Interpretable Hybrid Machine Learning Models Using FOLD-R++ and Answer Set Programming

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Introduction

In healthcare and various other domains, machine learning (ML) has become an increasingly indispensable tool for predictive analytics and decision support (Tonekaboni, Joshi, McCradden, and Goldenberg (2019)). Advanced ML models, particularly black-box models such as neural networks and ensemble methods, have shown impressive predictive capabilities. However, a challenge remains: the lack of interpretability and explainability. This limitation slows down the adoption of ML models in applications where understanding the reasoning behind a prediction is as important as the prediction itself (Arrieta et al. (2020)). In fields like medicine, decisions informed by ML models can have profound implications on patient outcomes. The ability to explain and justify predictions is therefore important for trust, accountability, and informed decision-making (Doshi-Velez and Kim (2017)).

Answer Set Programming (ASP), a form of declarative programming, provides a way to represent knowledge in transparent, human-understandable logical rules (Lifschitz (2019)). The FOLD-R++ algorithm uses ASP to learn default rules with exceptions from data (Wang and Gupta (2022)). These rules can complement black-box models by offering explanations for their predictions and therefore improving interpretability.

However, integrating ASP-derived rules with black-box ML models without changing their internal mechanisms remains challenging. While many existing hybrid approaches focus on integrating symbolic reasoning with neural networks (Garcez et al. (2019); Manhaeve, Dumancic, Kimmig, Demeester, and De Raedt (2018); Yang, Ishay, and Lee (2023)), fewer methods target other types of black-box models, such as support vector machines or ensemble methods. This gap is important because many real-world systems rely on non-neural classifiers.

This study proposes a hybrid approach that fills this gap by combining logical rules from FOLD-R++ with various black-box ML models. By using rules that capture domain knowledge, the hybrid system can correct ML model errors when the model is uncertain and provide human-readable explanations.

The following research questions guide this study:

RQ1: Does integrating interpretable ASP rules derived from FOLD-R++ improve the predictive performance of black-box ML models across various medical datasets?

RQ2: How does the hybrid model of ML and ASP improve the interpretability of predictions?

The remainder of this paper is organized as follows: first, related work on interpretability and hybrid models is reviewed. Then, the methodology is outlined, including data preparation, model training, and hybrid model implementation. Following that, the experimental findings are presented. Finally, the findings and implications are discussed to conclude the study.

By demonstrating how logical reasoning can improve both the performance and interpretability of various black-box ML models, particularly in the healthcare domain, this project contributes to the development of more reliable and transparent AI systems.

Background

The development of machine learning models that are both accurate and interpretable remains a foundational challenge in artificial intelligence (Guidotti et al. (2018)). While advanced ML techniques, such as deep neural networks and ensemble methods, achieve superior performance across diverse applications, they often function as "black-box" models, lacking transparency and making it difficult to understand and trust their decisions. This issue is particularly problematic in areas such as healthcare, where interpretability is important for ethical considerations, regulatory compliance, and fostering trust among clinicians and patients (Tonekaboni et al. (2019)).

Interpretability and Explainability

Interpretability refers to the extent to which a human can comprehend the cause of a decision made by a model, while explainability involves the extent to which the internal mechanics of a model can be explained in human-understandable terms (Gilpin et al. (2018); Xu et al. (2019)). For example, an interpretable model such as a decision tree provides a direct mapping from inputs to outputs. In contrast, explainability techniques apply to otherwise opaque models to explain their behavior post-hoc.

In healthcare, interpretability is vital. Clinicians must understand how a model arrived at a specific diagnosis to trust and effectively use it in decision-making (Tonekaboni et al. (2019)). Lack of transparency can lead to mistrust or rejection of ML systems (Arrieta et al. (2020)). Moreover, regulatory bodies increasingly require explanations for automated decisions, especially when they impact patient care (Palaniappan, Lin, and Vogel (2024)).

To address these issues, researchers have proposed various strategies. These include developing inherently interpretable models such as decision trees and rule-based systems (Rudin (2019)), and using post-hoc techniques like LIME (Ribeiro, Singh, and Guestrin (2016)) and SHAP (Lundberg (2017)) to explain predictions. However, there is often a trade-off between interpretability and performance. Simple models may not capture complex patterns in data, while complex models may be too opaque. Additionally, highly detailed explanations can overwhelm users (Xu et al. (2019)).

Symbolic Logic and Answer Set Programming

Symbolic logic provides a framework for building interpretable models by encoding knowledge in structured, human-readable formats. Answer Set Programming (ASP) is a form of declarative programming that combines logic programming with non-monotonic reasoning to effectively represent complex relationships and constraints (Lifschitz (2019)). ASP allows for the expression of knowledge through logical rules and facts, closely resembling human reasoning.

ASP is particularly suitable for tasks where interpretability is important. Applications of ASP span diverse areas, including planning, scheduling, and bio-informatics (Erdem, Gelfond, and Leone (2016)). In healthcare, ASP has been applied to model and reason about clinical guidelines (Spiotta, Terenziani, and Dupré (2017)), and solve scheduling problems (Erdem et al. (2016)).

FOLD-R++ Algorithm

The FOLD-R++ algorithm, introduced by Wang and Gupta (2022), extends the First-Order Logical Decision tree (FOLD) algorithm to learn default rules with exceptions from relational data, representing them in a form that is both human-readable and suitable for

reasoning with ASP. FOLD-R++ generates default rules capturing general patterns in the data, along with exceptions accounting for special cases or anomalies. The algorithm operates by recursively partitioning the data to construct a decision tree, similar to algorithms like ID3 or C4.5. However, FOLD-R++ transforms the decision tree into a set of default logical rules with exceptions, represented in ASP.

The algorithm starts with the entire dataset and considers all possible literals (attribute-value pairs or relational literals) that can be used to split the data. At each node, the literal that best separates the positive examples from the negative ones is chosen according to a heuristic. This literal becomes part of the condition in the rule. When a rule does not perfectly classify the data, the algorithm identifies exceptions to the rule. These exceptions are themselves induced as sub-rules using the same recursive process. Mechanisms for pruning unnecessary rules or exceptions are included to prevent overfitting. The final set of rules and exceptions is translated into an ASP program of the form:

label(X, Class) := conditions(X), not exceptions(X).

This means an instance X belongs to a class if it satisfies certain conditions and none of the exceptions apply.

Although newer algorithms in the same family, like FOLD-SE and FOLD-RM, offer advanced features, they were not selected due to accessibility constraints and alignment with the research focus. Specifically, FOLD-SE lacks a publicly available repository which limits integration into automated workflows. FOLD-R++ was chosen for its proven effectiveness and compatibility with the experimental setup.

Hybrid Models

Hybrid models that combine machine learning with symbolic reasoning aim to use the strengths of both approaches. Statistical ML models excel at capturing complex patterns and representations from large amounts of data but often lack interpretability. Symbolic reasoning provides transparency and the ability to incorporate domain knowledge but may struggle with noisy or high-dimensional data.

Most existing hybrid approaches focus on integrating symbolic reasoning with neural networks, creating neuro-symbolic systems. For instance, Garcez et al. (2019) discuss neuro-symbolic AI to combine learning and reasoning capabilities. Manhaeve et al. (2018) introduce DeepProbLog, integrating probabilistic logic programming with deep learning. In the context of ASP, Yang et al. (2023) propose NeurASP, a framework that combines neural networks with ASP.

These approaches often require modifications to the learning algorithms or network architectures, which can be complex and computationally intensive. They primarily focus on neural networks and do not address integration with other types of black-box ML models. There is a gap in research concerning the integration of symbolic reasoning with traditional classifiers and ensemble methods without altering their internal mechanisms.

This study addresses this gap by integrating interpretable ASP rules from FOLD-R++ with a variety of black-box ML classifiers, including support vector machines, random forests, knearest neighbors, and neural networks. This hybrid approach does not require changing the ML models, thus preserving their performance. The ASP component adds a layer of interpretability by offering human-understandable explanations for the predictions.

Methods

This section outlines the methodology used to develop and evaluate the hybrid model that integrates black-box ML models with interpretable rules generated by FOLD-R++ using ASP. The approach includes data preparation, model training, hybrid model implementation, experimental setup, and evaluation metrics.

Data Preparation

Five medical datasets from the UCI Machine Learning Repository (Kelly, Longjohn, and Nottingham (n.d.)) were selected:

- **Heart Disease:** Contains 303 instances with 14 commonly used attributes. It is used to predict the presence of heart disease in patients based on medical measurements.
- Autism Screening Adult: Includes 704 instances with 21 attributes, used to predict whether an individual is likely to have autism spectrum disorder based on screening test scores and demographic information.
- Breast Cancer Wisconsin: Consists of 569 instances with 30 numerical features computed from digitized images. The goal is to classify tumors as malignant or benign.
- Ecoli: Contains 336 instances with 8 attributes, used to classify protein localization sites within a cell.
- Chronic Kidney Disease: Contains 400 instances with 24 attributes, used to predict the presence of chronic kidney disease in patients based on clinical and laboratory findings.

Each dataset underwent preprocessing to handle missing values, encode categorical variables, and scale numerical features where necessary. Stratified sampling was used to split the datasets into training and testing sets to maintain class distribution. A different random seed was used for each experiment.

FOLD-R++

FOLD-R++ (Wang and Gupta (2022)) was used to induce ASP rules from the training data. In this study, original FOLD-R++ code was used and slightly refactored to fit the experimental setup. This included adding new functions to transform data into ASP-compatible formats and interface with Clingo. Additionally, a wrapper was created to handle the training of FOLD-R++, conversion of induced rules to ASP syntax, and prediction using Clingo. The training data was transformed into a format compatible with FOLD-R++, where each instance was represented as a set of logical facts with attributes and their values forming predicates. For example, an attribute-value pair such as age = 45 was converted into a predicate age(X,45).

FOLD-R++ induced rules of the form:

label(X, Class) := Conditions(X), not Exceptions(X).

Here, Conditions(X) represent the conditions under which an instance X belongs to a particular class, and Exceptions(X) are exceptions to these rules. The algorithm recursively constructs these rules and exceptions. The induced rules were converted into ASP syntax compatible with the Clingo solver (Gebser, Kaminski, Kaufmann, and Schaub (2019)). Numeric values were scaled by a factor 10 to handle the limitations of Clingo with floating-point numbers. The scaling was applied consistently to keep relationships between variables valid. Clingo was then used to apply the logical rules to the test data, reasoning over the facts representing each instance and the induced rules to infer the class labels.

ML Models

Four black-box ML models were used to provide baseline predictive performance:

• Random Forest (RF): An ensemble method that builds multiple decision trees using bootstrap aggregation (bagging) and random feature selection. It reduces variance and improves generalization.

• Support Vector Machine (SVM): A model that finds the optimal hyperplane that best separates classes in a high-dimensional space. The radial basis function (RBF) was used to capture non-linear relationships.

- K-Nearest Neighbors (KNN): A non-parametric method that classifies instances based on the majority class among the k-nearest neighbors in the feature space.
- Neural Network (MLPClassifier): A multi-layer perceptron that learns complex non-linear relationships through backpropagation. A configuration with one hidden layer containing 100 neurons and the ReLU activation function was used.

Default hyperparameters were used for all models unless adjustments were necessary for convergence or performance. Random seeds were set for model initialization and data splitting to ensure reproducibility across experiments. For models that provide probability estimates (e.g., RF, SVM with probability=True, MLP), the predict_proba method was used to obtain confidence scores for each class. For KNN, probabilities were derived from the proportion of neighbors belonging to each class.

Hybrid Model Implementation

The hybrid model integrates predictions from the ML models with the interpretable rules generated by FOLD-R++ using ASP. First, predictions and confidence scores from the ML model on the test set were obtained. Clingo was then used to apply the induced rules to the test instances and generate predictions.

A fixed confidence threshold of 0.6 was used to determine when to rely on the prediction of the ML model versus the ASP rules. If the confidence score of the ML model for a prediction was above 0.6, the ML prediction was used; otherwise, the prediction of the ASP rule was used. This approach ensures that the ASP rules intervene specifically when the ML model is uncertain. During development, both dynamic and fixed confidence thresholds were experimented with, but the dynamic threshold led to overfitting on the training data.

For each prediction corrected by the ASP rules, explanations were generated from the induced rules. These explanations highlight which logical conditions were met and which exceptions were not triggered.

Experimental Setup

Experiments were conducted to evaluate the performance of the ML models, the FOLD-R++ model, and the hybrid model. Ten experiments were conducted for each dataset and model combination. In each experiment, the dataset was split into training and testing sets using stratified sampling with an 80-20 split, using different random seeds to vary the splits and model initialization.

Performance metrics were averaged over the ten experiments, and standard deviations were calculated. The following metrics were assessed: accuracy, precision, recall, and F1 score.

Paired t-tests were conducted to determine whether the improvements observed with the hybrid model were statistically significant compared to the standalone ML models. A p-value threshold of 0.05 was used to determine statistical significance. If the ML model and hybrid model had the same accuracy in all experiments, the differences were zero, and the paired t-test could not be performed.

Due to variability in the induced ASP programs across different experiments - likely caused by randomness in data splitting - only the ASP programs and important rules from model-dataset combinations that showed statistically significant improvements were saved. The importance of each ASP rule was determined based on how frequently it contributed to correcting errors made by the ML models. Explanations were generated for instances where the hybrid

model corrected the prediction of the ML model, using the proof trees from the FOLD-R++ algorithm.

The implementation was done using Python, with libraries such as scikit-learn for ML models, SciPy for statistical tests, and clingo for ASP solving. Pandas and NumPy were used for data manipulation and numerical computations. The FOLD-R++ library was used to induce logical rules from data. The project was modularized into separate components for data loading, model training, hybrid integration, and evaluation to improve readability.

The source code is available on GitHub¹.

Results

This section presents the experimental results of evaluating the hybrid models that integrate black-box ML classifiers with interpretable rules derived from FOLD-R++ using ASP. The performance of the ML models and the hybrid model is compared across multiple medical datasets. Additionally, the role of ASP in improving interpretability and correcting errors made by the ML models is demonstrated through the application of logical rules and case studies.

Table 1 summarizes the average accuracy and F1 score of the ML models and the hybrid models across all datasets and experiments. Standard deviations are included to indicate variability in the results.

Dataset	Model	ML Acc (%)	Hybrid Acc (%)	ML F1 (%)	Hybrid F1 (%)
Heart					
	KNN	64.26 ± 5.38	64.26 ± 5.38	68.97 ± 4.49	68.97 ± 4.49
	MLP	80.93 ± 3.50	80.19 ± 4.94	81.22 ± 4.51	80.65 ± 5.70
	RF	79.44 ± 4.32	79.44 ± 5.69	81.24 ± 4.30	81.39 ± 5.69
	SVM	63.52 ± 5.24	71.30 ± 8.25	70.96 ± 4.82	75.14 ± 7.21
Autism					
	KNN	87.38 ± 1.56	87.38 ± 1.56	91.52 ± 1.11	91.52 ± 1.11
	MLP	97.52 ± 1.35	97.66 ± 1.21	98.30 ± 0.91	98.29 ± 0.82
	RF	97.38 ± 1.57	96.10 ± 1.35	98.20 ± 1.11	97.33 ± 0.94
	SVM	72.62 ± 1.74	94.04 ± 1.84	84.13 ± 1.17	96.01 ± 1.26
BreastW					
	KNN	94.36 ± 1.83	94.50 ± 2.10	91.62 ± 3.18	91.62 ± 3.18
	MLP	93.57 ± 2.33	94.43 ± 2.20	91.04 ± 3.56	91.86 ± 3.37
	RF	96.36 ± 2.60	95.50 ± 2.40	94.78 ± 3.69	93.63 ± 3.59
	SVM	95.21 ± 1.85	95.36 ± 1.94	93.11 ± 2.88	93.28 ± 3.15
Ecoli					
	KNN	65.74 ± 4.05	65.74 ± 4.05	57.46 ± 5.24	57.46 ± 5.24
	MLP	92.50 ± 3.57	94.71 ± 2.52	91.14 ± 4.51	93.93 ± 2.64
	RF	96.32 ± 2.62	96.47 ± 2.21	95.77 ± 2.97	95.96 ± 2.45
	SVM	57.06 ± 6.96	87.50 ± 15.14	23.37 ± 18.45	82.99 ± 21.55
Kidney					
	KNN	89.13 ± 2.13	62.00 ± 5.81	90.36 ± 2.07	76.01 ± 4.29
	MLP	95.25 ± 2.69	95.50 ± 2.30	96.05 ± 2.20	96.28 ± 1.87
	RF	100.00 ± 0.00	99.88 ± 0.40	100.00 ± 0.00	99.89 ± 0.34
	SVM	91.38 ± 2.60	93.13 ± 1.58	92.60 ± 2.36	94.27 ± 1.46

Table 1
Average Accuracy and F1 Score with Standard Deviations for ML and Hybrid Models

¹https://github.com/sannewielinga/mbai

The results indicate that, across several datasets, the hybrid models demonstrated an improvement in accuracy and F1 score over the standalone ML models. Notably, the SVM classifier showed significant improvements when combined with the ASP rules in the hybrid model.

Statistical Significance

Paired t-tests were conducted to determine whether the improvements observed with the hybrid models were statistically significant compared to the ML models. If the ML model and hybrid model have the same accuracy in all experiments, the differences were zero, and the paired t-test could not be performed (denoted as "N/A").

Table 2 presents	the	results	of the	he paired	t-tests.
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Dataset	Model	t-statistic	p-value	Significant
Heart	KNN	N/A	N/A	N/A
Heart	MLP	-0.53	0.606	No
Heart	RF	0.00	1.000	No
Heart	SVM	3.55	0.006	\mathbf{Yes}
Autism	KNN	N/A	N/A	N/A
Autism	MLP	1.00	0.343	No
Autism	RF	-3.04	0.014	Yes
Autism	SVM	32.12	1.35×10^{-10}	Yes
BreastW	KNN	N/A	N/A	N/A
BreastW	MLP	3.09	0.013	Yes
BreastW	RF	-2.54	0.032	Yes
BreastW	SVM	0.80	0.443	No
Ecoli	KNN	N/A	N/A	N/A
Ecoli	MLP	2.75	0.022	Yes
Ecoli	RF	0.36	0.726	No
Ecoli	SVM	7.30	4.58×10^{-5}	\mathbf{Yes}
Kidney	KNN	N/A	N/A	N/A
Kidney	MLP	0.69	0.509	No
Kidney	RF	-1.00	0.343	No
Kidney	SVM	3.74	0.005	\mathbf{Yes}

Table 2 Results of paired t-tests comparing ML models and hybrid models. N/A indicates the t-test could not be performed due to zero differences in all experiments. Significant results (p < 0.05) are highlighted in bold.

The results indicate that the improvements in accuracy and F1 score are statistically significant (p < 0.05) for datasets where the hybrid model outperformed the ML models. Specifically, significant improvements were observed for:

- Heart Disease Dataset: SVM classifier (p = 0.006)
- Autism Screening Dataset: SVM classifier (p < 1×10^{-10}) and RF (p = 0.014)
- Breast Cancer Wisconsin Dataset: MLPClassifier (p = 0.0013) and RF (p = 0.032)
- Ecoli Dataset: SVM classifier (p < 0.0001) and MLPClassifier (p = 0.022)
- Chronic Kidney Disease Dataset: SVM classifier (p = 0.005)

In datasets where the ML models already performed well, such as the Random Forest model on the Chronic Kidney Disease dataset, the hybrid model maintained similar performance. For KNN and MLP models, the performance was generally consistent with the ML models, with no significant improvements or declines.

Results by Dataset

The following subsections provide detailed analyses and case studies for each dataset where the hybrid model showed significant improvements. The case studies highlight how the ASP rules contributed to correcting misclassifications made by the ML models.²

Heart Disease Dataset. For the SVM classifier, the hybrid model improved accuracy from 63.5% to 71.3%. Key ASP rules included:

1. Rule for labeling "absent"

```
\begin{array}{l} \texttt{label}\left(X,\ \texttt{absent}\right) := \ \texttt{thal}\left(X,\ 3\right), \\ \texttt{maximum\_heart\_rate\_achieved}\left(\\ X,\ V\_\texttt{max\_hr\_1}\right), \\ V\_\texttt{max\_hr\_1} > 71.0\,, \\ \textbf{not}\ \mathtt{ab2}\left(X,\ \textbf{True}\right),\ \textbf{not}\ \mathtt{ab3}\left(X,\ \textbf{True}\right), \\ \textbf{not}\ \mathtt{ab4}\left(X,\ \textbf{True}\right),\ \textbf{not}\ \mathtt{ab5}\left(X,\ \textbf{True}\right), \\ \textbf{not}\ \mathtt{ab6}\left(X,\ \textbf{True}\right),\ \textbf{not}\ \mathtt{ab7}\left(X,\ \textbf{True}\right), \\ \textbf{not}\ \mathtt{ab8}\left(X,\ \textbf{True}\right). \end{array}
```

This rule states that if the attribute thal equals 3, the maximum heart rate achieved is greater than 71, and none of the exceptions apply, then the diagnosis is "absent" (no heart disease).

2. Exception rule ab2

```
ab2(X, True) :- chest\_pain(X, 4), \\ major\_vessels(X, V\_major\_vessels\_1), \\ V\_major\_vessels\_1 != 0, \\ not ab1(X, True).
```

This exception accounts for cases where patients exhibit chest pain type 4 and have a certain number of major vessels affect, which indicates a higher risk of heart disease.

An instance (patient34) was initially predicted as "absent" by the SVM model. The hybrid model corrected the prediction to "present" based on the rules. The patient had thal equal to 3 and a maximum heart rate achieved of 150 (greater than 71), but exceptions did not hold due to the absence of chest pain type 4 and no major vessels affected. This reasoning aligned with medical knowledge and resulted in a correct diagnosis.

Autism Screening Dataset. The SVM classifier showed significant improvement when combined with ASP rules, with accuracy increasing from 72.6% to 94.0%. Key ASP rules included:

1. Rule for labeling "NO"

```
\begin{array}{rll} \text{label}\left(X,\ NO\right) \ :- \ a5\left(X,\ V\_a5\_0\right), \\ & V\_a5\_0 \ != \ 1\,, \\ & \textbf{not} \ ab1\left(X,\ \textbf{True}\right), \\ & \textbf{not} \ ab2\left(X,\ \textbf{True}\right). \end{array}
```

This rule indicates that if the individual did not answer "1" to question 5 (a5), and exceptions ab1 and ab2 do not apply, then they are labeled as "NO" (not autistic).

2. Exception rule ab1

²Due to their size, the full ASP programs, including all induced rules and facts, are not included. They are available at https://github.com/sannewielinga/mbai

```
ab1(X, True) := a9(X,1),

a3(X,1),

a1(X,1),

a6(X,1).
```

This exception captures where affirmative answers to specific questions indicate strong autistic traits, overriding the general rule.

For example, for specific instance patient1, the values satisfied the rule: a5(X) was not equal to 1, and exceptions ab1 and ab2 did not hold. The ML model predicted the individual as "autistic", but the hybrid model corrected it to "non-autistic".

Breast Cancer Wisconsin Dataset. The performance of the MLP classifier improved with the hybrid model, increasing accuracy from 93.6% to 94.4%. Key ASP rules included:

1. Rule for labeling "Malignant"

A non-uniform cell size suggests malignancy unless exceptions apply. This rule aligns with medical knowledge that irregular cell sizes are indicative of cancerous cells.

2. Exception rule ab1

```
ab1(X, True) :- bare_nuclei(X, 1),
                cell size uniformity (X,
                V cell size uniformity 1),
                V_cell_size_uniformity_1 != 10,
                marginal_adhesion(X,
                V marginal adhesion 2),
                V marginal adhesion 2 != 10,
                clump thickness (X,
                V clump thickness 3),
                V clump thickness 3 != 7,
                cell size uniformity (X,
                V_cell_size_uniformity_4),
                V cell size uniformity 4 = 6,
                bland chromatin(X,
                V bland chromatin 5),
                V_bland_chromatin_5 != 5.
```

The exception handles cases where, despite non-uniform cell size, other features do not indicate malignancy.

For example, patient33 was initially misclassified as "benign" by the ML model but was correctly classified as "malignant" by the hybrid model. Here, cell_size_uniformity was equal to 5, which satisfied the condition of not being 1. Additionally, exceptions ab1 and ab2 did not hold.

Ecoli Dataset. The hybrid model improved SVM accuracy from 57.1% to 87.5%. Key ASP rules included:

1. Rule for labeling "cp"

$$\begin{array}{lll} \text{label}\,(X, & \text{cp}) & :- & \text{sn}\,(X, & V_\text{sn}_0)\,, & V_\text{sn}_0 \, \,! = \, \text{FECR}, \\ & & \text{alm1}\,(X, & V_\text{alm1}_1)\,, \\ & & V_\text{alm1}_1 <= \, 0.38\,, \\ & & \text{not} & \text{ab1}\,(X, & \text{True})\,. \end{array}$$

This rules states that if the sequence name (sn) is not "FECR", and the attribute alm1 is less than or equal to 0.38, and exception ab1 does not apply, then the sample is labeled as "cp".

2. Exception rule ab1

```
ab1(X, True) :- sn(X, V_sn_0), V_sn_0 != PTKB, \\ gvh(X, V_gvh_1), V_gvh_1 > 0.55, \\ mcg(X, V_mcg_2), V_mcg_2 > 0.41.
```

This exception accounts for cases where even if alm1 is low, certain combinations of other features (gvh, mcg) indicate that the sample should not be labeled "cp".

For example, patient48 was misclassified as "negative" by the ML model. The hybrid model corrected this to "positive", with the explanation being that the sequence name (sn) was not 'FECR', alm1 was 0.18 and therefore less than or equal to 0.38, and the exception was invalidated, satisfying the conditions.

Chronic Kidney Disease (CKD) Dataset. For the SVM classifier, the hybrid model improved accuracy from 91.4% to 93.1%. A key ASP rule includes:

1. Rule for labeling "ckd"

$$label(X, ckd) :- sc(X, V_sc_0), V_sc_0 > 1.2.$$

This rule indicates that if the serum creatinine level (sc is greater than 1.2, the patient is labeled as having chronic kidney disease.

An instance (patient70) was incorrectly predicted as "not ckd" by the SVM model. The hybrid model corrected this to "ckd" based on the ASP rule. The patient's sc value was 1.3, which exceeds the threshold.

Conclusion

This study investigated the integration of interpretable ASP rules derived from the FOLD-R++ algorithm with black-box ML models to improve predictive performance and interpretability in medical classification tasks. The study addressed two research questions.

First, regarding whether integrating interpretable ASP rules improves the predictive performance of black-box ML models across various medical datasets, the results demonstrate significant improvements. The hybrid model notably improved the accuracy and F1 scores of several ML classifiers, particularly the SVM, across multiple datasets. For example, in the Autism Screening Dataset, the hybrid model increased the accuracy of the SVM classifier from 72.6% to 94.0% (p < $1times10^{-10}$). Similarly, in the Ecoli dataset, the accuracy improved from 57.1% to 87.5% (p < 0.0001). These improvements suggest that the hybrid model was able to address limitations in certain ML models when dealing with complex or noisy data.

Second, concerning how the hybrid model improves the interpretability of predictions, the integration of ASP rules provides clear, human-readable explanations for each prediction. The logical rules derived from the FOLD-R++ algorithm align with domain knowledge, and make it easier to understand and trust the predictions. For instance, in the Chronic Kidney Disease dataset, the rule:

$$label(X, ckd) :- sc(X, V_sc_0), V_sc_0 > 1.2.$$

reflects the medical understanding that elevated serum creatinine levels (sc) are indicative of kidney dysfunction. Such rules improved the accuracy of predictions and provided an interpretable explanation aligned with medical knowledge. Such explanations are important in medical applications where transparency and trust are needed.

In summary, the hybrid model uses the strengths of both statistical learning and symbolic reasoning, resulting in improved predictive performance and interpretability.

While the hybrid model shows promising results, several limitations should be considered. As datasets become larger and more complex, the number of induced ASP rules can increase substantially. This may potentially affect interpretability. Managing and interpreting a large set of rules may become challenging for users. Additionally, heavy use of exceptions for capturing specific cases may cause the rules to overfit the training data. The variations in induced rules across different experiments suggest sensitivity of the FOLD-R++ algorithm to data splitting and randomness. Different training sets may lead to different rules being induced, which affects the consistency of the hybrid model. There may also be multiple hypotheses that fit the data equally well. Furthermore, the hybrid model did not consistently improve performance across all ML models and datasets. For some models, such as KNN and RF on certain datasets, the benefits were minimal or nonexistent. This indicates that the effectiveness of the hybrid approach may depend on the characteristics of both the dataset and the base ML model.

To build upon these findings, future research could focus on optimizing the rule induction process to improve scalability. Techniques such as rule pruning, clustering similar rules, or prioritizing the most impactful rules may help to improve interpretability further. Developing adaptive ways to handle the variability in induced rules and to determine the optimal confidence threshold could increase the robustness of the hybrid model. Applying the hybrid approach to other domains and combining it with additional explainable AI techniques may validate its generalizability further.

References

- Arrieta, A. B., Díaz-Rodríguez, N., Del Ser, J., Bennetot, A., Tabik, S., Barbado, A., . . . others (2020). Explainable artificial intelligence (xai): Concepts, taxonomies, opportunities and challenges toward responsible ai. *Information fusion*, 58, 82–115.
- Doshi-Velez, F., & Kim, B. (2017). Towards a rigorous science of interpretable machine learning. arXiv preprint arXiv:1702.08608.
- Erdem, E., Gelfond, M., & Leone, N. (2016). Applications of answer set programming. *AI Magazine*, 37(3), 53–68.
- Garcez, A. d., Gori, M., Lamb, L. C., Serafini, L., Spranger, M., & Tran, S. N. (2019). Neural-symbolic computing: An effective methodology for principled integration of machine learning and reasoning. arXiv preprint arXiv:1905.06088.
- Gebser, M., Kaminski, R., Kaufmann, B., & Schaub, T. (2019). Multi-shot asp solving with clingo. Theory and Practice of Logic Programming, 19(1), 27–82.
- Gilpin, L. H., Bau, D., Yuan, B. Z., Bajwa, A., Specter, M., & Kagal, L. (2018). Explaining explanations: An overview of interpretability of machine learning. In 2018 ieee 5th international conference on data science and advanced analytics (dsaa) (pp. 80–89).
- Guidotti, R., Monreale, A., Ruggieri, S., Turini, F., Giannotti, F., & Pedreschi, D. (2018). A survey of methods for explaining black box models. *ACM computing surveys (CSUR)*, 51(5), 1–42.
- Kelly, M., Longjohn, R., & Nottingham, K. (n.d.). The uci machine learning repository. https://archive.ics.uci.edu.
- Lifschitz, V. (2019). Answer set programming (Vol. 3). Springer Heidelberg.
- Lundberg, S. (2017). A unified approach to interpreting model predictions. $arXiv\ preprint\ arXiv:1705.07874$.
- Manhaeve, R., Dumancic, S., Kimmig, A., Demeester, T., & De Raedt, L. (2018). Deepproblog: Neural probabilistic logic programming. *Advances in neural information processing systems*, 31.
- Palaniappan, K., Lin, E. Y. T., & Vogel, S. (2024). Global regulatory frameworks for the use of artificial intelligence (ai) in the healthcare services sector. In *Healthcare* (Vol. 12, p. 562).

Ribeiro, M. T., Singh, S., & Guestrin, C. (2016). "why should i trust you?" explaining the predictions of any classifier. In *Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining* (pp. 1135–1144).

- Rudin, C. (2019). Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nature machine intelligence*, 1(5), 206–215.
- Spiotta, M., Terenziani, P., & Dupré, D. T. (2017). Temporal conformance analysis and explanation of clinical guidelines execution: An answer set programming approach. *IEEE Transactions on Knowledge and Data Engineering*, 29(11), 2567–2580.
- Tonekaboni, S., Joshi, S., McCradden, M. D., & Goldenberg, A. (2019). What clinicians want: contextualizing explainable machine learning for clinical end use. In *Machine learning for healthcare conference* (pp. 359–380).
- Wang, H., & Gupta, G. (2022). Fold-r++: a scalable toolset for automated inductive learning of default theories from mixed data. In *International symposium on functional and logic programming* (pp. 224–242).
- Xu, F., Uszkoreit, H., Du, Y., Fan, W., Zhao, D., & Zhu, J. (2019). Explainable ai: A brief survey on history, research areas, approaches and challenges. In *Natural language processing and chinese computing:* 8th ccf international conference, nlpcc 2019, dunhuang, china, october 9–14, 2019, proceedings, part ii 8 (pp. 563–574).
- Yang, Z., Ishay, A., & Lee, J. (2023). Neurasp: Embracing neural networks into answer set programming. arXiv preprint arXiv:2307.07700.