

# **CHIRPS: Explaining random forest classification**

Julian Hatwell<sup>1</sup> · Mohamed Medhat Gaber<sup>1</sup> · R. Muhammad Atif Azad<sup>1</sup>

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#### Abstract

Modern machine learning methods typically produce "black box" models that are opaque to interpretation. Yet, their demand has been increasing in the Human-in-the-Loop processes, that is, those processes that require a human agent to verify, approve or reason about the automated decisions before they can be applied. To facilitate this interpretation, we propose Collection of High Importance Random Path Snippets (CHIRPS); a novel algorithm for explaining random forest classification per data instance. CHIRPS extracts a decision path from each tree in the forest that contributes to the majority classification, and then uses frequent pattern mining to identify the most commonly occurring split conditions. Then a simple, conjunctive form rule is constructed where the antecedent terms are derived from the attributes that had the most influence on the classification. This rule is returned alongside estimates of the rule's precision and coverage on the training data along with counter-factual details. An experimental study involving nine data sets shows that classification rules returned by CHIRPS have a precision at least as high as the state of the art when evaluated on unseen data (0.91-0.99) and offer a much greater coverage (0.04-0.54). Furthermore, CHIRPS uniquely controls against under- and over-fitting solutions by maximising novel objective functions that are better suited to the local (per instance) explanation setting.

 $\textbf{Keywords} \ \ XAI \cdot Model \ interpretability \cdot Random \ forests \cdot Classification \cdot Frequent \\ patterns$ 

### 1 Introduction

Explainable Artificial Intelligence (XAI) is no longer just a research question (Doshi-Velez and Kim 2017); it is a concern of national defence and industrial strategy (Gunning 2017; Goodman and Flaxman 2016) and a topic of regular public discourse (Tierney 2017; O'Neil and Hayworth 2018). The challenge—to make AI explainable—arises because of a cognitive-representational mismatch; modern machine learning (ML) methods and models operate on dimensions, complexity and modes of knowledge representation that make them



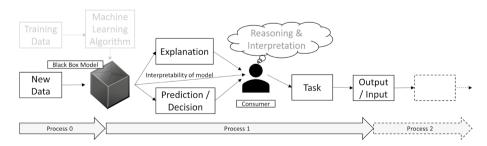
<sup>✓</sup> Julian Hatwell julian.hatwell@bcu.ac.uk http://www.bcu.ac.uk

Birmingham City University, Birmingham B5 5JU, UK

opaque to human understanding. Such models are termed "black boxes" (Freitas 2014; Lipton 2016).

Some have argued that classification performance improves only negligibly when we use complex, black box models instead of the classical methods such as linear discriminant analysis (Rudin 2018; Hand 2006); however, the majority still prefers to use the black box models such as Random Forests, Gradient Boosting Machines, Support Vector Machines and Neural Networks as the first choice methods for many applications. This preference may in part be thanks to the intense performance competitions—such as those hosted by Kaggle—as well as demands of commercial and critical applications. Research into these black boxes is motivated because they can achieve very high predictive accuracy that makes them suitable for such critical applications despite an almost complete loss of interpretability (Burrell 2016; Pasquale 2015; Hildebrandt 2012). Yet, this accuracyinterpretability trade-off (AITO) poses a barrier to adoption of these most accurate models in regulated industries where sensitive and personal data are used to make life-changing decisions about individuals (Goodman and Flaxman 2016). Automated decisions from a black box model are difficult to contest or defend; organisations that rely on such unexplainable decisions are at risk of non-compliance with data protection regulations (European Parliament and Council of the European Union 2018); moreover, organisations that fail to understand their automated decision making will not be able to identify or rectify mistakes and sources of bias. Black box models also face obstacles in the medical sector where automated diagnostics and personalised medicine offer untapped potential. Evidence in the literature shows that practitioners and clinicians are not yet ready to adopt models that do not provide clinical insight or do not easily align with prior knowledge, even if they are demonstrably more accurate. This lack of trust can impact negatively on patient outcomes (Jovanovic et al. 2016; Turgeman and May 2016; Letham 2015a; Subianto and Siebes 2007; Huysmans et al. 2006). XAI can improve trust where interpretation, interaction, intervention or expert verification by human agency is required. These scenarios can generally be described as Human-in-the-Loop (HIL) processes (DoD Modeling and Simulation (M&S) Glossary 1998), as illustrated in Fig. 1. A HIL process is any organisational process in which a human agent is required to complete a downstream task that depends on reasoning about an automated decision. HIL processes present a strong motivation for research in XAI and ML interpretability.

In this paper, we propose *Collection of High Importance Random Path Snippets* (CHIRPS), a novel, heuristic algorithm that provides instance-wise explanations of random forest (RF) classification. A CHIRPS explanation is in the form of a classification rule, supplemented by estimated performance measures (e.g. precision and coverage)



**Fig. 1** Process 0 represents submission of new data to the trained model for classification, Process 1 is a generic HIL process where the consumer must interpret the model output, and Process 2 is some downstream task that relies on the consumer's judgement



 Table 1
 An example of CHIRPS output for explaining an automated decision

Data set	Decision	Explanation	Contrast (%)	Confidence
adult	Income ≤ \$50 K	lcapitalgain ≤ $8.51 \land$ Relationship ≠ Husband $\land$ Educationnum ≤ $10.92$	-80.6 -24.9 -16.9%	Covers 39.4% of historical Matches 97.3 of covered Vote margin 40.0%

Table 2 A further example of CHIRPS output, illustrating diagnosis of a poor performing model

Data set	Decision	Explanation	Contrast (%)	Confidence
rcdv	Recid = Y	White = False	-19.8	Covers 19.4% of historical Matches 50.0% of covered Vote margin 2.7%

over the input space along with counter-factual detail. An example from the UCI Machine Learning Repository (Dheeru and Taniskidou 2017) adult data set is shown in Table 1. For this data set, the task is to build a model that can classify individuals according to whether they earn more or less than \$50K annually. The individual shown was classified by a random forest model as having income ≤ \$50K, and the CHIRPS explanation is a combination of three attributes: insufficient (log) capital gain, not married, and education level < 11, which indicates that this individual lacks a college degree on this ordered category. The explanation is immediately interpretable in the context a denial of credit decision, or similar downstream task. The Contrast column shows how far precision decreases when switching out each attribute term in the antecedent. This individual would surely receive a different result if they had saved more capital and, as such, this is an immediately actionable result.

We show a second example in Table 2 using the *rcdv* data set (ICPSR¹) relating to criminal recidivism in North Carolina during 1978 and 1980. For this data set, the task is to classify individuals as likely ("Y") or unlikely ("N") to reoffend. The individual shown has been classified as likely to re-offend. Without an explanation, the classification might not be called into question. However, the very dubious explanation White (race) = False is given, indicating that this single attribute was the deciding factor. In plain English, the model classified the individual as a risk of re-offending *because* they are African American! With the full detail of the explanation, we can see that this attribute was a very poor indicator. The vote margin within the black box model was borderline, at best. The automated decision taken about this individual appears to be little more than a random guess and worse still, this situation affects up to 20% of historical data. The explanation exposes serious flaws in the model itself, raising the necessity to reappraise the data set for bias, and to examine every stage of the model training. More broadly, this result highlights the ethical problems of relying on model classifications alone to make such life-changing decisions.



https://tinyurl.com/y8qvcgwu.

To achieve these results, CHIRPS looks at the decision paths taken by the RF to classify a single instance (the *explanandum*) in each base decision tree (DT) classifier, and retains only those paths that formed the majority vote. This step is justified because a rule based explanation must be locally accurate, meaning that the rule consequent *always* agrees with the model's classification (Lundberg and Lee 2017). The minority paths give a different classification and cannot form part of the explanation.

CHIRPS then employs Frequent Pattern (FP) mining to filter only the decision nodes that occur most frequently within the collection of decision paths. The most frequent nodes refer to attributes that contribute the most to the model's classification. The nodes (or terms) are greedily added into a single classification rule (CR); only the terms that improve the performance against the objective function are added. The "Contrast" analysis in Tables 1 and 2 shows how the rule's performance deteriorates when we exclude each individual term from the antecedent.

Our experimental study over nine data sets compares CHIRPS with four state of the art methods, that is, Anchors (Ribeiro et al. 2018), Bayesian Rule Lists (Letham 2015a, b), inTrees (Deng 2014) and defragTrees (Hara and Hayashi 2016). These methods generate a rule or cascading rule list (CRL), and so are directly comparable. They are also well cited in the literature. Our results show that CHIRPS is at least as good or significantly better in all quality measures in a comparative study that is broader in scope than much of the previous work in this research area. Furthermore, CHIRPS works well in multi-class problems and class-imbalanced problems, where other methods are inconsistent. Unlike some competing methods, CHIRPS does not require discretisation of continuous features as a preprocessing step, and therefore works directly with the model under scrutiny (MUS). We further show that using the traditional objective functions for finding optimal classification rules—precision and coverage—leads to over- and under-fitting solutions. We suggest novel counterparts that perform better in the local explanation setting.

The remainder of this paper is organised as follows: Sect. 2 discusses related work; Sect. 3 covers key concepts of Decision Trees and Random Forest models; Sect. 4 formalises the general problem of explaining classification models and the requirements of an effective solution; Sect. 5 shows how classification rules can be extended to meet all the requirements of explanation; Sect. 6 presents CHIRPS; Sects. 7 and 8 detail our experiments and discuss the results; and finally, Sect. 9 concludes the paper and presents some ideas for further work.

#### 2 Related work

In the last decade, many approaches have been taken to ML interpretability. There have been novel model types, designed for interpretability (Letham 2015b; Friedman and Popescu 2008; Riiping 2006; Waitman et al. 2006). The advantage of using such methods is early discovery of false assumptions and problems in the data set. Such methods can generate a sparse model that takes advantage of domain knowledge (Rudin 2018). Another approach is to extract an interpretable approximation from an already trained, black box model (Adnan and Islam 2017; Hara and Hayashi 2016; Deng 2014). Although all the methods mentioned so far are very different in their implementation, very many of the resulting models fall into the general category of rule sets or rule lists, especially Cascading (or falling) Rule Lists (CRL). This is because logical rules present an uncomplicated, semantic mapping between the inputs and outputs of classification and are considered by



many to provide the most intuitive explanations (Wang et al. 2017; Souillard-Mandar et al. 2016; Wang et al. 2016; Wang and Rudin 2015). CRL are ordered sets of classification rules (CR). CR are rules where the antecedent defines regions of the input space and the consequent is the expected class label in that region.

Bayesian Rule Lists (BRL) (Letham 2015a, b) and Brute (Waitman et al. 2006) are two well-known algorithms for generating a CRL directly from data. The objective is to create an interpretable model, as opposed to explaining an existing one. The complete set of CR is extracted from the data set and subjected to Frequent Pattern (FP) mining. Each method employs a probabilistic strategy to return a subset of mined rules of a user-defined, manageable size as the final model. Neither method modifies or constructs rules from sub-units. Aside from standard quality measures of the rules (precision and coverage), these methods provide a measure of uncertainty of the rule's classification. Brute uses several rounds of bootstrapping of the training data to extract CR for the FP mining. Rules that are similar and frequently occurring across replicates are retained, allowing antecedent terms with variance estimates. BRL, on the other hand, uses Monte-Carlo Markov Chains to return a distribution of rule lists. Individual rule lists from the chain can be used as spot estimates, or the distribution can output rules where the consequent is a probability distribution.

The RuleFit algorithm (Friedman and Popescu 2008) is notable for producing a novel rule-based model type, the predictive rule ensemble (PRE). The first step is to generate an intermediate specialised decision forest (DF). The maximum depth of each tree is a small, random integer, resulting in shallow decision trees with high variance that serve as a large pool of engineered, rule-based features. Next, a linear model (LM) is trained using all of the untransformed and engineered features together, while LASSO regularisation (Tibshirani 1996) ensures that the LM contains a minimal set of non-zero coefficients. These coefficients represent the contribution of the most important features. The rule-based terms in a PRE must be interpreted as oblique (non-orthogonal) parameters whose contribution is counted when the rule covers the instance. Questions remain about the interpretability of such oblique parameters in linear models (Huysmans et al. 2006).

Other methods generate a CRL as a proxy model from an existing MUS (that is always a DF of some kind), as opposed to learning directly from data. This approach is called decompositional (Andrews et al. 1995) because it reduces the search to the smallest information units of the model (e.g. the inner decision nodes of each base classifier in a decision tree ensemble). The purpose of the proxy is to explain the MUS through a more interpretable, simplified structure. The challenge for this approach is to maximise *fidelity* with the MUS. The related literature shows that such simplified, proxy models inevitably give a classification result that differs from the MUS for a proportion of instances. This phenomenon is a consequence of the AITO and such proxy models cannot be used to completely replace the original model. Less than perfect fidelity is a failure to explain individual instances (Rudin 2018); a situation that is unlikely to be acceptable in compliance and safety critical applications. Well known methods in this category include RF+HC (Mashayekhi and Gras 2015), ForEx++ (Adnan and Islam 2017), defragTrees (Hara and Hayashi 2016) and inTrees (Deng 2014). Each of these methods extracts all possible rules from root to leaf of each tree in the DF. The inTrees framework then uses FP mining to identify frequently occurring rules, while RF+HC and ForEx++ score each rule and apply a heuristic to identify a reduced rule set and defragTrees uses a Bayesian formulation. Based on the experimental results given in the relevant articles, the rule lists for RF+HC and ForEx++ remain too large to be considered truly interpretable. However, the stated aim of ForEx++ is knowledge discovery rather than interpretability per se and the authors further analysed the rule sets for patterns and trends.



Until recently, the interpretability gains of CRL were stated and accepted without much critique (Lipton 2016). However, to classify an instance, a CRL requires a top down evaluation; several rules may need to be parsed before finding one that covers an explanandum instance. The resulting explanation is the conjunction of the relevant rule and all preceding rules. Sometimes, there is no covering rule in the list and the model must default to the prior majority class. The interpretation of this default condition is *null*, "don't know," or "the model decided class  $y_k$  because this is true for the most instances." It is a trivial and under-fitting result that is unlikely to be acceptable in compliance and safety critical applications. To minimise these undesirable outcomes, a very long rule list may be required, reducing the comprehensibility of the CRL as a whole. So, CRL are straightforwardly interpretable only for easy to classify instances; those that are covered by a rule near the top of the list. A more realistic goal for CRL is to extract general and holistic insights about the model and data as stated in Adnan and Islam (2017), because they have significant disadvantages for explaining individual classifications. Decision Set based models (Lakkaraju et al. 2016) overcome this limitation, by generating an unordered rule set. As such, a decision set is an OR of ANDs where any one or more rules may resolve to true for an explanadum (Malioutov and Varshney 2013). These models usually require a user-defined and/ or domain informed prior to control the rule cardinality and number of rules generated (Wang et al. 2015); however, the main challenge of these methods is to find the optimal set that maximises coverage while minimising overlap (multiple rules covering the same instances). Overlap requires a tie-break that introduces uncertainty into the classification, while lack of coverage causes a default classification. These problems were recorded on up to 14% of test instances (Lakkaraju et al. 2016), which would be considered much too high for critical applications.

More recently, local explanation methods have emerged that sidestep the AITO altogether. They simplify and generalise per instance classifications (Ribeiro et al. 2018; Lundberg and Lee 2017; Ribeiro et al. 2016; Subianto and Siebes 2007). Local methods implicitly acknowledge that it is untenable to present a human interpretable view of the entire space of a black box model's behaviour (Lipton 2016). This approach allows the MUS to be tuned for optimal classification (or prediction) accuracy without being compromised by the explanation process; that is, there is no loss of fidelity. Several local methods have been proposed in a model-agnostic framework, probing the model's behaviour without needing to access the internal representation. They learn how the model's output changes over a perturbation distribution in the locality around the explanandum (according to some distance metric) and infer the importance of varying the inputs from the resulting output values. This approach, of learning from the model's behaviour, is described as didactic (Andrews et al. 1995). LIME (Ribeiro et al. 2016) is perhaps the most popular of these methods since its publication and recently Shapley values (Lundberg and Lee 2017) has also gained attention. These methods assign a real value to the most important attributes, hence are known as Additive Feature Attribution Methods (AFAM). An AFAM explanation is equivalent to a surrogate LM that approximates the behaviour of the classifier at the locality of the explanandum. The largest coefficients indicate largest contribution to the model's classification or prediction. LIME and Shapley Value explanations are intuitive for the end user, thanks to well-designed graphical outputs. However, it is not easy to know when one instance's explanation applies to other instances. This limitation was overcome in Anchors, which is a very recent extension to LIME. Anchors returns a single rule as an explanation, illustrating the enduring importance of logical rules despite the paradigm shift towards local explanations. Relevance of an explanation to other instances is determined unambiguously; either the rule is covering the new instance or it is not. Anchors



and LIME require all features to be discrete, and internally pre-process any continuous features into quartile bins by default, which can result in loss of information. These techniques have been shown to be effective in image and text classification but there are some limitations when applied to tabular data sets (Michal 2019). As described in Ribeiro et al. (2018) and Ribeiro et al. (2016), the perturbation distribution must be estimated from the joint distribution of the source data and this requires access to the training data set. In other words, these model-agnostic methods are not data-agnostic! If access to the training set is assumed, then the model-agnostic assumption of accessing only the inputs and outputs of the black box model is violated. This problem is overcome in LORE (Guidotti et al. 2018), which uses a genetic algorithm to generate a population of instances and allows for a worst case scenario where only information about the permissible range of values for each feature in the input space in known. This approach, however, is limited to binary classification and can take a prohibitively long time to run. Also, all of these local sampling techniques have been shown to introduce uncertainty and explanations with high variance for similar instances (Fen et al. 2019). This means they require additional checks to determine whether the selected attributes and features are stable over repeated trials. These results suggest that the model-agnostic assumption should be taken with caution.

We argue that the model-agnostic assumption is only required for a subset of problems in the context of HIL processes, such as model auditing by an external third party. HIL processes are frequently found in settings where the model and its training/test data are owned by the explainee. For example, a financial services company segmenting its loan applications by risk, or a medical enterprise implementing automated diagnostics. In these cases, there is no imperative to use a model-agnostic method, especially if a different approach gives better insight. Another problem with model-agnostic is that they explain correlations in the synthetic sample, but not necessarily what the black box model computes (Rudin 2018). This problem calls for a decompositional approach that explains each data instance separately and reveals the internals of the black box.

The very notion of interpretability in ML has been frequently ill-defined in the ML literature, with serious attempts at scientific rigour only appearing very recently (Doshi-Velez and Kim 2017; Bibal and Frenay 2016; Lipton 2016; Subianto and Siebes 2007). Taking an inter-disciplinary approach and drawing from the social sciences, Miller (2017) sets forth guiding principles for a form of explanation that reflects how people explain actions and reasoning to one another. Several other sources confirm that this is a desirable quality

(Woodward 2017; Wilkinson 2014; Salmon 1971; Hempel and Oppenheim Apr. 1948). These guiding principles suggest that explanations should be:

- minimally complete—neither under- nor over-fitting;
- contrastive—providing information about counter-factual cases;
- and a model of self—referring to historical data, not obscure parameters or synthetic distributions.

This research contributes a formalisation of explanations that align with these principles. Furthermore, our proposed method is the first explanation method to our knowledge that addresses directly the above principles. By relaxing the model-agnostic assumptions and given the realities of supervised learning on tabular data sets, our method offers the best of decompositional and didactic methods. Our rule-based explanations have no loss of fidelity, unlike global methods. When tested on unseen data and compared to state of the art methods, the rules are also more precise without tending to over-fit, and have higher coverage without tending to under-fit. These properties produce excellent robustness to class



imbalance where other methods struggle. Aside from LORE (Guidotti et al. 2018), ours is the only method to enhance the explanation with information about counter-factual cases but our method naturally addresses multi-class problems and classification uncertainty, while LORE only targets binary classification problems.

# 3 Decision trees and random forests

Before presenting our method in detail, we provide a brief overview of Decision Trees (DT) and, more specifically, the Classification and Regression Trees (CART) algorithm. CART models are the DT variant used in the original Random Forest (RF) algorithm (Breiman 2001). The CART algorithm is a heuristic method for inducing DT by top-down, greedy, recursive, and binary partitioning of the training data set. CART induction begins with a single (root) node that covers all training data instances. Using non-class attributes, CART proceeds by generating decision nodes that separate the instances into increasingly pure partitions according to their class label. On each iteration, candidate splits are evaluated for all nodes that are currently at the end of a decision path but do not yet meet the stopping criteria. The candidate split that would generate two child nodes with the lowest weighted total Gini Impurity  $I_G$  is always chosen and those child nodes are then added to the growing tree:

$$I_G(Q) = \sum_{k=1}^{K} p_k \cdot (1 - p_k) \tag{1}$$

where  $p_k$  is the proportion of instances having label  $y_k$  in a node Q and K is the number of classes.

Weighted Total 
$$I_G = \frac{I_G(Q_{\text{first}}) \cdot |Q_{\text{first}}|}{N} + \frac{I_G(Q_{\text{second}}) \cdot |Q_{\text{second}}|}{N}$$
 (2)

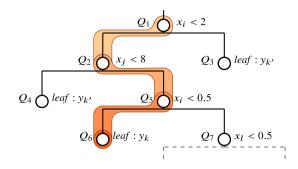
where  $\{Q_{\rm first},Q_{\rm second}\}$  is the set of child nodes that would be created by the candidate split and |Q| is the number of training instances covered by a node. This action occurs independently from any previous or subsequent iteration. There is no way to back out a previous move or find better splits by considering feature interactions. As such, this typifies a greedy heuristic; it is much more computationally efficient than an exhaustive search but has no guarantee of finding the optimal DT. The method is deterministic for a single tree and a static sample.

To classify a previously unseen instance, simply follow the path of that instance down the tree, beginning at the root and obeying the split condition of each decision node until a leaf node is reached. The split conditions are binary conditions that are either true or false for an instance. So, every instance can follow one and only one path, and arrive at one and only one leaf node. Each leaf node covers a subset of the training instances and returns the majority class label of those instances as the classification. See Fig. 2.

A RF is an ensemble of, typically, tens to thousands of base DT classifiers. The ensemble operates in parallel and classifies by majority vote. This improves classification performance in an ensemble compared to a single classifier, assuming each classifier in the ensemble performs somewhat better than a random guess and they are diverse (if not completely uncorrelated) in their errors. In an ensemble, erroneous classifications are outnumbered by correct classifications with very high probability, resulting in



Fig. 2 To classify an instance  $\mathbf{x} = \{\dots, x_i = 0.1, x_j = 10, \dots\}$ , we start at  $Q_1$  and follow the binary split conditions until we reach a leaf node,  $Q_6$  in this case, which returns the label  $y_k$  to the caller



a correct classification on aggregate. To promote the required structural diversity among the base classifiers, stochastic processes are introduced at two stages of DT induction. Firstly, each DT is induced on a uniform sample with replacement (bootstrap) of the training data set. Secondly, although it is still always the best  $I_G$  scoring candidate split that is added to the tree on each iteration, the candidate splits are limited to a random sub-sample of possible candidates. In other respects, tree induction is the same as described in earlier paragraphs except, to further increase the structural variance, it is common to avoid applying any stopping criteria. Under these conditions, trees are fully grown so that their leaves are pure; each leaf covers training instances of only a single class. The resulting trees can be very deep and bushy and individually over-fitting yet, as an ensemble, RF models constructed this way are highly competitive for accuracy among widely available ML methods (Fernandez-Delgado 2014) and are also robust to over-fitting (Breiman 2001), class imbalance, noise, non-informative features, anomalies and variations in the source data (Vens and Costa 2011), and more able to discover useful feature interactions over the whole sample of random trees. There are only two tuning parameters that control most of the variation in performance: the number of trees and the number of candidate features used to generate candidate splits. These properties make RF easy to deploy and popular in practice. In contrast to the relatively simple structure of an individual DT, the consensus is that RF are typical examples of uninterpretable, black box models; Breiman, the inventor of the original RF, described them as "impenetrable" (Breiman 2001). There are several methods for extracting a general measure of feature importance (Gain, Split Count, Permutation Error) but these deliver inconsistent results (Lundberg et al. 2017). Furthermore, these measures can only communicate that certain features were more useful in delivering the model's overall accuracy or error scores. This falls short of providing explanations that detail the contribution of specific attribute values to the classification output or determining the effect of changing the inputs to generate counter-factual classifications.

# 4 Problem formulation

Interpretability of ML models has been poorly defined in the ML literature until recently (Lipton 2016). In response, this section presents our requirements for local explanations, based on the guiding principles proposed in Miller (2017). We also scope these definitions to classification problems on tabular data sets.



# 4.1 The problem of classification

Let  $\mathcal{X} \in \mathbb{R}^P$  be a feature space where  $P \in \mathbb{N}$  is an arbitrary number of features. The jth feature is  $\mathcal{X}_j$ . An instance space  $\mathbf{X} \in \mathcal{X}$  of  $N \in \mathbb{N}$  instances is an  $N \times P$  matrix. Instance  $\mathbf{x}^{(i)} = [x_1^{(i)}, \dots, x_p^{(i)}]$  is the ith row vector of  $\mathbf{X}$  and  $\mathbf{X}_j = [x_j^{(1)}, \dots, x_j^{(N)}]^T$  is the column vector of the jth feature. An attribute  $x_j^{(i)}$  is the value at the jth feature of the ith instance. Let  $\mathcal{Y} = \{y_1, \dots, y_K\}$  be the space of K possible class labels, and  $\mathbf{Y} \in \mathcal{Y}$  be a vector of length N of known instance labels. There is an unknown, conditional distribution  $f = F(y|\mathbf{x})$  such that any randomly sampled, labelled instance space  $(\mathbf{X}, \mathbf{Y})$  has the joint distribution  $F(\mathbf{x}, y) = F(y|\mathbf{x}) \cdot F(\mathbf{x})$ . A classifier is a known function  $g : \mathcal{X} \longmapsto \mathcal{Y}, g \in \mathcal{G}$  selected from the hypothesis space  $\mathcal{G}$  by empirical risk minimisation (Vapnik et al. 1998) over a given, labelled instance space  $(\mathbf{X}, \mathbf{Y})$ , such that g approximates f and is expected to generalise to any random instance space, sampled from the same distribution:  $g(\mathbf{X}) \approx f(\mathbf{X}), \mathbf{X} \in \mathcal{X}$ 

# 4.2 The problem of explaining classifications

In Sect. 5 we will show that CR suit explanations; however, CR may not be the only valid or useful choice. Therefore, in this section we first build a theoretical framework for explanations in general. To aid the reader, we provide Table 3 as a key to the notation used that introduces new concepts in the remainder of this article.

We seek a function  $e: \mathcal{G}, x \mapsto \mathcal{E}$  whose output is  $E = e(g, \mathbf{x}), E \in \mathcal{E}_{g\mathbf{x}}$ , where  $\mathcal{E}_{g\mathbf{x}}$  is the space of possible explanations for a single black box classification event  $g(\mathbf{x})$ . E must be optimal for reliability, generality and interpretability. The trade-off between reliability and generality weighs upon most ML research but interpretability adds several dimensions. It is very difficult to define a general form for explanations that could apply to all situations (all hypothesis spaces and problem spaces). Measuring whether and how much a given E is informative requires the use of proxies that can only be compared between solutions of the same class, such as the number of non-zero linear coefficients (linear models), rule cardinality and number of rules (rule-based models), maximum tree depth or number of nodes (decision trees), number of support vectors in SVM (Bibal and Frenay 2016; Garcia 2009), or the number of relevant features from a tabular data set. This is not always satisfactory in high dimensional problems (Lipton 2016).

We identify the following requirements:

**Requirement 1** E must be minimally complete. We want E to have the smallest possible dimension dim(E) (perhaps measured as the above mentioned proxies). This requirement means that E must be the smallest subset of useful information encoded in  $(g, \mathbf{x})$  that maximises both reliability and generality. Consider, however, a classification task with class imbalance. A trivial or null explanation—one that states that the majority class was selected but gives no reasoning—could apply to every instance (maximum generality) and be valid for all the instances that receive the majority class label from the model (very high reliability). This situation is erroneous because it explains the classification event without any reference to the model's encoding of attribute differences between the classes—the relationship between  $\mathbf{X}$  and  $\mathbf{Y}$ . The implication is that all input values lead to the target



Table 3 Summary of notation

Symbol	Definition
N	The number of instances
P	The number of predictors/features
K	The number of classes
$e(g, \mathbf{x})$	A function that generates an explanation from a classifier and an instance
$\mathcal{E}_{g\mathbf{x}}$	The space of possible explanations that $e(g, \mathbf{x})$ can return
E	A concrete example of an explanation from $\mathcal{E}_{g\mathbf{x}}$ ; the output of $e(g,\mathbf{x})$
dim(E)	Returns the dimension of E e.g. rule cardinality, non-zero coefficients etc
$\mathbb{I}(a)$	Returns the binary truth of its argument
$\mathbb{P}(a)$	Returns the probability / proportion of its argument
L(a,b)	Returns the zero-one loss of its arguments
$r(E, \mathbf{z})$	A relevance function that determines if $E$ generalises to an instance $\mathbf{z}$
$\mathcal{Z}_E$	An input subspace of the input space $X$ over which $E$ generalises
$\mathbf{Z}_{E}$	An instance subspace of the data set $X$ over which $E$ generalises
R(E)	Local risk—the expected loss of <i>E</i> over $\mathcal{Z}_E$
$R_{\rm emp}(E)$	Local, empirical risk—the estimated loss of E over $\mathcal{Z}_E$
$\mathcal{Z}_E^{'}$	The counter-facutal relevance subspace of $E$
$\mathbf{Z}_{E}^{'}$	The counter-factual instance subspace of $E$
$c_i^{\text{lwr}}, c_i^{\text{upr}}$	Lower and upper bounds defined over a feature $j$
$C_{\mathcal{Z}_{F}}$	A set of upper/lower bounds that define the relevance space of $E$
$\zeta(g, \mathbf{Z}_E, \mathbf{x})$	Stability—a precision-like quality measure for explanations
$\xi(g,\mathbf{X},\mathbf{Z}_E,\mathbf{x})$	Exclusive coverage—a coverage-like quality measure for explanations
$(j, v, \tau)$	Detail of a given node in a decision path: a triple of (feature index, threshold value, Boolean test)
$ps_n$	A given path snippet, comprising one or more node detail triples
ρ	A user-defined target stability. An early stopping parameter

class, which is false. This is an under-fitting scenario, equivalent to a classification model with constant output. So, *E* must reduce the problem dimensionality but must remain informative to some extent; *E* may not be trivial.

**Requirement 2** There must be some function r that determines when  $E = e(g, \mathbf{x})$  is relevant to any instance other than the explanandum instance  $\mathbf{x}$  in the reduced dimension of the solution space  $\mathcal{E}_{g\mathbf{x}}$  (Req 1):

$$r(E, \mathbf{z}) = \begin{cases} 1 \text{ if } E \models \mathbf{z} \\ 0 \text{ otherwise} \end{cases}$$
 (3)

where  $\mathbf{z} \neq \mathbf{x}$ ,  $\mathbf{z} \in \mathcal{X}$  and  $a \models b$  (a models b) means a is a logical conjunction and every part of a is true of b. Thus, the relevance subspace of E can be determined from r:

$$\mathcal{Z}_E = \{ \mathbf{z} : r(E, \mathbf{z}) = 1, \ \mathbf{z} \in \mathcal{X} \}, \ \mathcal{Z}_E \text{ is continuous.}$$
 (4)

Note,  $E \in \mathcal{E}_{g\mathbf{x}}$  means that E is an explanation of  $\mathbf{x}$ , therefore  $r(E, \mathbf{x}) = 1$  and  $\mathbf{x} \in \mathcal{Z}_E$  are always true.



**Requirement 3** *E* must have maximal local reliability. The term *local* refers to everything inside the relevance subspace. Perfect local reliability means that  $g(\mathbf{z}) = g(\mathbf{x})$ ,  $\mathbf{z} \in \mathcal{Z}_E$  but this may not be possible while simultaneously satisfying minimal completeness. We can proceed by minimising local risk:

$$R(E) = \int L(g(\mathbf{z}), g(\mathbf{x})) d\mathbf{z}, \ \mathbf{z} \in \mathcal{Z}_E, \ E \in \mathcal{E}_{g\mathbf{x}}, \tag{5}$$

$$L(a,b) = \begin{cases} 0 \text{ if } a = b \\ 1 \text{ if } a \neq b \end{cases}$$
 (6)

Typically in ML research, the true distribution of z is unknown. Therefore, the risk must be estimated empirically from an instance space X of observed data. X could be the training set used to train g or any i.i.d. random sample from the same distribution. The relevant instance space is:

$$\mathbf{Z}_{E} = \{ \mathbf{z} : \mathbf{z} \in \mathcal{Z}_{E} \cap \mathbf{X} \}. \tag{7}$$

Then, empirical local risk can be estimated by:

$$R_{\text{emp}}(E) = \frac{1}{|\mathbf{Z}_E|} \sum_{i=1}^{|\mathbf{Z}_E|} L(g(\mathbf{z}^{(i)}), g(\mathbf{x})); \mathbf{z}^{(i)} \in \mathbf{Z}_E, E \in \mathcal{E}_{g\mathbf{x}},$$
(8)

which is related to precision, by way of reversing the zero-one loss function:

$$\mathbb{P}\left(g(\mathbf{z}^{(i)}) = g(\mathbf{x})\right) = \left(1 - R_{\text{emp}}(E)\right) \\
= \frac{1}{|\mathbf{Z}_{E}|} \sum_{i=1}^{|\mathbf{Z}_{E}|} 1 - L\left(g(\mathbf{z}^{(i)}), g(\mathbf{x})\right) \\
= \frac{1}{|\mathbf{Z}_{E}|} \sum_{i=1}^{|\mathbf{Z}_{E}|} \mathbb{I}\left(g(\mathbf{z}^{(i)}) = g(\mathbf{x})\right); \mathbf{z}^{(i)} \in \mathbf{Z}_{E}, E \in \mathcal{E}_{g\mathbf{x}}$$
(9)

where the final term is equivalent to the standard definition of precision.

**Requirement 4** E must be as general as possible given maximal local reliability. This means its relevance subspace covers the largest continuous volume of the feature space that achieves the same precision or better than any other relevance subspace. The E that satisfies this requirement meets the following criteria:

$$|\mathbf{Z}_E| > |\mathbf{Z}_{E'}|, \ \mathbb{P}\left(g(\mathbf{Z}_E) = g(\mathbf{x})\right) \geq \mathbb{P}\left(g(\mathbf{Z}_{E'}) = g(\mathbf{x})\right), \ E \neq E', \ E, E' \in \mathcal{E}_{g\mathbf{x}}. \tag{10}$$

**Requirement 5** E must not be tautological, meaning that it generalises to a set of instances not limited to the singleton explanandum  $\mathbf{x}$ . An E that does not generalise beyond the singleton  $\mathbf{x}$  is an erroneous situation that trivially explains the classification event  $g(\mathbf{x})$  by the uniqueness of  $\mathbf{x}$  in the data set. This is the local explanation equivalent of over-fitting. Such over-fitting could arise at a complex or noisy decision boundary. In the most extreme case, where  $g(\mathbf{x}) = y_k$  while for every near neighbour  $g(\mathbf{z}) \neq y_k$ , equation (8) is trivially maximised if  $\mathbf{x}$  is the only member of  $\mathbf{Z}_E$  and plummets when any  $\mathbf{z} \neq \mathbf{x}$  is included in  $\mathbf{Z}_E$ . In Sect. 5, we introduce a novel objective function, *stability* to gracefully handle this problem.



**Requirement 6** It must be possible to present E with contrastive, counter-factual information. That is, we assume that the form of explanation reveals the minimal changes to the inputs that give different results. In Sect. 5 we show how this is defined for CR specifically. Some authors posit that the counter-factual cases are any changes in the attributes of an instance that would result in a different classification (Guidotti et al. 2018; Subianto and Siebes 2007). However, such a definition can only apply to discrete, nominal and deterministic predictors. In the case of continuous predictors with complex decision boundaries, such as the mixed Gaussian process shown in Fig. 4, there could be several non-contiguous or interleaved regions of the input space (Ho and Basu 2002) that classify identically; in these cases a change of the minimal attribute set may not always result in a different class assignment. We can, however, expect a change in precision outside the relevance space and there is support for such models that offer measures of uncertainty rather than crisp boundaries in the literature (Proenca and Leeuwen 2019; Letham 2015a, b; Waitman et al. 2006). Therefore, we propose a task dependent definition of contrastive explanations: counter-factual cases should be *demonstrably* different from observed cases. This difference is manifested as a drop in precision below some user-defined tolerance  $\delta$ . That is  $\mathbb{P}(g(\mathbf{Z}_{E}') = g(\mathbf{x})) \le \mathbb{P}(g(\mathbf{Z}_{E}) = g(\mathbf{x})) - \delta \text{ where}$ 

$$\mathbb{P}\left(g(\mathbf{Z}_{E}') = g(\mathbf{x})\right) = \frac{1}{|\mathbf{Z}_{E}'|} \sum_{i=1}^{|\mathbf{Z}_{E}'|} \mathbb{I}\left(\left(g(\mathbf{z}^{(i)}) = g(\mathbf{x})\right)\right), \ \mathbf{z}^{(i)} \in \mathbf{Z}_{E}', \ \mathbf{Z}_{E}' = \{\mathbf{z} \in \mathcal{Z}_{E}' \cap \mathbf{X}\}$$

$$(11)$$

This quantity is the precision of the counter-factual instance space  $\mathbf{Z}_E'$ , and  $\mathbf{Z}_E'$  is the counter-factual relevance space. Note,  $\mathbf{Z}_E'$  is a space, or set of spaces covered by minimal changes to E. It is not equivalent to  $\{\mathbf{X} \setminus \mathcal{Z}_E\}$ , which is the entire input space not covered by E. If the latter were true, then each unique explanation would be a global model describing the entire input space by itself and its complement. Rather, the benefit of counter-factual information is to identify the boundary outside which E is no longer reliable.

**Requirement 7** E should be a "model-of-self" that explains the model from the data. Model g is the output of a learning algorithm (a function) that was parameterised by the training data (X, Y). E should frame the explanation in terms of the influence of (X, Y) over the original learning algorithm. This requirement is met *de facto* by the empirical formulations given.

In the following sections, we show how CHIRPS using CR as the form of explanation, is designed to meet these requirements. As our experimental study shows, competing methods that do not explicitly address them all have a tendency to converge to under- or over-fitting solutions.

# 5 Extending classification rules as explanations

Frequent Patterns (FP), Association Rules (AR) and Classification Rules (CR) are all modes of expressing relationships between patterns in a data set. A pattern is formed from  $k \ge 1$  attributes, and referred to as a k-item set. The  $support\ count = \sigma(fp)$  is the number of instances in a data set that match the pattern fp, while  $support(fp) = \frac{\sigma(fp)}{N}$  is the fraction of instances containing fp. A pattern is said to be frequent if its support exceeds minsup, a user-defined threshold. AR describe associations over the whole data set between



individual items within a k > 1 item set. For example, for a 2-item set fp =  $\{Z, Y\}$ , there is a relationship expressed as the rule:  $Z \Longrightarrow Y$ . Here, Z is called the antecedent and Y the consequent. Such an AR has a level of *confidence* or *precision*, which is equal to the conditional probability  $\mathbb{P}(Y|Z) = \frac{support(\{Z,Y\})}{support(Z)}$ , where  $support(Z) = \mathbb{P}(Z)$  is the support of the antecedent alone (also called the coverage). A CR is simply an AR where Z is a set of conditions defined on one or more features  $\{X_1, \ldots, X_P\}$  of a data set, and Y is a class label. It is trivial to derive a CR from the decision path of a DT (Quinlan 1987): Using the example from Fig. 2, the following is a CR:

$$\{\mathbf{x} : \min(\mathcal{X}_i) \le x_i < 0.5, \ 8 \le x_i \le \max(\mathcal{X}_i)\} \implies y_k \tag{12}$$

# 5.1 Meeting the requirements for explanations

We can find CR that conform to our formulation of an explanation, given in Sect. 4, if we set  $Z = \mathcal{Z}_E$ , a relevance subspace, and  $Y = g(\mathbf{x})$ , the output of the model. Then, the CR is simply  $\mathcal{Z}_E \implies g(\mathbf{x})$ . Req 2 is satisfied by this formulation because we can define the relevance evaluation function as:

$$r(E, \mathbf{z}) := \prod_{j=1}^{P} \mathbb{I}\left(\max\left(c_{j}^{\text{lwr}}, \min(\mathcal{X}_{j})\right) \le z_{j} \le \min\left(c_{j}^{\text{upr}}, \max(\mathcal{X}_{j})\right)\right),$$

$$c_{j}^{\text{lwr}}, c_{j}^{\text{upr}} \in C_{\mathcal{Z}_{F}}, \mathbf{z} \in \mathcal{X}$$

$$(13)$$

where  $C_{\mathcal{Z}_E}$  is the set of parameters that define the lower and upper bounds of each feature. For a feature space with P features, any  $\{c_j^{\text{lwr}}, c_j^{\text{upr}}, j \in P\}$  may be undefined, in which case the interval begins and/or ends with the domain of  $\mathcal{X}_j$ . Minimising dim(E) requires  $|C_{\mathcal{Z}_E}|$  to be as small as possible, though it may not be zero (Req 1). The best case is  $|C_{\mathcal{Z}_E}| = 1$  and the worst case is  $|C_{\mathcal{Z}_E}| = 2P$ .

To find candidates  $E \in \mathcal{E}_{gx}$  that meet the requirements, we propose an iterative, breadth-first search heuristic as follows: at iteration i=0,  $E^{(i)}$  is a trivial or empty rule. In other words, the antecedent  $C_{\mathcal{Z}_{E^{(0)}}} = \emptyset$  while the consequent is g(x). Thus coverage is complete at the start and will be iteratively reduced in a trade off (Req 4) with precision. In each subsequent iteration i+1 we either add a new parameter or update an existing one that strictly increases the precision. However, to avoid tautological solutions (Req 5), we cannot use high precision as an optimisation target for this procedure because this measure can be trivially maximised with singletons or very small, overfit subspaces. We therefore propose *stability*, a novel objective function that penalises explanations that explain only a small number of instances.

**Definition 1** *Stability* takes the form  $\zeta : \mathcal{G}, \mathcal{X}, x \longmapsto \mathbb{R} \in (0, 1)$ .

$$\zeta(g, \mathbf{Z}_{E}, \mathbf{x}) = \frac{\left|\left\{\mathbf{z} : g(\mathbf{z}) = g(\mathbf{x}), \ \mathbf{z} \in \mathbf{Z}_{E} \setminus \mathbf{x}\right\}\right| + 1}{\left|\mathbf{Z}_{E}\right| + K} = \frac{\left|\left\{\mathbf{z} : g(\mathbf{z}) = g(\mathbf{x}), \ \mathbf{z} \in \mathbf{Z}_{E}\right\}\right|}{\left|\mathbf{Z}_{E}\right| + K}$$

$$(14)$$

where *K* is a regularising constant and equals the number of possible classes.

The middle formulation in equation (14) shows how this measure relates to requirement 5; we calculate the precision of  $g(\mathbf{z}) = g(\mathbf{x})$  inside the relevant instance space, excluding



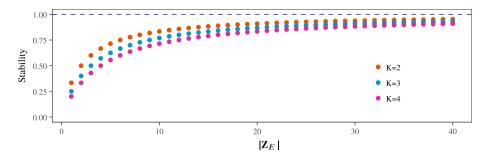


Fig. 3 Maximum achievable stability (the discrete points) when all instances are given the same classification, for relevant instance spaces containing from one to forty instances and  $K \in \{2, 3, 4\}$ . The dashed line shows precision, which is always exactly 1.0 in these circumstances, no matter how small the instance space

**Table 4** Demonstrating stability for K = 2 with examples

	Rule-instar	Rule-instance table		Values	
	Covered	Not covered			
Iteration i			,		
Target class	20	780	Stability	0.870	
Other class	1	199	Precision	0.952	
			Recall	0.025	
			F-1	0.049	
$Iteration \ i+1$					
Target class	1	799	Stability	0.333	
Other class	0	200	Precision	1.0	
			Recall	0.001	
			F-1	0.002	

**x** itself. We apply additive smoothing as  $\frac{n+1}{m+K}$ . Then, the numerator simplifies as shown in the final form. Therefore, stability is similar to using precision with a Laplace correction (Clark and Boswell 1991) but with a more severe penalty. Due to the division by K, trivial relevance spaces (of size 1) only get a stability of 33% or less for  $K \ge 2$ . The function profile shown in Fig. 3 makes this clear.

We illustrate the benefit of this novel function with an example given in Table 4. At iteration i, there are twenty-one covered instances  $\mathbf{z} \in \mathbf{Z}_{E^{(i)}}$ . For all but one of these  $g(\mathbf{z}) = g(\mathbf{x})$ . This could be an optimal solution but the search continues to iteration i+1. The rule takes a new, more specific parameter and  $\mathbf{Z}_{E^{(i+1)}}$  now covers just one instance. If we are optimising for precision,  $E^{(i+1)}$  would be considered better than  $E^{(i)}$  because precision is trivially maximised to 1.0. Stability, on the other hand, has fallen well below any tolerable level, so instead we keep  $E^{(i)}$  as the explanation. It is important to realise that better recognised statistics such as *recall* and *F-1 measure* are unsuitable in this setting; since, the table shown in the examples is not a confusion matrix. Rather, we have tabulated the instance classification versus the rule coverage. We seek to maximise *covered*, *target class* and minimise *covered*, *other class*. We can tolerate high numbers of instances in the *not covered* column because we assume these instances will be covered by another explanation. Another perspective is that stability approaches precision asymptotically



as  $|\mathbf{Z}_E| \to \infty$  but when  $|\mathbf{Z}_E|$  diminishes so does the maximum stability; maximum stability  $= \frac{1}{K}$  when  $|\mathbf{Z}_E| = 1$ . This behaviour acts as a brake that prevents the algorithm from adding more parameters and converging on singletons. This is achieved non-parametrically, without the need for user intervention.

We introduce another, novel quality measure by returning to the minimal completeness requirement (Req 1). This states that there must be at least one *informative* parameter that can distinguish between differently classified instances. In situations of severe class imbalance, precision and coverage could simultaneously be trivially maximised by a *null* solution that covers the entire input space. As we show in our experimental results, classimbalance can lead to such under-fitting solutions in several competing methods. To guard against this, we propose a further, novel objective function, *exclusive coverage* in equation (15) that penalises high coverage against a lack of discrimination between classes.

**Definition 2** Exclusive coverage takes the form  $\xi: \mathcal{G}, \mathcal{X}, \mathcal{X}, x \longmapsto \mathbb{R} \in (0, 1)$ . Exclusive coverage is calculated as coverage, the fraction of all instances covered by the rule excluding the explanandum. This is similar to the relation between stability and precision. Additionally, however, the value is weighted by the ratio of *not covered, other class* to *not covered, other class* + *covered, other class* (equivalent of "true negative rate"). This measure increases with the number of differently classified instances outside the relevant instance space  $\mathbf{Z}_E$ .

$$\xi(g, \mathbf{X}, \mathbf{Z}_{E}, \mathbf{x}) = TNR \cdot \frac{|\mathbf{Z}_{E} \setminus \mathbf{x}| + 1}{|\mathbf{X}| + K} = TNR \cdot \frac{|\mathbf{Z}_{E}|}{|\mathbf{X}| + K}, \ \mathbf{Z}_{E} \subseteq \mathbf{X}$$

$$TNR = \frac{|\{\mathbf{z}' : \mathbf{z}' \notin (\mathbf{Z}_{E}) \land g(\mathbf{z}') \neq g(\mathbf{x})\}|}{|\{\mathbf{w} : \mathbf{w} \in (\mathbf{X}) \land g(\mathbf{w}) \neq g(\mathbf{x})\}|}$$
(15)

where TNR is the so-called "true negative rate" described above.

We illustrate the benefit of this novel function with an example given in Table 5. In this highly imbalanced class example, at iteration 0, the *null* rule covers all instances. Precision and stability are very high, perhaps above a threshold that could trigger an early stopping condition. Coverage is trivially maximised at 1.0. To report such a result would lead to a misleading representation of the rule quality. It is clearly an under-fitting solution. So we must add a term to the rule, even one that may dramatically decrease stability, precision and, of course, coverage. An example of a possible subsequent state is shown at iteration 1. At this point, the search for additional rule terms that can increase stability should continue. So, at iteration 2, another rule term is added. This results in a more specific rule that has slightly reduced coverage, but slightly increased exclusive coverage. This example shows how using exclusive coverage as a quality measure helps to disqualify under-fitting solutions.

We reiterate the importance of using appropriate quality measures for explanations and how these differ from measures typically associated with classification accuracy (precision, recall, F-1 score). These novel functions are central to the contribution of this research.

### 5.2 Providing contrastive and counter-factual information

Counter-factual examples illustrate changes in the inputs that will give different results. We have defined this in Req 6 as ensuring that the MUS's outputs are demonstrably different



**Table 5** Demonstrating Exclusive Coverage with Examples for K = 2

	Rule-instar	nce table	Measure	Values
	Covered	Not covered		
Iteration 0			1	
Target class	950	0	Stability	0.948
Other class	50	0	Precision	0.950
			TNR	0.0
			Excl. Cov.	0.0
			Coverage	1.0
Iteration 1				
Target class	200	750	Stability	0.881
Other class	25	25	Precision	0.889
			TNR	0.5
			Excl. Cov.	0.112
			Coverage	0.225
Iteration 2				
Target class	190	760	Stability	0.918
Other class	15	35	Precision	0.927
			TNR	0.7
			Excl. Cov.	0.143
			Coverage	0.205

For clarity, we have included the TNR which is the ratio *bottom leftlbottom row total*. The unweighted, intermediate term (not shown) is identical to coverage at three decimal places

for instances in the counter-factual space  $\mathcal{Z}'$ . This contrastive output may be a change of class label, or a significant drop in precision, that is, confidence in the given classification. Recall that the motivation for implementing local, per instance explanations is to avoid generalising the output of the MUS (model g) for the entire input space. We seek an explanation that is valid in the locality of the instance and we seek to avoid developing a global proxy of the MUS with all the disadvantages discussed in Sect. 2. The minimal completeness criterion means that it is necessary to show a decrease in precision below a user-defined tolerance only for spaces defined by a change to a single parameter in  $C_{\mathcal{Z}_E}$ , all others remaining identical. To obtain the complete set of adjacent spaces, we switch the position of each parameter  $c \in C_{\mathcal{Z}_E}$ , one at a time, such that a  $c_j^{\text{upr}}$  replaces  $c_j^{\text{lwr}}$  or vice versa. This is illustrated in Algorithm 1 and visually in two dimensions in Fig. 4 where an unseen instance  $\mathbf{x}$  is classified as belonging to the triangle class. A candidate explanation, the optimal relevance subspace  $\mathcal{Z}_E = \{\mathbf{z}: a \leq z_1 \leq b, c \leq z_2 \leq d\}$  is defined around  $\mathbf{x}$  by the parameters  $\{a, b, c, d\}$ . If the intervals [a, b] or [c, d] are any wider, there will be a drop in precision. If the intervals are any tighter, coverage decreases without improving precision. By Algorithm 1, the adjacent (counter-factual) spaces are:

$$\mathcal{Z}'_{E} = \left\{ A = \{ \mathbf{z} : z_{1} \le a, c \le z_{2} \le d \}, \ B = \{ \mathbf{z} : b \le z_{1}, c \le z_{2} \le d \}, \right.$$

$$C = \left\{ \mathbf{z} : a \le z_{1} \le b, z_{2} \le c \right\}, \ D = \left\{ \mathbf{z} : a \le z_{1} \le b, d \le z_{2} \right\} \right\}$$

$$(16)$$



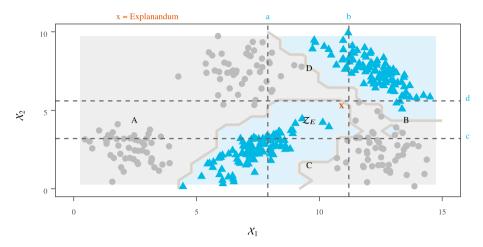


Fig. 4 A model with a complex boundary trained on a synthetic data set which has two classes, shown as triangles and circles and the candidate relevance space  $\mathcal{Z}_E$  is defined by four parameters a, b, c and d

```
Algorithm 1 Get Adjacent Space for a Relevance Space
 1: procedure Get Adjacent Spaces(C_{Z_E})
          Adjacent Spaces ← []
                                                                                                                                                         ▶ Empty List
 3.
          for all c_j \in C_{Z_E} do
              C \leftarrow C_{Z_E}

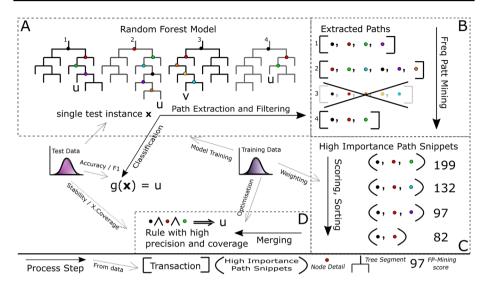
if c_j is an upper bound of X_j then
 4:
                                                                                                                          ▶ Copy of relevance space parameters
 5:
                   c_i^{\text{lwr}} of C \leftarrow c_j; c_i^{\text{upr}} of C \leftarrow \max(X_j)
 6:
 7:
                     _{i}^{\text{upr}} \text{ of } C \leftarrow c_{j}; c_{i}^{\text{lwr}} \text{ of } C \leftarrow \min(X_{j})
 8:
 9:
               Append C to Adjacent Spaces
          Return(Adjacent Spaces)
10.
```

Provided the precision of the explanations representing each of these subspaces falls below the user-defined tolerance, all the requirements are satisfied. If a counter-factual space has a precision above the tolerance, the space can be merged with  $\mathcal{Z}_E$  by removing the defining parameter from the rule antecedent.

### 6 CHIRPS

We propose our novel procedure to search for CR that meet the requirements for local explanations. CHIRPS is a concrete implementation of the function  $e(g, \mathbf{x})$  and the heuristic search introduced in Sects. 4 and 5. CHIRPS assumes g is a random forest model, which defines CHIRPS as a model-specific method. Each step is illustrated in the conceptual diagram in Fig. 5 and detailed in the following sections. To explain the classification of an unseen instance, the original training set can be used in the rule finding step. The test set, originally used for assessing the classification accuracy of g, can be used to verify quality of the resulting explanations, using a leave-one-out procedure: One instance is classified and explained, while the remaining instances are kept aside and contribute no information to the explanation. These remaining instances can then be





**Fig. 5** Conceptual diagram of CHIRPS in four steps: A. Path Extraction and Filtering, B. FP Mining, C. Scoring and Ranking, D. Merging and Pruning

used to determine stability and exclusive coverage scores for that individual rule. Thus each instance of the test set constitutes an experimental unit. Performance of an explanation algorithm is then the aggregate score over all these units.

### 6.1 Path extraction and filtering

The first step is to classify the explanandum instance  $\mathbf{x}$  and simultaneously extract the decision path of every DT. This is simply a matter of tracking the detail of each node. Without loss of generality, the node detail can always be posed as the evaluation of an inequality  $x_j < v$ , where j is a feature index and  $v \in \mathbb{R}$ . Let  $\tau \in \{0,1\}$  be the binary truth of the evaluation. Thus, each node detail is the triple  $(j,v,\tau)$ . Assuming nominal values are binary encoded, we can represent node detail for any data type with this structure. The interpretation depends on the domain of  $\mathcal{X}_j$ . The following examples are for illustrative purposes and are non-exhaustive:

$$(i, 0.5, 1) \land \mathcal{X}_i \in \{0, 1\} \implies x_i = 0 \text{ (binary false)}$$
  
 $(j, 0.5, 0) \land \mathcal{X}_j \in \mathbb{R} \implies 0.5 \le x_j \le max(\mathcal{X}_j) \text{ (real valued interval)}$   
 $(l, 3.5, 0) \land \mathcal{X}_l \in \{1, 2, 3, 4, 5\} \implies x_l \in \{4, 5\} \text{ (likert score } \ge 4)$ 

There is only one possible path for  $\mathbf{x}$  down each tree so the rest of the model is ignored (of course, for a different instance, a different set of paths are extracted). Trees have a number of nodes in  $\mathcal{O}(2^n)$  where n is the maximum tree depth, compared to paths that are  $\mathcal{O}(n)$ , so this step reduces the search space logarithmically while retaining all the information about  $g(\mathbf{x})$ . A second level of filtering is achieved by retaining only decision paths that agreed with the majority vote. Trees that voted for a minority class represent noise in the model. Their contribution was made redundant by the majority vote system.



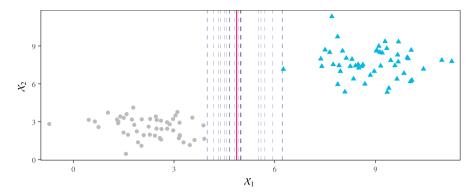


Fig. 6 Simulation of discretising by the median (solid line) of twenty axis aligned splits (dashed lines) that all represent the same decision; they are sampled uniformly from inside the margin between two clusters that are linearly separable on continuous feature  $\mathcal{X}_1$ 

# 6.2 Frequent pattern mining

In this section, we explain how FP mining is very well suited to extracting knowledge from random forests. Treating the RF model as a sample of a tree-structured random variable, certain stochastic phenomena have been demonstrated (Paluszynska 2017; Louppe 2017; Biau 2012; Vens and Costa 2011; Ishwaran 2007). As described in Sect. 3, CART adds decision nodes to a growing tree that minimise the total, weighted  $I_G$  score on each iteration. Therefore, features with the greatest power to discriminate between classes occur with greatest probability at shallow levels because they are selected whenever they appear as candidates. This results in a smaller mean depth of nodes involving those features. Every root node in the RF has probability p = 1 of being included in the set of decision paths of any instance. The probability of being included falls exponentially with each tree level because the number of alternative paths grows at  $\mathcal{O}(2^n)$  for n levels. So nodes involving the most discriminating features will appear in the collection of paths with very high probability. Also, the weighted total  $I_G$  of a candidate split is conditional on all nodes above it in the same path. This means that features that interact have a greater chance of co-occurring in any given path, with these co-occurrences showing increased frequency over the whole collection. These properties suggest that frequency based filtering will be very effective at selecting the most important decision nodes. Furthermore, instances with more attributes in common are more likely to follow a similar path through each tree, resulting in solutions that are highly generalisable.

In addition to the above properties, note that FP mining requires a transaction list as input. A transaction list is a very suitable representation for the set of extracted and filtered decision paths. Each decision path can be considered as a transaction. Each transaction is a set of items, being the triples  $(j, v, \tau)$  described in the previous section. The whole triple is the underlying unit for pattern matching. To execute a reasonable FP-mining task of these units, it is necessary to resolve the potentially very large number of unique values resulting from real-valued features. The cut-point v chosen independently by each DT might be anywhere in a location that separates the classes. That is to say, many unique values may all represent the same decision boundary. So, this uniqueness presents a problem. Before performing the FP mining, all triples matching  $(j, \bullet, \tau)$ —where  $\bullet$  is any value—are discretised. This is illustrated in Fig. 6. Increasing



the number of discrete values may improve results with more complex boundaries, so we use a binning function where number of bins can be set as a user-defined tuning parameter.

The output of FP mining is a list of FP that exceeded the minimum support, further filtering the search space prior to the rule building step. The support value of each item set is also returned as a score. Since these *k*-item sets may represent non-contiguous nodes in a path, we name these objects *high importance random path snippets* or simply, path snippets.

# 6.3 Ranking

Even though the previous two steps have dramatically reduced the search space, finding the minimal set of snippets that maximises stability and exclusive coverage is a multi-objective, combinatorial problem. To avoid an exhaustive search we rank the snippets according to a heuristic score. The RF+HC method (Mashayekhi and Gras 2015) also uses a score function for rule ranking, so that function was considered first. Unfortunately, it demonstrates undesirable behaviour for our needs. Firstly, the penalty increases with rule length because rule length appears in the denominator. This is the wrong direction because, under FP mining, higher cardinality snippets naturally have lower support than those with lower cardinality (Agrawal et al. 1994). Those longer snippets that have passed our support threshold contain the most useful feature interactions. Secondly, the penalty depends on rule accuracy and coverage because the number of covered and correct instances appear in the numerator. We need to separate these effects. Consequently, we developed a unique ranking system that uses cardinality adjusted support with regularisation.

$$Score(ps, w, sup, \alpha) = w \cdot sup \cdot \frac{(|ps| - \alpha)}{|ps|}$$
 (18)

where ps is the path snippet,  $| \cdot |$  is the cardinality, or length of  $\cdot$  and the remaining variables are tunable parameters:

- $sup \in \{1, support(ps)\}$ . If set to 1 then the effect is neutral.
- $\alpha$  is a real valued constant to adjust the support based on path snippets cardinality. Higher order interactions are favoured when  $0 \le \alpha$ . The effect is neutral when  $\alpha = 0$
- w is a regularising weight (with a neutral default = 1). Our early investigations indicated that performance improved when each ps's score was weighted by the following Kullback-Leibler (KL) Divergence:

$$w_{ps} = D_{KL}(P \parallel Q) = -\sum_{x \in \mathcal{X}} P(x) \log \left(\frac{P(x)}{Q(x)}\right). \tag{19}$$

where P, Q are the posterior class distribution when each snippet is used to partition the training data, and prior class distribution, respectively. The KL-Divergence measures the information lost if a distribution Q is used, instead of another distribution P to encode a random variable. Our sensitivity analysis shows that the use of this weight reduces the variance of stability for a large sample of test instances (see Sect. 8.2).



# 6.4 Merging and pruning

Following the heuristic steps outlined in Sect. 5, the path snippets from the ranked list are merged into a CR using a simple, greedy algorithm. Section 7 details our experimental results, showing that this solution is fast and beats competing methods without requiring a more sophisticated optimisation algorithm. A walk-through of the major steps is given here. Also, see Algorithm 2.

```
Algorithm 2 Rule Merging
 1: procedure RuleMerge(g, X, x, (ps_1, ps_2, ..., ps_n), \rho, \alpha)
                                                                                                                                                                       ▶ iteration number
 3:
           C_{Z_{E^{(i)}}} \leftarrow \emptyset
                                                                                                                                                                                \triangleright Z_{E_0} = X
 4:
           s_i \leftarrow \zeta(g, \mathbf{X}, \mathbf{X}, \mathbf{x})
                                                                                                                  ▶ Prior estimate. See Step 2 notes for bootstrap options
 5:
           while s_i < \rho and length(ps_1, ..., ps_n) > 0 do
                \mathbf{Z} \leftarrow \mathbf{X} \cap (C_{\mathcal{Z}_{E^{(i-1)}}} \cup ps_1)
                                                                                                                                     ▶ Instance space of candidate explanation
 8.
                if \zeta(g, \mathbf{X}, \mathbf{Z}, \mathbf{x}) > s_{i-1} then
                                                                                                                                        ▶ See Step 2 notes for bootstrap options
                      C_{Z_{E^{(i)}}} \leftarrow C_{Z_{E^{(i-1)}}} \cup ps_1
 9.
                                                                                                                                                                              ▶ update rule
                       s_i \leftarrow \zeta(g, \mathbf{X}, \mathbf{Z}, \mathbf{x})
10:
                      for all ps \in (ps_1, \ldots, ps_n) do
11:
                                                                                                                                   > remove redundant path snippets from list
12.
                           if ps \subseteq C_{\mathcal{Z}} then
13:
                                (ps_1, \ldots, ps_n) \leftarrow (ps_1, \ldots, ps_n) \setminus ps
14:
                 else(ps_1, \ldots, ps_n) \leftarrow (ps_1, \ldots, ps_n) \setminus ps
                                                                                                                                        ▶ Remove ps1 if no increase to stability
           return C_{\mathcal{Z}_{E^{(i)}}}
15:
```

**Step 1** Starting breadth first with a non-informative, *null* explanation:

$$E^{(i)} = \mathcal{Z}_{E^{(i)}} \implies g(\mathbf{x}), \ C_{\mathcal{Z}_{E^{(i)}}} = \emptyset, \ i = 0$$

$$(20)$$

where i is the iteration number. The initial relevance subspace has no defining parameters and so covers the entire input space  $\mathcal{X}$  and the relevant instance space  $\mathbf{Z}_{E^{(0)}} = \mathbf{X}$  is equal to the entire training set. The prior stability  $s_0$  can be a point estimate:  $\zeta(g, \mathbf{Z}_{E^{(0)}}, \mathbf{x})$ , or estimated with confidence intervals using the bootstrap:  $\frac{1}{B}\sum_{b=1}^{B}\zeta(g, \mathbf{Z}_{E^{(0)}}^{*b}, \mathbf{x})$ , where B is the number of bootstraps and  $\mathbf{Z}_{E^{(0)}}^{*b}$  is the bth bootstrap sample of the relevant instance space.

**Step 2** On each iteration *i*, a candidate subspace is formed from  $C_{\mathcal{Z}_{E^{(i-1)}}} \cup ps_1$  where  $ps_1$  is the path snippet currently at the top of the ranked list. The stability of the candidate and current subspaces are compared, using the bootstrap formulation:

$$p = \frac{1}{B} \sum_{b=1}^{B} \mathbb{I}\left(\zeta(g, \mathbf{Z}_{E^{(i)}}^{*b}, \mathbf{x}) > \zeta(g, \mathbf{Z}_{E^{(i-1)}}^{*b}, \mathbf{x})\right)$$
(21)

If p exceeds some confidence level (e.g. 0.95) then  $ps_1$  is added to the rule, otherwise  $ps_1$  is simply discarded and the current rule carries over to the next iteration. Note, on each iteration,  $ps_1$  either becomes part of the growing rule or it is discarded. In both case it is removed from the list on each iteration and the next path snippet in the list becomes the next  $ps_1$  as it takes the top position.

**Step 3** To reduce the overall number of iterations, any path snippets that are merely subsets of the current rule are deleted from the ranked list. To ensure that the relevance



Iteration i		Iteration i + 1		Pruning Stage One	
Attribute	State	Attribute	State	Attribute	State
black		black		black	True
white	False	white	False	white	
asian pac islander	False	asian pac islander	False	asian pac islander	
amer indian eskimo False		amer indian eskimo	amer indian eskimo False		
other		other False other		other	

**Table 6** Hypothetical example of pruning stage one for *race* feature

If n-1 attributes are marked False, the remaining one must be the True value

subspace coverage decreases monotonically, snippets containing split conditions on continuous features whose bounds fall outside the current subspace are also deleted from the ranked list.

Steps 1–3 iterate until a user-defined target stability  $\rho$  is met or the list is exhausted, after which two pruning steps are enacted. Pruning Stage One deals with the way CART, and consequently RF reduces all nominal features to a series of binary splits. For example, suppose an instance x in the adult data set has the attribute black for feature race. We represent this as  $\mathbf{x} = \{\dots, \mathcal{X}_h = 1, \mathcal{X}_i = 0, \mathcal{X}_l = 0, \mathcal{X}_m = 0, \mathcal{X}_n = 0, \dots\}$ where the binary encoded attributes are: h = black, j = white, l = asian pac islander, m = amer indian eskimo, n = other. Because of the high variance of the base classifiers in RF models, there is no guarantee that a triple (h, 0.5, 0) for the true binary evaluation of race = black is added to the growing rule on any iteration. Instead, it is possible that one or more triples indicating the false evaluations from this related set are added to the rule. Should it happen that triples for all the false evaluations are added, the rule can be pruned. To facilitate this pruning step, CHIRPS maintains a map of the state (True, False or empty) of each attribute of nominal features in the data set. Table 6 shows such a map for the running example. On iteration i, the rule contains the triples (j,0.5,1), (l,0.5,1), (m,0.5,1) from previous iterations and the state map reflects that three out of the five attributes are false. The rule currently expresses the disjunction  $(race = black \lor race = other)$ . On iteration i + 1, triple (n, 0.5, 1) is added to the rule and attribute other is set to false in the map. Consequently, race = black must be true for this x. Four triples can be replaced with (h, 0.5, 0), giving a rule that is logically identical yet more terse.

```
Algorithm 3 Rule Pruning Stage One
 1: procedure Disjoint Set Prune(C_{\mathcal{Z}_E}, \text{State Map})
         for all Feature ∈ State Map do
                                                                                                                                                   ▶ See Table 6
 3:
              N \leftarrow count unique Attribute values
              if \sum \mathbb{I}(\text{State is False}) = N - 1 then
 4:
 5:
                   for all c = (i, v, \tau) \in C_{Z_E} where i \in Attribute indices do
                       C_{\mathcal{Z}_E} \leftarrow C_{\mathcal{Z}_E} \setminus c
 6:
 7:
                       insert (j, 0.5, 0) into C_{Z_E} where j = \text{Attribute} and State is empty
         return C_{Z_F}
 8:
```



Table 7	An example of CHIRPS before pruning stage two	
---------	---	--

Data set	Decision	Explanation	Contrast (%)	Confidence
adult	Income ≤ \$50K	lcapitalgain ≤ $8.51 \land$ Relationship ≠ Husband $\land$ Educationnum ≤ $10.92 \land$ Sex = Male	-80.6 -24.9 -16.9	Covers 39.4% of historical Matches 97.3% of covered Vote margin 40.0%

Pruning Stage Two removes any triples that fail to meet the minimal completeness requirement. These may be added to the growing rule because of the fast but greedy rule merge algorithm (Algorithm 2). Confounding, or highly colinear features can be included as a result of this implementation. Therefore, at the end of the routine, we test all the adjacent subspaces, as per Algorithm 1. If stability decreases by  $<\delta$  (a user-defined parameter) in any of these adjacent subspaces, that triple can be removed from the rule. The result is a shorter rule and a larger subspace whose stability within the user-defined tolerance of the unpruned rule's stability. A bootstrap formulation can be used here, similar to equation (21):

$$p = \frac{1}{B} \sum_{b=1}^{B} \mathbb{I}\left(\zeta(g, \mathbf{Z}_{E}^{*b}, \mathbf{x}) - \delta < \zeta(g, \mathbf{Z}_{E'}^{*b}, \mathbf{x})\right)$$
(22)

```
Algorithm 4 Rule Pruning Stage Two
 1: procedure Minimal Completeness Prune(g, C_{Z_E}, \mathbf{X}, \mathbf{x}, \delta)
         removeList \leftarrow empty list
 3:
          Adjacent Spaces \leftarrow Adjacent Spaces(C_{Z_E})
                                                                                                                                                       ▶ Algorithm 1
 4:
          for all (c, \mathbf{Z}') \in (C_{\mathcal{Z}_E}, \text{ Adjacent Spaces}) do
 5:
              if If p > 0.95 then
                                                                                                                                                      ► Equation (22)
                   append c to removeList
 7:
          C_{\mathcal{Z}_E} \leftarrow C_{\mathcal{Z}_E} \setminus removeList
         return C_{\mathcal{Z}_E}
 8:
```

For example, returning to our opening illustration, suppose the merging step finished on the output shown in Table 7 and the user-defined tolerance  $\delta = 0.1$ . Pruning Stage Two would result in the final term being removed, before returning the output given in Table 1.

#### 6.5 Output

The final output of each CHIRPS explanation contains the found rule, along with quality measures. The final rule and counter-factual cases are compared in a way that aids the end user in validating the importance of each rule term. Two such examples from our experimental results were presented in Tables 1 and 2 in Sect. 1.

# 6.6 Computational complexity

In practice, the most computationally demanding step is FP mining. We implement the *FP-Growth* (Pei and Han 2000) algorithm, which is known to be the fastest among competing



Table 8 Data sets used in the experiments

Data set	Target	Classes	Class balance	Features	Of which categorical	N
adult	income	2	0.77:0.23	14	9	48,842
bank	y	2	0.89: 0.11	20	11	45,307
car	acceptability	2	0.71:0.29	7	7	1728
cardio	NSP	3	0.78:0.14:	22	1	2126
			0.08			
credit	A16	2	0.57:0.43	16	10	690
german	rating	2	0.70:0.30	21	14	1000
lending	loan_status	2	0.79:0.21	75	9	2105 <sup>a</sup>
nursery	decision	4	0.33:0.33:	9	9	12,958
			0.31:0.02			
rcdv	recid	2	0.38:0.62	19	19	18,876

<sup>&</sup>lt;sup>a</sup>The number of instances in the original data set is 842000 and was down sampled to N = 2105 for these experiments

**Table 9** Methods used in the experiments

Method	Platform	G/L	Scope	Continuous features?	Ref.
defragTrees	Py 3.x & Hybrid	Global	Regression & Classification	Yes	Hara and Hayashi (2016)
inTrees	R	Global	Regression & Classification	Yes	Deng (2014)
BRL	R, Py 2.x	Global	Binary Classification	No	Letham (2015b)
Anchors	Py 3.x	Local	Multi-Class Classification	No	Ribeiro et al. (2018)
CHIRPS	Ру 3.х	Local	Multi-Class Classification	Yes	

algorithms; with FP-Growth, CHIRPS achieves a competitive time per explanation without significantly compromising quality. We managed the computational efficiency of the whole procedure by tuning the *minsup* hyper-parameter.

# 7 Experiments

In an experimental study involving nine data sets, detailed in Table 8, we compared CHIRPS with competing state of the art methods, detailed in Table 9. We assessed the standard quality measures, precision and coverage, along with our proposed, novel quality measures, stability and exclusive coverage, which are more sensitive to over- and underfitting solutions. We also conducted a sensitivity analysis of the effect of various tuning parameters on CHIRPS performance, using a grid search. In the interests of reproducibility, we publish our source code and preprocessed data in our GitHub repository.<sup>2</sup>



<sup>&</sup>lt;sup>2</sup> https://tinyurl.com/yxuhfh4e.

# 7.1 Hardware setup

The experiments were conducted using both Python 3.6.x and R 3.5.x environments, depending on the availability of open source packages for the benchmark methods. The hardware used was a TUXEDO Book XP1610 Ultra Mobile Workstation with Intel Core i7-9750H @ 2.60–4.50GHz and 64GB RAM using the Ubuntu 18.04 LTS operating system.

#### 7.2 Data sets

Nine data sets, detailed in Table 8, were included, all from UCI Machine Learning repository (Dheeru and Taniskidou 2017) except *lending* (Kaggle) and *rcdv* (ICPSR<sup>3</sup>). These were selected to be a mix of binary and multi-class problems, to exhibit different levels of class imbalance, to be a mixture of discrete and continuous features, and to be a contextual fit (i.e. credit and personal data) where possible. Three of these data sets (*adult*, *lending* and *rcdv*) are those used in Ribeiro et al. (2018) and were chosen to draw direct comparisons. A subsample of the exceptionally large *lending* data set was taken, down to the number shown in Table 8. Identical training and test data sets were made available to both R and Python environments by sampling the row index numbers without replacement and cutting the resulting index vector into two pieces of size 70% and 30%. These vectors were used to index the preprocessed .csv files. We did not implement any stratification or class balancing.

#### 7.3 Selection of benchmark methods

To make direct comparisons with CHIRPS, we selected benchmark methods that either output a rule list, or a single rule (in the case of Anchors Ribeiro et al. 2018). Readers that have some familiarity with XAI may question the ommission of LIME (Ribeiro et al. 2016) and Shapley values (Lundberg and Lee 2017), which are two of the most discussed local explanation methods. However, as the authors of Lundberg and Lee (2017) make clear, these methods are of a different class, described as *additive feature attribution methods* (AFAM). AFAM comprise a linear model (LM) with coefficients and parameters relating the importance of various attributes to the model's classification of the explanandum. There is no obvious way to apply the local LM for one instance to any other instances in order to calculate the quality measures such as precision and coverage. Fortunately, Anchors (Ribeiro et al. 2018) has been developed by the same research group that contributed LIME. Anchors can be viewed as a rule-based extension of LIME and its inclusion into this experimental study provides a useful comparison to AFAM research. The selected methods are detailed in Table 9.

### 7.4 Random forest model training and performance

We present the performance scores of the trained models in Table 10. It is important to note that although the model training is part of the experimental setup, these scores are

https://tinyurl.com/y8qvcgwu



 Table 10
 Random forest

 performance scores

Run-time environment  Used by			Python 3.x Undiscretised CHIRPS and defragTrees		Python 3.x Discretised Anchors		R 3.5.x  BRL & inTrees	
adult	0.86	600	0.85	0.54	0.84	0.44	0.87	0.54
bank	0.92	1600	0.90	0.24	0.92	0.23	0.90	0.40
car	0.98	800	0.97	0.94	0.97	0.94	0.99	0.97
cardio	0.94	600	0.93	0.82	0.90	0.71	0.93	0.80
credit	0.88	400	0.86	0.73	0.87	0.77	0.86	0.72
german	0.76	1600	0.78	0.43	0.75	0.38	0.75	0.33
lending	0.95	1200	0.97	0.88	0.96	0.86	N/A	
nursery	0.99	1600	0.95	0.92	0.96	0.94	0.95	0.91
rcdv	0.67	1400	0.66	0.19	0.61	0.11	0.64	0.18

secondary to the current research and are not part of the research contribution. We only provide this level of detail to demonstrate that the trained models reasonably approximate the underlying data sets; however, an explanation method could just as well be applied to a poorly performing model.

We left the mtry parameter as the default and tuned the ntree hyper-parameter, using a search of the following values  $ntree \in \{200, 400, ..., 1600\}$  to achieve the minimum number of base classifiers that delivered the best accuracy on Out of Bag (OOB) instances. For each base DT, the OOB instances are those instances that were not used in the sample on which that DT was trained. The selected value for ntree was used to train a model in the three run-time environments. We show the best OOB accuracy achieved and the winning ntree setting. We also show generalisation accuracy scores for the three resulting models. This is measured using the held out test set (note; this is a purely informative score and does not leak information about the test set into the subsequent explanations). Cohen's  $\kappa$  is also displayed, as this is a useful measure in multi-class problems and class imbalanced data.  $\kappa$  corrects for chance agreement, which can be high in such cases. Values close to zero indicate a high degree of chance agreement. Cohen's  $\kappa$  is calculated as:

$$\kappa = \frac{N\sum_{i=1}^{K} N_{ii} - \sum_{i=1}^{K} N_{i+} N_{+i}}{N^2 - \sum_{i=1}^{K} N_{i+} N_{+i}}$$
(23)

where K is the number of classes, N is the total number of instances,  $N_{ij}$  is the number of instances in cell ij of the confusion matrix and  $N_{i+}, N_{+j}$  are the ith row and jth column marginal totals respectively.

# 7.5 CHIRPS tuning parameters

CHIRPS offers several tunable hyper-parameters that have an effect on the solution. We used the following parameter options in a grid search to find the combination with the highest mean training score (estimated during the rule merge phase on the training data)



and compared this explainer with the other methods. See Sect. 6 for details about these parameter settings:

- Number of bins for discretisation of continuous features in the extracted paths: bins ∈ {4,8}
- 2. Minimum support level for FP mining:  $minsup \in \{0.1, 0.2\}$
- 3. Score function parameters:
  - (a) Neutral or weighted:  $w \in \{1, D_{KL}\}$
  - (b) Neutral or weighted by path snippet support:  $sup \in \{1, support\}$
  - (c) Neutral or penalising short path snippets:  $\alpha \in \{0, 0.1, 0.5, 0.9\}$ .

After concluding the state of the art comparison, we used the grid search results from the above settings to provide a sensitivity analysis of the various parameters. We were able to search a sizeable parameter space for CHIRPS.

# 7.6 Benchmarks methods tuning parameters

The inTrees, BRL and defragTrees methods each offer a tuning parameter set that controls the breadth of the search space for generating the rule list (proxy model). The number and cardinality of rules, and the number and maximum depth of trees extracted from the MUS are among the most important of these parameters. We expound further on these settings later in Sect. 7.7. Anchors, in contrast, does not generate a proxy model. Anchors has one parameter—the precision guarantee threshold—that directly affects the target precision. An automated search would always choose the parameter setting that results in the highest training precision, making such a search redundant for the Anchors method. However, since Anchors guarantees a minimum precision, setting this parameter too high can easily result in over-fitting. Therefore, we kept the default value of 0.95 used in the original paper (Ribeiro et al. 2018).

# 7.7 Limitations of the comparative study

In this section, we describe certain limitations of the comparative study and how we mitigated any of them.

### 7.7.1 Scalability of the benchmark methods

Unfortunately, BRL, defragTrees and inTrees manifested serious scalability issues for the larger data sets. All but the most restrictive settings resulted in very long computation times ending in fatal errors (system crashes, non-recoverable memory allocation errors, etc). These fatal errors occurred despite using hardware of a very high specification and made it impossible to automate a grid search for the best parameter set, as was conducted for CHIRPS. These methods are well cited in the literature and such problems with scalability were entirely unexpected. We increased our original hardware specification and engaged in a laborious and very time consuming manual search to select best performing parameters that successfully ran to completion on the selected hardware.



**Table 11** Tuning parameter settings for the benchmark methods

data	defragTrees		inTrees		BRL		
	maxdepth	ntree	maxdepth	ntree	lambda	eta	maxlen
adult	8	400	8	120	10	1	8
bank	4	_	8	80	10	5	4
car	_	_	8	_	10	5	8
cardio	_	_	8	_	5	1	4
credit	_	_	8	_	5	1	4
german	_	_	8	_	5	1	4
lending	_	_	N/A		N/A		
nursery	8	_	8	_	10	5	8
rcdv	8	200	8	140	10	1	4

The final selections of the parameters are shown in Table 11. Here, '-' indicates the parameter was unrestricted or left at the default, and so takes on the equivalent value in Table 10. The remaining entries show that it was necessary to restrict the search space (quite severely, in some cases) for all the three globally interpretable methods. On the data sets *adult*, *bank*, *nursery* and *rcdv*, the defragTrees method never ran to completion whichever settings were chosen for its in-built tuning parameters. Consequently, a simplified random forest had to be generated with the maximum tree depth and the number of trees shown. For inTrees, *ntree* and *maxdepth* the parameters refer to in-built parameters that dictate how much of the MUS shall be mined for rules. The inTrees method was not able to traverse the fully-grown random forest for any data set. For *adult*, *bank* and *nursery*, the number of trees considered also had to be restricted. For BRL, *lambda* is a prior on the expected number of rules in the final list, *eta* is a prior on the average rule cardinality and *maxlen* is a hard limit on the individual rule cardinality. It is clear from these final parameter settings that BRL was only able to consider limited orders of feature interaction for all the data sets.

These important limitations to scalability are not mentioned in the original research nor subsequent citations for any of these three algorithms. When making comparisons against CHIRPS and Anchors with respect to the quality measures and computation times, our study demonstrates that defragTrees, BRL and inTrees require very restrictive compromises to the search space and complexity of the MUS and do not provide real equivalence in delivering explanations.

#### 7.7.2 Run-time envorinments

Note that defragTrees worked natively in Python or in a hybrid mode, calling Python from R. BRL was available in R and Python 2.x only, so the R version was selected to avoid setting up a third environment. In the experiments, CHIRPS and defragTrees both used the same random forest model, with the exceptions noted in Table 11.

#### 7.7.3 Disretisation of data

Anchors and BRL only handle discrete features; therefore, to use Anchors we are forced to train a separate model on a discretised data set, using the default quantile binning function



provided by the authors of Ribeiro et al. (2018). This required a second Python run-time environment. BRL learns a proxy model directly from the training data, quantile binning was also used to preprocess the data for BRL.

# 7.7.4 Adaptation of BRL to multi-class classification

BRL is included in the experiments because it has a robust statistical foundation (Yang et al. 2017; Wang et al. 2017, 2016; Wang and Rudin 2015; Letham 2015b). However, it can only perform binary classification in the available open source library. Since BRL is a probabilistic classifier, we constructed *K* one-versus-all classifiers for the multi-class data sets *cardio* and *nursery*. Classification is done by selecting the classifier that yields the highest probability for its positive class. To explain the classification, we simply performed a reverse lookup to that classifier and extracted the firing classification rule as an explanation. This *K* one-versus-all approach is a commonly used technique for converting a binary classifier into a multi-class classifier. For example, it is used in XGBoost (Friedman 2001) but we have not found examples in the literature of its application to BRL. Nevertheless, the accuracy of this multi-class BRL classifier on the *cardio* and *nursery* data sets was in line with the "out of the box" algorithm on the binary class data sets used in our study, so we have included the results.

# 7.7.5 High dimensionality of the *lending* data set

We also found that the randomForest library for R has a hard limit on the number of features of the data set. This limit ruled out the *lending* data set. Consequently, the results for this data set are not represented for either BRL or inTrees. This is a limitation of the runtime environment, not the predictive/explanatory algorithm.

#### 8 Discussion

In this section, we discuss the results and their significance.

# 8.1 Comparative analysis

Explanations relate to the model's output  $g(\mathbf{X})$  and not the true labels (which are unknown in real-world applications). Therefore, we cannot use a batchwise comparison of predicted values versus true values, as is typical in ML model evaluation. Instead, we assess the explanations by classifying and explaining instances from the test set *one at a time* and scoring against the remaining test instances that were not involved in generating each explanation. This gives an unbiased estimate for each individual case. We now report on the aggregate scores of this leave-one-out testing procedure.

BRL, defragTrees and inTrees produce simplified, proxy models. These proxy models are not expected to make the same classification as the MUS for 100% of instances. It is therefore necessary to check the *fidelity* as an additional quality metric for these models when assessing their global performance:



Table 12	Fidelity of the globally
interpreta	able methods BRL,
defragTre	ees and inTrees

Data	BRL	defragTrees	inTrees
adult	0.91	0.94	0.90
bank	0.97	0.99	0.94
car	0.97	0.74	0.99
cardio	0.88	0.85	0.91
credit	0.89	0.93	0.87
german	0.81	0.80	0.88
lending	N/A	0.85	NA
nursery	0.93	0.73	0.91
rcdv	0.88	0.89	0.83

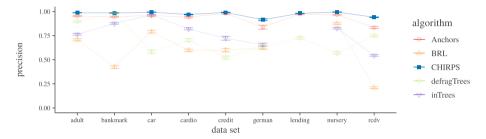


Fig. 7 Mean precision for the five methods over nine data sets

$$fid(u, g, \mathbf{X}) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}(u(\mathbf{x}^{(i)}) = g(\mathbf{x}^{(i)})), \ \mathbf{X} = {\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}}$$
 (24)

where u is the surrogate model approximating g. By design, both Anchors and CHIRPS always score 1 for fidelity across any instance space because they are always locally accurate (Lundberg and Lee 2017)—the consequent of the output rule is always  $g(\mathbf{x})$ . A fidelity score significantly less than 1.0 is a serious problem in applications requiring an explanation; since, for any instance where  $u(\mathbf{x}) \neq g(\mathbf{x})$ , the proxy does not even agree with the MUS classification. The fidelity for each of the globally interpretable algorithms is given in Table 12.

We assume that the acceptable level should be a problem or domain specific consideration. The only guidance we found in the literature suggests that when measuring the quality of explanations, the misclassified instances should receive a negative score (Lipton 2016). It is not clear what the magnitude of this penalty should be. We suggest 0 on precision and stability for each such individual case, as this will penalise the aggregate quality measure. Taking these penalties into account, we show visual comparisons of the mean (with standard errors  $\frac{\sigma}{\sqrt{N}}$ ) of precision, stability, coverage and exclusive coverage scores for all methods on each data set in Figs. 7, 8, 9, and 10. We have added guidelines to assist the reader in comparing scores across the data sets. The tabulated results are provided in the "Appendix".

These visual comparisons illuminate the utility of our novel quality measures. Take, for example, the very high coverage scores for BRL and defragTrees in several data sets. Here is a clear sign of under-fitting, since precision is approximately equal to the prior



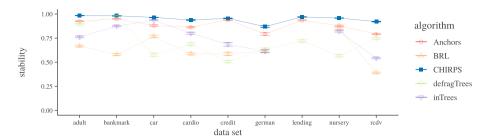


Fig. 8 Mean stability

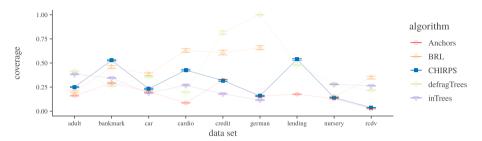


Fig. 9 Mean coverage

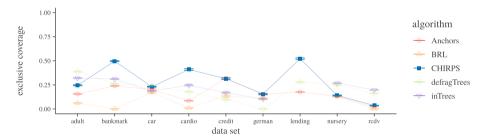


Fig. 10 Mean exclusive coverage

proportion of majority class instances. This is most notable for defragTrees on the *german* data set where mean coverage is 1.0, indicating that only the empty, default rule has been found. It would be erroneous to state that this high coverage score is better than a lower coverage when the latter is combined with high precision and stability. Our novel alternative, exclusive coverage, favours solutions where the number of *covered*, *other class* instances is lower (see Sect. 5). The consistency of CHIRPS under both ordinary coverage and exclusive coverage shows that it is extremely well safeguarded against under-fitting. The benefit of stability is a little more subtle here, but the effect is clearer when we consider how close the precision measurements are for CHIRPS and Anchors on several data sets. CHIRPS explanations generally cover far more target class instances, as shown in Fig. 11. This is because CHIRPS is guarded against over-fitting by design. On the other hand, Anchors implements a precision guarantee by design. In order to meet this guarantee, Anchors will produce an over-fitting rule that uniquely identifies the target instance when



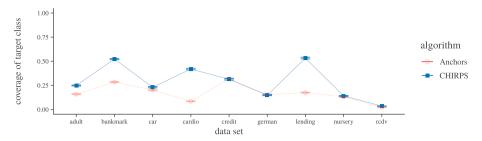


Fig. 11 Mean coverage of target class instances

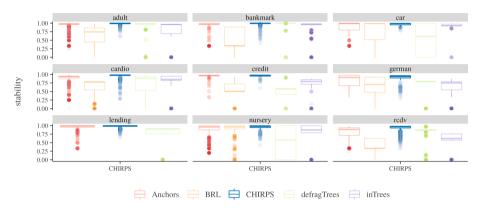


Fig. 12 Stability scores shown as boxplots

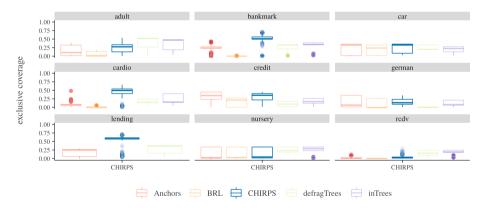


Fig. 13 Exclusive coverage scores shown as boxplots

no other explanation can be found. Stability scores between these two methods are better separated than precision scores wherever Anchors has over-fit more frequently.

We also present boxplots of stability and exclusive coverage in Figs. 12 and 13 to provide a visual analysis of the distributions. We can see that the results for CHIRPS are closest to the ideal for stability, close to 1.0 with the smallest variance. The results for exclusive coverage are less clear cut on visual inspection. To test for statistical significance



**Table 13** Top two algorithms by mean rank (mrnk) stability for each data set

Data	1st	mrnk	2nd	mrnk	Z	p val
adult	CHIRPS	1.26	Anchors	2.76	80.93	≈ 0*
bank	defragTrees	1.15	CHIRPS	2.10	49.82	$\approx 0^*$
car	CHIRPS	1.94	Anchors	2.17	2.31	0.011
cardio	CHIRPS	1.28	Anchors	2.71	16.13	$\approx 0^*$
credit	Anchors	1.37	CHIRPS	1.70	2.08	0.019
german	CHIRPS	1.14	Anchors	2.19	5.68	$\approx 0^*$
lending	CHIRPS	1.15	CHIRPS	1.87	12.93	$\approx 0*$
nursery	Anchors	2.43	CHIRPS	2.45	0.47	0.318
rcdv	CHIRPS	1.25	Anchors	2.49	41.86	$\approx 0^*$

A significant result in the post hoc pairwise test is indicated by \* and the winning algorithm formatted in boldface

of these results, we use the Friedman test for comparing stability and exclusive coverage among the algorithms. The Friedman test is a non-parametric equivalent to ANOVA. It is an extension of the rank sum test for multiple comparisons and is recommended for comparison of classification algorithms (Demsar 2006). The original Friedman test produces an approximately  $\chi^2$  distributed statistic, but this is known to be very conservative. Therefore, we use the modified F-test given in Demsar (2006), because we have very large values for N, i.e., the count of instances in the test set. The null hypothesis of this test is that there is no significant difference between the mean ranks R of the algorithms. The null is rejected when  $F_F$  exceeds the critical value for an F distributed random variable with the first degrees of freedom  $\mathrm{df}_1 = k - 1$  and the second  $\mathrm{df}_2 = (k - 1)(N - 1)$ , where k is the number of algorithms:

$$F_F = \frac{(N-1)\chi_F^2}{N(k-1) - \chi_F^2}, \quad \chi_F^2 = \frac{12N}{k(k+1)} \left[ \sum_{j=1}^k R_j^2 - \frac{k(k+1)^2}{4} \right]$$
 (25)

For all data sets, our tests returned vanishingly small p values,  $p \approx 0$ , providing very strong evidence against the null hypothesis. We conclude that, for each data set, at least two algorithms differ significantly in their mean ranks for stability and exclusive coverage. This result is expected, based on the visual inspection of the plots. We ran the recommended pairwise, post-hoc comparison test with the Bonferroni correction proposed in Demsar (2006):

$$z = \operatorname{diff}_{ij} / \sqrt{\frac{k(k+1)}{6N}}, \ \operatorname{diff}_{ij} = R_i - R_j$$
 (26)

where  $R_i$  and  $R_j$  are ranks of two algorithms and z is distributed as a standard normal under the null hypothesis that the pair of ranks are not significantly different. It is sufficient for this study to demonstrate whether the top scoring algorithm was significantly greater than the second place algorithm on our quality measures of interest. We, therefore, report for stability and exclusive coverage on the mean ranks, z and the p value of a two-tailed z-test only for the top two methods for each data set. See Tables 13 and 14.

When assessing stability, we see that CHIRPS significantly outranks the next best algorithm for five out of nine data sets. Of the remaining four data sets, CHIRPS ranks first or second but the difference between the top two is not significant in three of them.



**Table 14** Top two algorithms by mean rank (mrnk) exclusive coverage for each data set

Data	1st	mrnk	2nd	mrnk	z	p val
adult	defragTrees	1.31	inTrees	2.37	56.89	≈ 0*
bank	CHIRPS	1.22	inTrees	2.94	56.15	$\approx 0^*$
car	Anchors	2.52	CHIRPS	2.75	2.35	0.009
cardio	CHIRPS	1.51	inTrees	2.37	9.66	$\approx 0^*$
credit	Anchors	2.06	CHIRPS	2.12	0.40	0.343
german	CHIRPS	2.05	Anchors	2.24	1.47	0.071
lending	CHIRPS	1.17	defragTrees	2.05	15.60	$\approx 0^*$
nursery	inTrees	1.59	defragTrees	2.67	30.14	$\approx 0^*$
rcdv	inTrees	1.30	defragTrees	1.80	16.86	$\approx 0^*$

A significant result in the post hoc pairwise test is indicated by \* and the winning algorithm formatted in boldface

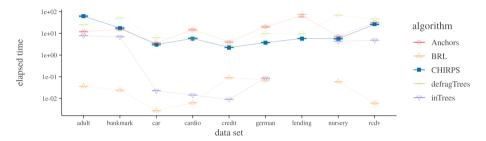


Fig. 14 Mean elapsed time per explanation (s). Note, the y-axis is log scaled

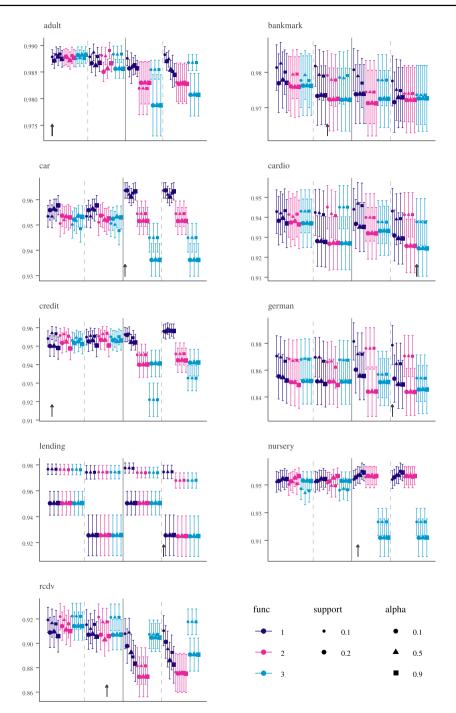
Only in final data set, defragTrees significantly outranks CHIRPS. For exclusive coverage, CHIRPS significantly outranks the next best algorithm on four out of nine data sets; although, CHIRPS is ranked second on two data sets, the difference with the top ranked algorithm is not significant. On the remaining three data sets defragTrees and inTrees dominate but they do not perform well for precision or stability measures on the same data sets.

Finally, we visually compare the computation time (Fig. 14). On seven out of nine data sets, CHIRPS came third out of the five algorithms. The slowest CHIRPS performance was on the adult data set where the mean computation time was 47.01 s per explanation, while the fastest was on the credit data set at 0.29 s per explanation. It is likely that the wide variation in timings relates to complexity of the MUS, which in turn depends on characteristics and size of the data set. While BRL and inTrees were often much faster, we remind the reader that only CHIRPS and Anchors could scale to work on the four most challenging data sets. In contrast, BRL, defragTrees and inTrees could not run unless the tuning parameters were set to significantly constrain the model complexity (e.g. a limited number of trees, a limited maximum tree depth or rule cardinality). These scalability issues demonstrate that the three methods cannot truly explain the MUS, only a very simplified proxy. The end user must consider whether this situation, along with less than perfect fidelity, would meet their critical requirements.

### 8.2 Sensitivity analysis

CHIRPS as a multi-step procedure has several tuning parameters that may be important for optimising the results. We investigated the effect of the tuning parameters with a grid





**Fig. 15** Sensitivity analysis of CHIRPS to the available tuning parameters, showing mean stability on the y-axis, measured on the test set by leave-one-out evaluation and an arrow on each panel indicating the parameter set that was picked from the best estimated (training) score



search as described in Sect. 7.5. The results are visualised in Fig. 15. The points show the mean stability scores on unseen data, along with standard error bars. Note, in the legend "func" indicates the score function configuration: (1) Support,  $\alpha$  (snippet length) and Weights, (2)  $\alpha$  and Weights, (3) Weights only. The left half of each panel contains the KL-div weighted scores, while the right half is unweighted scores. The binning (discretisation) function is set to 4 in the left quadrant of each half panel, and 8 on the right. In each panel, an arrow indicates the parameter set that gave the top mean rank on the training data, i.e., the final score after merging and pruning. This would suggest that the training scores alone provide an excellent predictor of the best parameter settings. There was no "universal" parameter set that did well on all data sets, however, the following general advice applies:

- A round of parameter tuning prior to implementation is very likely to yield improved performance in production, possibly increasing stability measures by a few percentage points.
- Lower support always yields better training scores for precision and stability. However, decreasing the support results in increasing the computation time per instance. The best trade off between these two variables will be a problem specific choice.
- The D<sub>KL</sub> weighting usually reduces the variance of the results. Varying the score function does not usually have a significant effect when this weighting is set.
- However, in a few cases, greater stability is achievable with neutral weights. This setting should be investigated for critical problems where very small improvements are still significant.
- Discretisation settings make no difference for data sets that contain only categorical variables.

# 9 Conclusions and future work

We have expounded the rapidly developing research area of eXplainable Artificial Intelligence (XAI) and the need to interpret and explain black box models. Furthermore, we have made a case for relaxing the requirement to be model-agnostic; typically, a model and training data are "owned" by an actor or organisation wishing to adopt predictive analytics. In these cases, decompositional methods that unpack the internal representation of a model are viable alternatives, especially if they outperform the model-agnostic approach. At the same time we have set out the need for additional requirements that have not been addressed in previous research. For example, concretely addressing the tendency to overand under-fit, and providing a format for counter-factual information. From this foundation, we have proposed a novel formulation for explanations of black box classifiers on tabular data sets and an optimisation framework, including novel objective functions (stability and exclusive coverage) to generate better solutions.

The major contribution of this paper is the novel method, CHIRPS, for returning rule-based local explanations from Random Forests. Our experimental study shows that this method outperforms both local, model-agnostic methods, and globally interpretable methods. CHIRPS is able to discover classification rules that are extremely precise, yet surprisingly general on a variety of data sets. The classification rules are enhanced with rich information about the contrastive, counter-factual cases, providing additional intuition for the end user.



Our experimental study revealed scalability issues in competing methods. Overcoming these issues required prior restrictions such as reducing the number of trees by orders of magnitude, the maximum tree depths to little more than decision stumps, or setting the maximum cardinality of rules considered, thereby limiting higher order interactions. These settings place arbitrary limits on the solution space and put a distance between the model under scrutiny (the model to be explained) and the proxy model comprising the explanations themselves. We suggest that classification-rule-based explanation methods have many advantages over additive feature attribution methods (e.g. easy applicability to other instances) but to make some of the classification-rule-based methods truly scalable, there are open challenges for algorithmic optimisation.

Directions for future work are adapting CHIRPS to boosting classifiers, and variants of the RF algorithm that use unbiased alternatives to CART. Replacing the simple greedy algorithm with modern multi-objective optimisation methods (e.g. genetic algorithms) is another avenue of research.

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# **Appendix**

See Tables 15, 16, 17, and 18.

**Table 15** Each explanation was generated from one held out instance and the precision measured on the remaining held out data

	Anchors	BRL	CHIRPS	defragTrees	inTrees
adult	$0.9530 \pm 0.0052$	$0.7063 \pm 0.0100$	$0.9861 \pm 0.0009$	$0.8949 \pm 0.0076$	$0.7628 \pm 0.0092$
bank	$0.9457 \pm 0.0052$	$0.4247 \pm 0.0138$	$0.9838 \pm 0.0017$	$0.9841 \pm 0.0035$	$0.8754 \pm 0.0079$
car	$0.9575 \pm 0.0089$	$0.7904 \pm 0.0139$	$0.9928 \pm 0.0010$	$0.5837 \pm 0.0168$	$0.9638 \pm 0.0048$
cardio	$0.9419 \pm 0.0085$	$0.5971 \pm 0.0122$	$0.9687 \pm 0.0032$	$0.7031 \pm 0.0143$	$0.8196 \pm 0.0104$
credit	$0.9805 \pm 0.0084$	$0.5988 \pm 0.0188$	$0.9901 \pm 0.0020$	$0.5225 \pm 0.0152$	$0.7226 \pm 0.0203$
german	$0.8373 \pm 0.0207$	$0.6250 \pm 0.0190$	$0.9145 \pm 0.0090$	$0.6341 \pm 0.0186$	$0.6557 \pm 0.0162$
lending	$0.9732 \pm 0.0063$	N/A	$0.9801 \pm 0.0017$	$0.7259 \pm 0.0124$	N/A
nursery	$0.9662 \pm 0.0055$	$0.8759 \pm 0.0091$	$0.9944 \pm 0.0008$	$0.5693 \pm 0.0124$	$0.8259 \pm 0.0084$
rcdv	$0.8332 \pm 0.0097$	$0.2100 \pm 0.0093$	$0.9398 \pm 0.0034$	$0.7484 \pm 0.0095$	$0.5436 \pm 0.0082$

The mean  $\pm$  standard errors are shown. The winning scores are printed in bold face



**Table 16** Each explanation was generated from one held out instance and the stability measured on the remaining held out data

	Anchors	BRL	CHIRPS	defragTrees	inTrees
adult	$0.9253 \pm 0.0045$	$0.6677 \pm 0.0090$	$0.9830 \pm 0.0010$	$0.8946 \pm 0.0076$	$0.7625 \pm 0.0092$
bank	$0.9495 \pm 0.0093$	$0.5801 \pm 0.0093$	$0.9819 \pm 0.0018$	$0.9832 \pm 0.0035$	$0.8750 \pm 0.0079$
car	$0.8806 \pm 0.0075$	$0.7674 \pm 0.0134$	$0.9649 \pm 0.0015$	$0.5779 \pm 0.0166$	$0.9356 \pm 0.0047$
cardio	$0.8626 \pm 0.0072$	$0.5871 \pm 0.0111$	$0.9374 \pm 0.0042$	$0.6867 \pm 0.0140$	$0.7999 \pm 0.0103$
credit	$0.9405 \pm 0.0070$	$0.5853 \pm 0.0179$	$0.9549 \pm 0.0031$	$0.5006 \pm 0.0135$	$0.6858 \pm 0.0192$
german	$0.7926 \pm 0.0133$	$0.6164 \pm 0.0186$	$0.8691 \pm 0.0089$	$0.6305 \pm 0.0185$	$0.6132 \pm 0.0150$
lending	$0.9347 \pm 0.0051$	N/A	$0.9699 \pm 0.0020$	$0.7203 \pm 0.0123$	N/A
nursery	$0.8777 \pm 0.0062$	$0.8494 \pm 0.0089$	$0.9581 \pm 0.0019$	$0.5674 \pm 0.0123$	$0.8206 \pm 0.0084$
rcdv	$0.7926 \pm 0.0066$	$0.3913 \pm 0.0062$	$0.9212 \pm 0.0034$	$0.7465 \pm 0.0095$	$0.5430 \pm 0.0082$

The mean ± standard errors are shown. The winning scores are printed in bold face

**Table 17** Each explanation was generated from one held out instance and the coverage measured on the remaining held out data

	Anchors	BRL	CHIRPS	defragTrees	inTrees
adult	$0.1613 \pm 0.0047$	$0.2022 \pm 0.0101$	$0.2506 \pm 0.0050$	$0.4149 \pm 0.0052$	$0.3823 \pm 0.0048$
bank	$0.2918 \pm 0.0056$	$0.4586 \pm 0.0157$	$0.5272 \pm 0.0055$	$0.2609 \pm 0.0032$	$0.3444 \pm 0.0042$
car	$0.2036 \pm 0.0071$	$0.3843 \pm 0.0148$	$0.2320 \pm 0.0058$	$0.3584 \pm 0.0039$	$0.1878 \pm 0.0036$
cardio	$0.0866 \pm 0.0030$	$0.6890 \pm 0.0188$	$0.4256 \pm 0.0082$	$0.1963 \pm 0.0021$	$0.2685 \pm 0.0062$
credit	$0.3212 \pm 0.0099$	$0.6079 \pm 0.0252$	$0.3180 \pm 0.0076$	$0.8159 \pm 0.0172$	$0.1789 \pm 0.0055$
german	$0.1568 \pm 0.0092$	$0.6579 \pm 0.0213$	$0.1584 \pm 0.0049$	$1.0000 \pm 0.0000$	$0.1154 \pm 0.0049$
lending	$0.1764 \pm 0.0042$	N/A	$0.5380 \pm 0.0087$	$0.5380 \pm 0.0059$	N/A
nursery	$0.1303 \pm 0.0049$	$0.1502 \pm 0.0059$	$0.1409 \pm 0.0046$	$0.2742 \pm 0.0021$	$0.2798 \pm 0.0028$
rcdv	$0.0237 \pm 0.0009$	$0.3480 \pm 0.0151$	$0.0368 \pm 0.0012$	$0.2173 \pm 0.0038$	$0.2631 \pm 0.0023$

This was repeated for entire held out data, or one thousand instances (whichever was the smaller). The mean  $\pm$  standard errors are shown

**Table 18** Each explanation was generated from one held out instance and the exclusive coverage measured on the remaining held out data

	Anchors	BRL	CHIRPS	defragTrees	inTrees
adult	$0.1556 \pm 0.0045$	$0.0618 \pm 0.0025$	$0.2457 \pm 0.0048$	$0.3873 \pm 0.0049$	$0.3196 \pm 0.0051$
bank	$0.2387 \pm 0.0033$	$0.0006 \pm 0.0001$	$0.4969 \pm 0.0048$	$0.2609 \pm 0.0032$	$0.3106 \pm 0.0039$
car	$0.2028 \pm 0.0071$	$0.1720 \pm 0.0060$	$0.2306 \pm 0.0057$	$0.2409 \pm 0.0026$	$0.1860 \pm 0.0035$
cardio	$0.0851 \pm 0.0029$	$0.0097 \pm 0.0007$	$0.4098 \pm 0.0078$	$0.1777 \pm 0.0023$	$0.1777 \pm 0.0023$
credit	$0.3177 \pm 0.0098$	$0.1342 \pm 0.0087$	$0.3138 \pm 0.0075$	$0.0979 \pm 0.0053$	$0.1688 \pm 0.0050$
german	$0.1534 \pm 0.0090$	$0.1099 \pm 0.0069$	$0.1546 \pm 0.0048$	$0.0000 \pm 0.0000$	$0.1031 \pm 0.0039$
lending	$0.1757 \pm 0.0042$	N/A	$0.5215 \pm 0.0082$	$0.2789 \pm 0.0045$	N/A
nursery	$0.1302 \pm 0.0049$	$0.1332 \pm 0.0048$	$0.1487 \pm 0.0046$	$0.2492 \pm 0.0023$	$0.2675 \pm 0.0027$
rcdv	$0.0233 \pm 0.0009$	$0.0001 \pm 0.0000$	$0.0363 \pm 0.0012$	$0.1623 \pm 0.0023$	$0.1967 \pm 0.0016$

This was repeated for entire held out data, or one thousand instances (whichever was the smaller). The mean  $\pm$  standard errors are shown



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