Given these two clauses, \(c_1 = \neg \alpha \land \beta; c_2 = \alpha, \) and their probabilities, \(P(c_1) = 0.6, P(c_2) = 0.8,\) the complete conjunction set \(\mathcal{W} = \{\neg \alpha \land \neg \beta, \neg \alpha \land \beta, \alpha \land \gamma, \alpha \land \beta \land \gamma\}\). Truth assignments satisfying \(\alpha \land \beta, \neg \alpha \land \beta,\) and \(\alpha \land \neg \beta\) satisfy \(c_1\) and truth assignments satisfying \(\alpha \land \beta\) and \(\alpha \land \neg \beta\) satisfy \(c_2\). \(K\) is consistent iff \(\pi_1 = \pi(\alpha \land \beta), \pi_2 = \pi(\alpha \land \beta), \pi_3 = \pi(\alpha \land \beta),\) and \(\pi_4 = \pi(\neg \alpha \land \neg \beta)\) s.t. \(\sum_{j=1}^{4} \pi_j = 1, \pi_1 + \pi_3 + \pi_4 = 0.6\) and \(\pi_1 + \pi_2 = 0.8, L_K\) is:

\[
\minimise: ||\omega(c_1) - 0.6| + |\omega(c_2) - 0.8|
\]

subject to:

\[
\omega(c_1) \leq \omega(\neg \alpha) + \omega(\beta); \quad \omega(c_2) \leq \omega(\alpha);
\]

\[
\omega(c_1) \geq \omega(\neg \alpha); \quad \omega(c_1) \geq \omega(\beta); \quad \omega(c_2) \geq \omega(\alpha);
\]

\[
1 = \omega(\alpha) + \omega(\neg \alpha); \quad 1 = \omega(\beta) + \omega(\neg \beta);
\]

\[
0 \leq \omega(\alpha) \leq 1; \quad 0 \leq \omega(\beta) \leq 1.
\]

A solution to \(L_K\) is:

\[
\omega(-\alpha \lor \beta) = 0.6; \quad \omega(\alpha) = 0.8; \quad \omega(\neg \alpha) = 0.2; \quad \omega(\beta) = 0.6; \quad \omega(\neg \beta) = 0.4.
\]

It is easy to see that \(K\) is consistent, and for all literals \(z\) in \(K\), \(\omega(z)\) is a probability assignment for \(z\). Definition 4 gives a means of performing probabilistic inference, as this Example can be seen as modus ponens, i.e., from \((\alpha \land \beta) = \gamma\) where \(P(\alpha \lor \beta) = 0.6, P(\alpha) = 0.8,\) we infer \(\omega(\beta) = 0.6\).

In general, for a literal \(z\) in a KB \(K\), it may be the case that no \(\pi\) exists such that \(\omega(z)\) equals the probability computed from \(\pi\). For example, consider:

**Example 5.** Let \(K = \{c_1 \ldots c_4\}, in which \(c_1\) is \([1.0, 0]\) \(\alpha \lor \beta; c_2\) is \([1.0, 0]\) \(\alpha \lor \gamma; c_3\) is \([1.0, 0]\) \(\beta \lor \gamma; c_4\) is \([1.0, 0]\) \(\alpha \lor \beta \lor \gamma\),

Then, \(\omega(c_1) = 1, \omega(\alpha) = \omega(\beta) = \omega(\gamma) = 0.5\) is a solution to \(L_K\) where the objective function attains 0. However, \(\omega(z) \neq P(z), for z = \alpha, \beta, \gamma\).

This shows that \(L_K\) has a feasible region larger than the solution space of \(\pi\). However, since linear programming algorithms look for solutions at the boundary of variables, we do not see such solutions in practice. Indeed, the Gurobi solver finds \(\omega(z) = P(z) = 1, for z = \alpha, \beta, \gamma, which are in the solutions computed with Nilsson’s method.\)
Relations between literal probability found via computing exact solutions from the distribution over the complete conjunction set and solutions found in L_K are as follows.

**Lemma 1.** If \( K \) is consistent, then solutions for all \( \omega(z) z \in Z \) exist s.t. Eqn. (2) minimises to 0.

**Proof.** (Sketch.) Eqn. (2) minimises to 0 only when \( \omega(c_i) = p_i \) for all \( c_i \). If \( K \) is consistent, then there is an assignment of values to the literal probabilities that satisfies the constraints, i.e., for all literals \( z \) and all clauses \( c \), \( \omega(z) = P(z) \) and \( \omega(c) = P(c) \) minimise (2) to 0. \( \square \)

**Corollary 1.** Given a KB \( K \), if \( L_K \) does not minimise to 0, then \( K \) is not consistent.

**Proof.** (Sketch.) By the contrapositive of Lemma 1, if there is no assignment that solves the linear programming problem, then there is no exact solution for \( \pi \). \( \square \)

**Proposition 3.** Given a KB \( K \) with \( n \) propositional variables \( x_1, \ldots, x_m \), each \( \omega(x_i) \) in \( L_K \) can be computed in polynomial time wrt. \( n \).

**Proof.** (Sketch.) Let \( n \) be the number of unknowns in \( L_K \), \( m \) the number of clauses in \( K \), \( n = 2n + m \). Linear Programming is polynomial time solvable. \( \square \)

It is theoretically interesting to ask, for consistent KBs, what the error bound between literal probability computed with Nilsson’s method and our linear programming method is, subject to a chosen linear programming solver. However, in the context of this work, answering such question is less important as KBs generated by our approach are not necessarily consistent. For such KBs, Nilsson’s approach gives no solution thus these is no “error bound” exists.

With a means to reason with KBs, we are ready to answer queries. Algorithm 4 defines the query process. Let \( L_K \) be the linear system constructed from \( K \). Given a query \( Q \) with feature-value pairs \( a_1, \omega_1, \ldots, a_m, \omega_m \), we amend \( L_K \) by inserting \( \omega(a_i, v_j) = 1 \) and \( \omega(a_i, v_j) = 0 \), where \( v_j \) is a possible value of \( a_i, v_j \neq v_j \), for all \( a_i, v_j \) in \( Q \). \( \omega(P\{\}) \) computed in \( L_K \) answers whether \( Q \) is positive. Since the solution of \( \omega(P\{\}) \) can be a range, we compute the upper and lower bounds of \( \omega(P\{\}) \) by maximising and minimising \( \omega(P\{\}) \) subject to minimising Eqn.(2), respectively, and use the average of the two. It returns positive when the average is greater than 0.5. The intuition of our approach is that, for a query \( x \), to evaluate whether \( K, x \models \mathcal{P} \), we compute \( \omega(P\{\}) \) in \( L_K \), in which \( K \) is treated “ defeasibly” s.t. the probabilities of a clauses in \( K \) can be relaxed whereas the query \( x \) is treated “strictly” as constraints in \( L_K \). Example 6 illustrates the query process.

**Example 6.** (Example 2 cont.) For query 0101, we add the following equations as constraints to \( L_K \):

\[
\begin{align*}
\omega(a_1, 0) &= 1, & \omega(a_1, 1) &= 0, & \omega(a_2, 0) &= 0, & \omega(a_2, 1) &= 1, \\
\omega(a_3, 0) &= 1, & \omega(a_3, 1) &= 0, & \omega(a_4, 0) &= 0, & \omega(a_4, 1) &= 1.
\end{align*}
\]

The computed \( \omega(P\{\}) \) is no greater than 0.5, representing a negative classification.

**Algorithm 4 Query Knowledge Base**

1: procedure QueryKB(query, \( L_K \))
2: for each feature \( a \) in query do
3: for each possible value \( v \) of \( a \) do
4: if \( a \) has value \( v \) in query then
5: \( \omega(a_{a,v}) = 1 \) to \( L_K \)
6: else
7: \( \omega(a_{a,v}) = 0 \) to \( L_K \)
8: return \( \omega(P\{\}) \) computed in \( L_K \)

The proposed querying mechanism differs fundamentally from that of decision trees. A decision tree query can be viewed as finding the longest clause in the KB that matches with the query in and checking whether its probability is greater than 0.5. For instance, for query 0101, a decision tree query returns positive as the longest matching clause in “\( \text{POS} \lor \neg a_4 \)” has probability 1. However, our approach considers probabilities from other clauses in the \( K \) and produces a different answer.

Since KB constructed with Algorithm 3 contains far more clauses than Algorithm 2, to improve query efficiency, for a given query \( Q \), we can construct a KB that only contains clauses directly relevant to \( Q \), as shown in Example 7, and perform query on this subset of clauses, as shown in Algorithm 5. The query performed on the relevant KB gives the same result as in the full KB, \( K_0 \), as irrelevant clauses give no additional constraint to \( \omega(P\{\}) \).

**Algorithm 5 Construct Relevant Knowledge Base**

1: procedure QueryRelevant\( (Q, K_0) \)
2: \( \text{featVals} \leftarrow \{a \mid \text{feature } a \text{ has value } v \text{ in } Q \} \)
3: \( S \leftarrow \text{PowerSet(}\text{featVals} \) \( \setminus \{\} \) \)
4: for each key \( a \) in \( S \) do
5: for each clause in \( K_5 \) do
6: if clause contains key then
7: Insert clause to relevantKB
8: return relevantKB

**Example 7.** (Example 6 cont.) relevantKB for query 0101 is follows:

\[
\begin{align*}
\text{PO} & \lor \neg a_4 \lor \neg a_3 \lor \neg a_1 \lor \neg a_2, \quad \text{PO} \lor \neg a_4 \lor \neg a_3, \\
\text{PO} & \lor \neg a_3, \quad \text{PO} \lor \neg a_4 \lor \neg a_1, \\
\text{PO} & \lor \neg a_3 \lor \neg a_1, \quad \text{PO} \lor \neg a_4 \lor \neg a_2, \\
\text{PO} & \lor \neg a_4 \lor \neg a_3, \quad \text{PO} \lor \neg a_3 \lor \neg a_1 \lor \neg a_2 \lor \neg a_4.
\end{align*}
\]

Overall, our method is non-parametric so no tuning is required. Query generalization is the result of restricting the solution space of \( \omega(P\{\}) \) through clauses describing subsets of the query. In Example 7, 0101 is not in the training set. However, the relations between its substrings and \( \text{PO} \) are described by clauses in the KB. Jointly, these clauses decide \( \omega(P\{\}) \), which approximates \( P(P\{\}) \) for this query.

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4In line 6, a clause containing a key is defined syntactically, e.g., “\( \text{PO} \lor \neg a_1 \lor \neg a_2 \lor \neg a_4 \)” contains \{\( \neg a_1 \lor \neg a_2 \lor \neg a_4 \)\}.  
5In line 6, a clause containing a key is defined syntactically, e.g., “\( \text{PO} \lor \neg a_1 \lor \neg a_2 \lor \neg a_3 \lor \neg a_4 \)” contains \{\( \neg a_4 \lor \neg a_3 \lor \neg a_1 \lor \neg a_2 \lor \neg a_4 \)\}.  

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Explanation and Knowledge Incorporation

Several methods for comparing feature importance as a form of explanation have been introduced in the literature. Some of these methods, e.g. (Zhao and Hastie 2019) and (Apley and Zhu 2016), study the relation between features and the overall classification for all training cases. They are “global” methods in the sense that they answer the question: “Which feature has the strongest correlation with the class label in a dataset?” Whereas other methods, notably Shaply Value based approaches (Strumbelj and Kononenko 2014; Lundberg and Lee 2017; Lundberg et al. 2020), study feature value contribution for individual instances. They are “local” and answer: “For a given query instance, how much contribution does each of its feature value make?” In this sense, ours is a local approach that explains query instances.

One advantage of the presented classification method is that it supports partial queries, which are queries with missing values, as the probability of POS can be computed without values assigned to all features. Explanation computation can be supported with partial queries in our approach. Algorithm 6 outlines one approach. Given a query Q with n features, to find the k most decisive features, we construct sub-queries s.t. each sub-query contains exactly k feature-value pairs in Q. If Q yields a positive classification, then the sub-query that maximises $\omega(\text{POS})$ is an explanation; otherwise, the sub-query that minimises $\omega(\text{POS})$ is. Since we know that there are $\binom{n}{k}$ different sub-queries in total, the order of sub-query evaluation can be strategised with methods such as hill climbing for more efficient calculation. Although in principle, Algorithm 6 could work with any classification technique supporting partial queries, our proposed method does not require reconstructing the trained model for testing each of the sub-queries, making the explanation generation convenient. The explanation approach is illustrated in Example 8.

**Algorithm 6 Explanation Computation**

1: procedure COMPUTEEXPLANATION(Q, L_k, k)  
2: $S \leftarrow \{q \in Q \in 2^Q, \text{SIZE}(q) = k\}$  
3: if QUERYKB(Q, L_k) > 0.5 then  
4: return $\arg \max_{q \in S} \text{QUERYKB}(q, L_k)$  
5: else  
6: return $\arg \min_{q \in S} \text{QUERYKB}(q, L_k)$

**Example 8.** (Example 6 cont.) To compute the single most decisive feature, we let $k = 1$. $S$ contains four feature-value pairs: $q_1 = \{a_1, 0\}$, $q_2 = \{a_2, 1\}$, $q_3 = \{a_3, 0\}$, $q_4 = \{a_4, 1\}$. Let $\omega_1, i = 1 \ldots 4$ be $\omega(\text{POS})$ computed with $q_1 \ldots q_4$, respectively. We have $\omega_1 = 0.33$, $\omega_2 = 0.5$, $\omega_3 = 0.5$, and $\omega_4 = 1$. Thus, the computed explanation for the classification is $a_4, 0$. We read this as: $0 \ldots \cdot$ is responsible for 0101 being negative.

This matches with our intuition well as for each of the other choices, there are at least as many positive samples as negative ones.

Note that there is a subtle difference between our approach and Shaply Value based methods. Upon computing a $k$-feature explanation, our approach considers $\binom{n}{k}$ $k$-feature coalitions and select the “most decisive” coalition. Whereas Shaply Value approaches consider each feature individually and returns the set of $k$ most decisive features.

Incorporating domain knowledge to complement data-driven machine learning is supported by our approach. Since a KB consists of probabilistic clauses, any knowledge $K'$, about either a specific query or the overall model, can be used alongside $K$, as long as it is represented in clausal form. In other words, Equation 1 can be revised to

$$\mathcal{M}(D), K', x \models \text{POS}. \quad (7)$$

Two advantages of our approaches is (1) incorporated knowledge is used in the same way as clauses learned from data; and (2) since the inference process tolerates inconsistency, incomplete or imperfect knowledge can be incorporated. For instance, suppose we somehow know it is “mostly true” that a string is positive if either its 3rd or 4th digit is 0. If we liberate “mostly true” as, saying, probability 0.9, this can be represented as $a_3 \lor a_4 \rightarrow \text{POS}$, so we insert $[0.9] \cdot \text{POS} \lor \neg a_3 \land \neg a_4$ into $K$ to complement clauses learned from data. Although similar clauses or even the same clause with different probabilities may already exist in the KB, our ability of tolerating inconsistencies could accommodate such knowledge, as shown in the next section.

Performance Analysis

Definition 4 gives an efficient system construction. As shown in Figure 2, we can solve KBs containing up to 10,000 variables and 10,000 clauses within a few seconds on a single CPU workstation with an Xeon 2660v2 processor and 32GB RAM. The ability of approaching KBs of such large sizes enables solving practical classification tasks.

![Figure 2: Experiment results from KB with different sizes.](https://www.kaggle.com/c/titanic)

To evaluate the proposed classifiers, we first conduct experiments on six real data sets, with results shown in Table 2. For each data set, we measure the performance with the $F_1$ score, taken as the average of 50 runs for each data set. Our approaches are Tree (Algorithm 2) and Direct (Algorithm 3). We use CART (a decision tree algorithm), multi-layer perceptron (MLP) neural networks (with two hidden layers with 12 and 10 nodes, respectively), random forest (with 100 trees) and support vector machine as our comparison baselines. The six real data sets include the Titanic data set and Mushroom, Nursery and HIV-1 protease cleav-
age data sets from the UCI Machine Learning Repository (Dua and Karra Taniskidou 2017), the UK parliament bill data set reported in (Cyras et al. 2019) as well as an image data set for vehicle classification. For the Titanic data set, we used seven discrete features – ticket class, sex, age (discretized to 4 categories), number of siblings, number of parents, passenger fare (discretized to 3 categories), and port of embarkation. For the Mushroom data set, we used the first 11 features. For the multi-class data set Nursery, we randomly selected two classes and discarded others. For the Parliament bill, we used five features – House of Commons or House of Lords, type of bill, number of sponsors, bill subject, and final stages of the bill. The vehicle image data set contains 1635 images with 767 of them being cars and the rest busses and trucks. Feature extraction has been applied with 12 features created for each image. They are: number of pixels of the object, shape coefficient 1-5, mean and standard deviation of RGB channels. Each data set has been pre-processed such that the positive and the negative samples are balanced by randomly replicating samples in the smaller class. For all data set, the ratio between training and testing is 70% to 30%. Overall, we see that Direct gives satisfactory performance.

To evaluate our explanation approach, we first compare Direct with the state of the art Shapley Value based approach SHAP (Lundberg et al. 2020), using the Titanic and Mushroom data sets. The results are shown in Figure 3, with Figure 3(a)(b) showing the results from the Titanic data set and Figure 3(c)(d) from the Mushroom. Figure 3(a) shows the percentage of the same features suggested as explanations for different explanation lengths (i.e., \( k = 1, 2, 3, 4, 5 \)). For example, when \( k = 1 \) (computing one-feature explanations), 75% of all instances have the same feature chosen as the explanation by both approaches. When \( k = 2 \) (computing two-feature explanations), there are 72% and 25% instances found with the same 1 and 2 features, respectively. Figure 3(b) shows the percentage of each feature being selected as an explanation across all instances. We see that when \( k = 1 \), ours and SHAP both suggest that feature 2 explains the classification result for over 70% instances. When \( k = 2 \), the two approaches agree that feature 2 is an explanation while differing on the choice for the other feature.

Results presented in Figure 3 shows that our approach gives similar results to SHAP. As there is no explanation ground truth in these data sets, it is impossible to decide who gives “correct” explanations. To address this, we performed further experiments with synthetic data sets with known explanation ground truth. Specifically, we created four synthetic data sets of integer strings, Syn 10/4, Syn 10/8, Syn 12/4, and Syn 12/8, with the following rules. For each data set, we set a (random) seed string of the same length as strings in the data set from the same alphabet. For instance, for the “Syn 10/4” data set with 10 bits strings where each bit can take 4 possible values, 3232411132 is the seed. (Here, the size of the alphabet is 4. Each 10-bit string denotes a data instance with 10 features s.t. each feature takes its value from \{1,2,3,4\}. A string \( s \) in the data set is labelled positive if \( s \) match bits in the seed for exactly five places. E.g., 3133421242 is positive and 3133421232 is negative (it shares 6 bits as the seed rather than 5). For each string classified as positive, we compute a \( k \)-bit explanation. An explanation is correct if the seed string has the same values for the bits identified as the explanation. The accuracy of an explanation is defined as the number of correct bits over the length of explanation. For instance, for \( k = 5 \), we have

| Query | Explanation | Seed | Accuracy |
|-------|-------------|------|----------|
| Syn 10/4 | 0.71 | 0.78 | 0.62 | 0.70 |
| Syn 10/8 | 0.92 | 0.95 | 0.89 | 0.94 |
| Syn 12/4 | 0.79 | 0.87 | 0.70 | 0.84 |
| Syn 12/8 | 0.77 | 0.83 | 0.73 | 0.80 |

Table 3: Experiment results (F1 scores) with synthetic data sets and several baseline algorithms.

| Data Set | Titanic | Mushroom | Nursery | HIV-1 | Bill | Vehicle |
|----------|---------|----------|---------|-------|------|---------|
| Tree     | 0.79    | 0.99     | 0.99    | 0.87  | 0.98 | 0.95    |
| Direct   | 0.79    | 0.99     | 0.99    | 0.97  | 0.99 | 0.96    |
| CART     | 0.82    | 0.99     | 0.99    | 0.94  | 0.99 | 0.98    |
| MLP      | 0.81    | 0.99     | 0.99    | 0.73  | 0.98 | 0.96    |
| Forest   | 0.82    | 0.99     | 1       | 0.98  | 0.99 | 0.98    |
| SVM      | 0.78    | 0.99     | 0.99    | 0.99  | 0.99 | 0.97    |

Table 4: Explanation accuracy on four syntactic data sets and various explanation lengths \( k \).
classification. Table 4 shows that although our approach (Direct) and SHAP both can identify part of the seed string from each query instances, hence computing correct explanations, ours gives higher accuracy across the board.

To demonstrate the effect of knowledge incorporation, we gradually add clauses drawn from sub-strings derived from the seed to the KB. The result is shown in Figure 4(a). Tested on the data set with string length 10, size of alphabet 4 with the Tree algorithm, we see that the classification performance improves as the number of true clauses inserted grows. To show that the knowledge incorporation is resilient to pollution, we insert clauses of a random length between 1 and 10 with a random probability to pollute the KB. As shown in Figure 4(b), for the same data set, the classification performance deteriorates gradually as the number of random clauses grows.

Related Work

Probabilistic logic programming, or ProbLog, (Fierens et al. 2015) provides a means to do logic programming with probabilities. Our work differs from ProbLog in several ways. (1) ProbLog develops Logic Programming and uses grounded predicates with closed world assumption to allow negations whereas we use propositional clauses with classical negations; (2) ProbLog uses Sato’s distribution semantics and assumes all atomic variables,
Recall clauses with associated probabilities are turned into systems with the Logic Solver (NILS) approach. Although in both works (Henderson and Khardon 2020), mathematical programming has been studied recently in the context of classification as the independence assumption does not hold between the class labels and feature values or, in general, values across different features. When independence cannot be assumed, systems constructed with NILS contain $k$th order equations with $2^k - 1$ unknowns for each $k$ literal clauses. Such high order equations with high number of unknowns are difficult to solve numerically. Comparing with NILS, the construction given in Definition 4 “hides” the complexity introduced by conditionals in NILS with inequalities and ensures polynomial complexity. Moreover, NILS does not tolerate inconsistency whereas our approach does.

More generally, developing intelligent system based on reasoning with KB has been explored in the past, see e.g., (McCarthy 1968; Nilsson 1991). Some of the early works on learning KB from data use classical logic, e.g., (Khardon and Roth 1994) or default logic (Roth 1996). A comprehensive review on combining logic and probability is beyond the scope of this section. For broader discussions on this topic, see e.g., (Bacchus 1990) for probabilistic logic, (Chavira and Darwiche 2008) for weighted model counting, and (Gogate and Domingos 2016) for probabilistic graphical models with logical structures. The problem of testing a KB’s consistency is known as the probabilistic satisfiability (PSAT) problem. Works dedicated to solving PSAT include (Cozman and di Ianni 2015; Finger and Bona 2011; Georgakopoulos et al. 1998). Since most of these compute exact solutions over consistent KBs by solving an NP problem, they are not suitable for classification.

In explainable machine learning, there has been significant interest in providing explanations for classifiers; see e.g., (Biran and Cotton 2017) for an overview. Works have been proposed to use simpler thus weaker classifiers to explain results from stronger ones, e.g., (Féraud and Cléro 2002). Recent works on model-agnostic explainers (Ribeiro et al. 2016; Ribeiro et al. 2018) focus on adding explanations to existing (black-box) classifiers. (Alonso et al. 2018) use KB based classifiers to explain results obtained from MLP and random forests. LIME (Ribeiro et al. 2016) augment the data with randomly generated samples close to the instance to be explained and then construct a simple thus explainable classifier to generate explanations. (Robnik-Šikonja and Kononenko 2008) works by decomposing a model’s predictions based on individual contributions of each feature. (Shih et al. 2018) explains Bayesian network classifiers by compiling naïve Bayes and latent-tree classifiers into Ordered Decision Diagrams. (Lundberg et al. 2020) provides explanations for decision trees based on the game-theoretic Shapley values.

(Berrar et al., 2019), (Sachan et al. 2018) and (Vo et al. 2017) are some recent work on incorporating knowledge into machine learning. (Yu 2007) contains a survey, categorising methods into four groups based on use of knowledge: (1) to prepare training samples, (2) to initialise the hypothesis or hypothesis space, (3) to alter the search objective and (4) to augment the search process. Our approach fundamentally differs from those as we represent knowledge in the same format as the model learned from data and reason with both uniformly.

**Conclusion**

We present a non-parametric classification technique that gives explanations to its predictions and supports knowledge incorporation. Our approach is based on approximating literal probabilities in probabilistic logic by solving linear systems corresponding to KBs, which are either directly learned from data or augmented with additional knowledge. Our linear program construction is efficient and our approaches tolerate inconsistency in a KB. As a stand-alone classifier, our approach matches or exceeds the performance of existing algorithms on both synthetic and non-synthetic data sets. At the same time, our approaches generate explanations in the form of “most decisive” features. Upon comparing with a state-of-the-art Shapley Value based explanation method, SHAP, our approach finds similar explanation as SHAP on real data sets. On four synthetic data sets with known explanation truth, our approach is shown to be superior as it achieves higher accuracy. Overall, we envisage our approaches to be most useful for classification tasks where there exists knowledge to complement data and explanations are required to ensure usability.

There are four research directions that we plan to explore. Firstly, this work focuses on developing the underlying explainable classification techniques. We will apply techniques developed practical applications and perform user studies in the future. Secondly, we will study semantics for inconsistent KBs. Thirdly, we will study richer explanation generation with with (probabilistic) logic inference. Lastly, we would like to develop other suitable representations for
knowledge incorporation.

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