
An empirical study on hyperparameter tuning of decision trees

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Abstract

Machine learning algorithms often contain many hyperparameters whose values affect the predictive performance of the induced models in intricate ways. Due to the high number of possibilities for these hyperparameter configurations, and their complex interactions, it is common to use optimization techniques to find settings that lead to high predictive accuracy. However, we lack insight into how to efficiently explore this vast space of configurations: which are the best optimization techniques, how should we use them, and how significant is their effect on predictive or runtime performance? This paper provides a comprehensive approach for investigating the effects of hyperparameter tuning on three Decision Tree induction algorithms, CART, C4.5 and CTree. These algorithms were selected because they are based on similar principles, have presented a high predictive performance in several previous works and induce interpretable classification models. Additionally, they contain many interacting hyperparameters to be adjusted. Experiments were carried out with different tuning strategies to induce models and evaluate the relevance of hyperparameters using 94 classification datasets from OpenML. Experimental results indicate that hyperparameter tuning provides statistically significant improvements for C4.5 and CTree in only one-third of the datasets, and in most of the datasets for CART. Different tree algorithms may present different tuning scenarios, but in general, the tuning techniques required relatively few iterations to find accurate solutions. Furthermore, the best technique for all the algorithms was the Irace. Finally, we find that tuning a specific small subset of hyperparameters contributes most of the achievable optimal predictive performance.

keywords: Decision trees, hyperparameter tuning, hyperparameter importance, J48, CART, CTree

1 Introduction

Many Machine Learning (ML) algorithms able to deal with classification tasks can be found in the literature. Although high predictive accuracy is the most frequently used measure to evaluate these algorithms, in many applications, easy interpretation of the induced models is also an important requirement. Good predictive performance and model interpretability are found in one of the most successful set of classification algorithms: Decision Tree (DT) induction algorithms [1].

When applied to a dataset, these algorithms induce a model represented by a set of rules in a tree-like structure (as illustrated in Figure 1). This structure elucidates how the induced model predicts the class of a new instance, more clearly than many other model representations, such as an Artificial Neural Network (ANN) [2] or Support Vector Machines (SVMs) [3]. As a result, DT induction algorithms are among the most frequently used ML algorithms for classification tasks [4, 5].

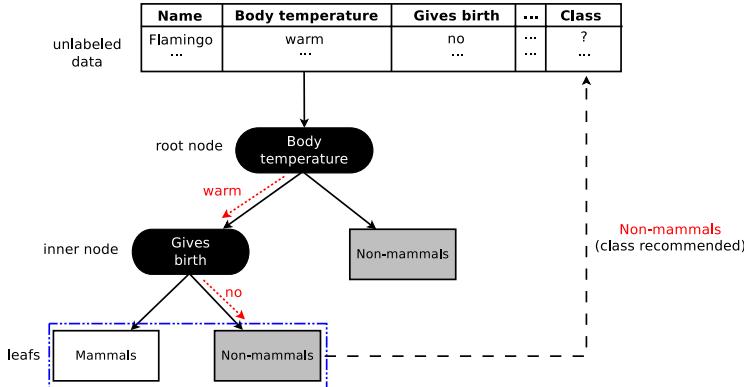


Figure 1: Example of a decision tree. Unlabeled data is provided to the tree, that iteratively selects the most promising attribute until a leaf is reached. At the end, the class is recommended. Adapted from [6].

DT induction algorithms have several other advantages over many ML algorithms, such as robustness to noise, tolerance against missing information, handling of irrelevant and redundant predictive attribute values, and low computational cost [1]. Their importance is demonstrated by the wide range of well-known algorithms proposed in the literature, such as Breiman et al.'s Classification and Regression Tree (CART) [7] and Quinlan's C4.5 algorithm [8], as well as some hybrid-variants of them, like Naïve-Bayes Tree (NBTree) [9], Logistic Model Tree (LMT) [10] and Conditional Inference Trees (CTree) [11].

Similarly to most ML algorithms, DT induction algorithms have hyperparameters whose values must be set. Due to the high number of possible configurations, and their large influence on the predictive performance of the induced models, hyperparameter tuning is often warranted [12, 13, 14, 15]. The tuning task is usually investigated for “black-box” algorithms, such as ANNs and SVMs, but not for DTs. There are some prior studies investigating the evolutionary design of new DT induction algorithms [16, 17], but only few on hyperparameter tuning for them [18, 19, 20].

This paper investigates the effects of the hyperparameter tuning on the predictive performance of DT induction algorithms, as well as the impact hyperparameters have on the final predictive performance of the induced models. For such, three DT induction algorithms were chosen as study cases: two of the most popular algorithms in Machine Learning [4] - the J48 algorithm, a WEKA [21] implementation for the Quinlan's C4.5 [8]; the Breiman et al.'s CART algorithm [7]; and the algorithm “Conditional Inference Trees (CTree)” [11], a more recent implementation that embeds statistical tests to define whether a split must occur (similar to CHAID) [22].

A total of six different hyperparameter tuning techniques (following different learning biases) were selected: a simple Random Search (RS), three commonly used meta-heuristics - Genetic Algorithm (GA) [23], Particle Swarm Optimization (PSO) [24], and Estimation of Distribution Algorithm (EDA) [25], Sequential Model-based Optimization (SMBO) [26], and Iterated F-race (Irace) [27]¹.

¹These techniques will be described on the next sections.

Experiments were carried out with a large number of heterogeneous datasets, and the experimental results obtained by these optimization techniques are compared with those obtained using the default hyperparameter values recommended for C4.5, CART and CTree.

In many situations, the analysis of the global effect of a single hyperparameter, or interactions between different hyperparameters, may provide valuable insights. Hence, we also assess the relative importance of DT hyperparameters, measured using a recent functional ANOVA framework [28].

In all, the main contributions of this study are:

- Large-scale comparison of different hyperparameter tuning techniques for DT induction algorithms;
- Comprehensive analysis of the effect of hyperparameters on the predictive performance of the induced models and the relationship between them;

The current study also extends a previous investigation [29]. This extended version reviews previous studies performing hyperparameter tuning of C4.5 (J48); includes two additional tree algorithms - CART and CTree; includes two state-of-art optimization techniques in the experiments (SMBO and Irace); presents a more detailed methodology (with all implementation choices), and improves the experimental analysis, mainly the experiments considering the relative importance of the DT algorithm hyperparameters. All the code generated in this study is available to reproduce our analysis - and extend it to other classifiers. All experiments are also available on OpenML [30].

The remainder of this paper is structured as follows: Section 2 covers related work on hyperparameter tuning of DT induction algorithms, and Section 3 introduces hyperparameter tuning in more detail. Section 4 describes our experimental methodology, and the setup of the tuning techniques used, after which Section 5 analyses the results. Section 6 validates the results from this study. Finally, Section 7 summarizes our findings and highlights future avenues of research.

2 Related work

A large number of ML studies investigate the effect of hyperparameter tuning on the predictive performance of classification algorithms. Most of them deal with the tuning of “black-box” algorithms, such as SVMs [31] and ANNs [32]; or ensemble algorithms, such as Random Forest (RF) [33, 34] and Boosting Trees [35, 36]. They often tune the hyperparameters by using simple techniques, such as Pattern Search (PS) [37] and Random Search (RS) [32], but also more sophisticated ones, such as meta-heuristics [15, 31, 38, 39, 40], SMBO [12, 41], racing algorithms [42, 43] and Meta-learning (MtL) [44]. However, when considering DT induction algorithms, there are far fewer studies available.

Recent work has also used meta-heuristics to design new DT induction algorithms combining components of existing ones [17, 45]. The algorithms created are restricted by the existing components, and since they have to optimize the algorithm and its hyperparameters, they have a much larger search space and computational cost. Since this study focuses on hyperparameter tuning, this section does not cover DT induction algorithm design.

2.1 C4.5/J48 hyperparameter tuning

Table 1 summarizes studies performing hyperparameter tuning for the C4.5/J48 DT induction algorithm. For each study, the table presents which hyperparameters were investigated (following the J48 nomenclature also presented in Table 4²), which tuning techniques were explored, and the number and source of datasets used in the experiments. Empty fields in the table mean that the procedures used in that specific study could not be completely identified.

Schauerhuber et. al. [46] presented a benchmark of four different open-source DT induction algorithm implementations, one being J48. In this study, authors assessed the algorithms performances on 18 classification datasets from the UCI repository. The authors tuned two hyperparameters: the pruning confidence (C) and the minimum number of instances per leaf (M).

²The original J48 nomenclature may also be checked at <http://weka.sourceforge.net/doc.dev/weka/classifiers/trees/J48.html>.

Table 1: Some properties of the related studies that performed C4.5 (J48) hyperparameter tuning. The hyperparameters abbreviations are explained according to the reference description at the text.

Reference	Hyperparameter									Tuning Technique	Number of Datasets	
	C	M	N	O	R	B	S	A	J	U		
Schauerhuber et. al. (2008) [46]	•	•									GS	18 (UCI)
Sureka & Indukuri (2008) [47]											GA	
Stiglic et. al. (2012) [48]	•	•				•	•				VTJ48	71 (UCI)
Lin & Chen (2012) [49]	•	•									SS	23 (UCI)
Ma (2012) [50]	•	•									GP	70 (UCI)
Auto-WEKA [51, 52]	•	•			•	•	•	•	•	•	SMBO	21
Molina et. al. (2012) [19]	•	•									GS	14
Sun & Pfahringer (2013) [53]							•				PSO	466
Reif et. al. (2014) [20]	•										GS	54 (UCI)
Sabharwal et. al. (2016) [54]	•	•									DAUP	2 artificial 4 real-world
Tantithamthavorn et. al. (2016) [55]	•										caret	18
Delgado et. al. (2014) [56]												
Wainberg et. al. (2016) [57]	•	•										121 (UCI)

Sureka & Indukuri [47] used a GA (see Section 3.3) to recommend an algorithm and its best hyperparameter values for a problem. They used a binary representation to encode a wider hyperparameter space, including Bayes, Rules, Network and Tree-based algorithms, including J48. However, the authors do not provide more information about which hyperparameter, ranges, datasets or evaluation procedures were used to assess the hyperparameter settings. Experiments also showed that the algorithm can find good solutions, but requires massive computational resources to evaluate all possible models.

Stiglic et. al. [48] presented a study tuning a Visual Tuning J48 (VTJ48), i.e., J48 with predefined visual boundaries. They developed a new adapted binary search technique to perform the tuning of four J48 hyperparameters: the pruning confidence (C); the minimum number of instances per leaf (M); the use of binary splits (B) and subtree raising (S). Experimental results on 40 UCI [58] and 30 bioinformatics datasets demonstrated a significant increase in accuracy in visually tuned DTs, when compared with defaults. In contrast to classical ML datasets, there were higher gains in bioinformatics datasets.

Lin & Chen [49] proposed a novel Scatter Search (SS)-based algorithm to acquire optimal hyperparameter settings, and to select a subset of features that results in better classification performance. Experiments with 23 UCI datasets demonstrated that the hyperparameter settings for C4.5 algorithm obtained by the new approach, when tuning the ‘C’ and ‘M’ hyperparameters, were better than those obtained by baselines (defaults, simple GA and a greedy combination of them). When feature selection is considered, classification accuracy rates on most datasets are increased.

Ma [50] leveraged the Gaussian Process (GP) algorithm to optimize hyperparameters for some ML algorithms (including C4.5 and its hyperparameters ‘C’ and ‘M’) for 70 UCI classification and regression datasets. GPs were compared with Grid Search (GS) and RS methods (see Section 3.1). GPs found solutions faster than both baselines with comparably high performances. However, compared specifically to RS, GPs seems to be better for more complex problems, while RS is sufficient for simpler ones.

Sabharwal et. al. [54] proposed a method to sequentially allocate small data batches to selected ML classifiers. The method, called “Data Allocation using Upper Bounds” (DAUP), tries to project an optimistic upper bound of the accuracy obtained by a classifier in the full dataset, using recent evaluations of this classifier on small data batches. Experiments evaluated the technique on 6 classification datasets and more than 40 algorithms with different hyperparameters, including C4.5 and its ‘C’ and ‘M’ hyperparameters. The proposed method was able to select near optimal classifiers with a very low computational cost compared to full training of all classifiers.

In Tantithamthavorn et. al. [55], the authors investigated the performance of prediction models when tuning hyperparameters using “*caret*”³ [59], a ML tool. A set of ML algorithms, including J48 and its ‘C’ hyperparameter, were tuned on 18 proprietary and public datasets. In a comparison with defaults from *caret* using the AUC⁴ measure, the tuning produced better results.

Wainberg et. al. [57] reproduced the benchmark experiments described in [56]. They evaluated 179 classifiers from 17 different learning groups on 121 datasets from UCI. The hyperparameters of the J48 algorithm were manually tuned.

Other studies used hyperparameter tuning methods to generate Meta-learning (MtL) systems [19, 20, 51, 52, 53]. These studies search the hyperparameter spaces to describe the behavior of ML algorithms in a set of problems, and later recommend hyperparameter values for new problems. For example, Molina et. al. [19] tuned two hyperparameters of the J48 algorithm (‘C’ and ‘M’) in a case study with 14 educational datasets, using GS. They also used a set of meta-features to recommend the most promising set of <algorithm, hyperparameters> pairs for each problem. The proposed approach, however, did not improve the performance of the DTs with defaults.

Sun & Pfahringer [53] also used hyperparameter tuning in the context of MtL. The authors proposed a new meta-learner for algorithm recommendation, and a feature generator to construct the datasets used in experiments. They searched 20 ML algorithm hyperparameter spaces, one of them the C4.5 and its ‘B’ hyperparameter. The PSO technique (see Section 3.4) was used to generate a meta-database for a recommendation experiment. Similarly, Reif et. al. [20] implemented an open-source MtL system to predict accuracies of target classifiers, one of them the C5.0 algorithm (a version of the C4.5), with its pruning confidence (C) tuned by GS.

A special case of hyperparameter tuning is the Combined Algorithm Selection and Hyper-parameter Optimization (CASH) tool, introduced by [51] as the Auto-WEKA⁵ framework, and updated recently in [52]. Auto-WEKA applies SMBO (see Section 3.2) to select an algorithm and its hyperparameters to new problems based on a wide set of ML algorithms (including J48). In addition to the previously mentioned hyperparameters (C, M, B and S), Auto-WEKA also searches for the following HP values: whether to collapse the tree (0), use of Laplace smoothing (A), use of MDL correction for the info gain criterion (J) and generation of unpruned trees (U).

2.2 CART hyperparameter tuning

Table 2 summarizes previous studies on hyperparameter tuning for the CART algorithm. For each study, the table presents which hyperparameters, tuning techniques, and the number and source of datasets explored in the experiments.

Table 2: Summary of previous studies on CART hyperparameter tuning. The hyperparameter nomenclature adopted is explained according to the reference description in the original text.

Reference	cp	Hyperparameter					Tuning Technique	Number of Datasets
		min split	min bucket	max depth	weights leaf	max leaf		
Schauerhuber et. al. [46]	•						GS	18 (UCI)
Sun & Pfahringer (2013) [53]	•						PSO	466
Bermudez-Chacon et. al.(2015) [60]	•	•	•	•	•	•	RS SH PD	29 (UCI) 7 (other)
Auto-skLearn [44, 61]	•		•	•	•	•	SMBO	140 (OpenML)
Levesque et. al. (2016) [62]	•	•	•		•		SMBO	18 (UCI)
Tantithamthavorn et. al. (2016) [55]	•						caret	18 (various)
Delgado et. al. (2014) [56]	•							
Wainberg et. al. (2016) [57]	•			•				121 (UCI)

³<https://cran.r-project.org/web/packages/caret/index.html>

⁴Area under the ROC curve

⁵<http://www.cs.ubc.ca/labs/beta/Projects/autoweka/>

In Schauerhuber et. al. [46], the authors added CART/rpart to their benchmark analysis. They manually tuned only the complexity parameter ‘cp’. Sun et. al. [53] investigated the tuning of CART hyperparameters, in particular its `minsplit` hyperparameter, over 466 datasets (some of which are artificially generated) using PSO. This hyperparameter controls the minimum number of instances necessary for a split to be attempted. The hyperparameter settings assessed during the search were used to feed a meta-learning system. In Tantithamthavorn et. al. [55], the authors did a similar study, but focused on the complexity parameter ‘cp’.

In Bermudez-Chacon et. al. [60], the authors presented a hierarchical model selection framework that automatically selects the best ML algorithm for a particular dataset, optimizing its hyperparameter values. Algorithms and hyperparameters are organized in a hierarchy, and an iterative process makes the recommendation. The optimization technique used for tuning is considered a component of the framework, and three choices are available: RS, Shrinking Hypercube (SH) and Parametric Density (PD) optimization methods. The technique encapsulates a long list of algorithms, including CART and some of its hyperparameters: ‘`minsplit`’; the minimum number of instances in a leaf (‘`minbucket`’); the maximum depth of any node of the final tree (‘`maxdepth`’); weighted values to leaf nodes (‘`weights_leaf`’); the maximum number of leafs (‘`maxleafs`’) and the maximum number of features from dataset used in trees (‘`maxfeatures`’).

In Feurer et. al. [44, 61], the authors used the SMBO approach to select and tune algorithm from the “scikit learn”⁶ framework, hence Auto-skLearn⁷. The only DT induction algorithm covered here is CART. CART with some hyperparameters manually selected was also experimentally investigated in [56, 57].

Levesque et. al. [62] investigated the use of hyperparameter tuning and ensemble learning for tuning CART hyperparameters when models induced by CART were part of an ensemble, using SMBO. Four hyperparameters were tuned in the process: ‘`minsplit`’, ‘`minbucket`’, ‘`maxdepth`’ and the ‘`maxleaf`’. The tuning resulted in a significant improvement in generalization accuracy when compared with the Single Best Model Ensemble and Greedy Ensemble Construction techniques.

2.3 CTree hyperparameter tuning

Table 3 summarizes previous studies on hyperparameter tuning for the CTree algorithm [11]. For each study, the table presents which hyperparameters were investigated, which tuning techniques were explored, and the number (and source) of datasets used in the experiments. Studies at the table with no technique specified used a manual selection process.

Table 3: Summary of previous studies on CTree hyperparameter tuning. The hyperparameter nomenclature adopted is explained according to the reference description in the original text.

Reference	Hyperparameter					Tuning Technique	Number of Datasets
	min criterion	min split	min stump	mtry	max depth		
Schauerhuber et. al. (2008) [46]	•						18 (UCI)
Delgado et. al. (2014) [56] Wainberg et. al. (2016) [57]		•			•		121 (UCI)
Sarda-Espinoza et. al. (2017) [63]	•				•	GS	4 (private)

Schauerhuber et. al. [46] also included the CTree algorithm in their benchmark study. In their study, only the ‘`mincriterion`’ hyperparameter is manually tuned for 18 UCI datasets. This hyperparameter defines the value of the statistic test ($1 - p.value$) that must be exceeded for a split to occur.

A CTree implementation is also explored in the benchmark studies presented by [56, 57]. Two hyperparameters are tuned manually: the ‘`mincriterion`’ and the maximum tree depth (‘`maxdepth`’). Experiments were performed with a total of 121 UCI heterogeneous datasets.

⁶<http://scikit-learn.org/>

⁷<https://github.com/automl/auto-sklearn>

Sarda-Espinoza et. al. [63] applied conditional trees to extract relevant knowledge from electrical motors' data. The final models were obtained after tuning two hyperparameters via GS: 'mincriterion' and 'maxdepth'. The resulting models were applied to four different private datasets.

2.4 Literature Overview

The literature review indicates that hyperparameter tuning for DT induction algorithm could be more deeply explored. We found eleven studies investigating some tuning for the J48 algorithm, six for CART and only three for the CTree algorithm. These studies neither investigated the tuning task itself nor adopted a consistent procedure to assess candidate hyperparameter settings while searching the hyperparameter space:

- some studies used hyperparameter sweeps;
- some other studies used simple CV resamplings;
- a few studies used nested-CV procedures, but only used an inner holdout and they did not repeat their experiments with different seeds⁸; and
- some studies did not even describe which experimental methodology was used.

Regarding the search space, most studies concerning C4.5/J48, CART and CTree hyperparameter tuning investigated only a small subset of the hyperparameter search spaces (as shown in Tables 1, 2 and 3). Furthermore, most of the studies did the tuning manually, used simple hyperparameter tuning techniques or searched the hyper-spaces to generate meta-information for Meta-learning (MtL) and CASH systems.

This paper overcomes these limitations by investigating several techniques for DT hyperparameter tuning, using a reproducible and consistent experimental methodology. It presents a comparative analysis for each of the investigated algorithms (C4.5, CART and CTree), and analyzes the importance and relationships between many hyperparameters of DT induction algorithms.

3 Hyperparameter tuning

Many applications of ML algorithms to classification tasks use hyperparameter default values suggested by ML tools, even though several studies have shown that their predictive performance mostly depends on using the right hyperparameter values [44, 51, 61]. In early works, these values were tuned according to previous experiences or by trial and error. Depending on the training time available, finding a good set of values manually may be subjective and time-consuming. In order to overcome this problem, optimization techniques are often employed to automatically look for a suitable set of hyperparameter settings [12, 41].

The hyperparameter tuning process is usually treated as a black-box optimization problem whose objective function is associated with the predictive performance of the model induced by a ML algorithm, formally defined as follows:

Let $\mathcal{H} = \mathcal{H}_1 \times \mathcal{H}_2 \times \dots \times \mathcal{H}_k$ be the hyperparameter space for an algorithm $a \in \mathcal{A}$, where \mathcal{A} is the set of ML algorithms. Each \mathcal{H}_i represents a set of possible values for the i^{th} hyperparameter of a ($i \in \{1, \dots, k\}$) and can be usually defined by a set of constraints. Additionally, let \mathcal{D} be a set of datasets where $\mathbf{D} \in \mathcal{D}$ is a dataset from \mathcal{D} . The function $f : \mathcal{A} \times \mathcal{D} \times \mathcal{H} \rightarrow \mathbb{R}$ measures the predictive performance of the model induced by the algorithm $a \in \mathcal{A}$ on the dataset $\mathbf{D} \in \mathcal{D}$ given a hyperparameter configuration $\mathbf{h} = (h_1, h_2, \dots, h_k) \in \mathcal{H}$. Without loss of generality, higher values of f mean higher predictive performance.

Given $a \in \mathcal{A}$, \mathcal{H} and $\mathbf{D} \in \mathcal{D}$, together with the previous definitions, the goal of a hyperparameter tuning task is to find $\mathbf{h}^* = (h_1^*, h_2^*, \dots, h_k^*)$ such that

$$\mathbf{h}^* = \arg \max_{\mathbf{h} \in \mathcal{H}} f(a, \mathbf{D}, \mathbf{h}) \quad (1)$$

⁸Since the stochastic nature of the often used tuning algorithms, experimenting with different seeds (for random generator) is desirable.

The optimization of the hyperparameter values can be based on any performance measure f , which can even be defined by multi-objective criteria. Further aspects can make the tuning more difficult, like:

- hyperparameter configurations that lead to a model with high predictive performance for a given dataset may not lead to high predictive performance for other datasets;
- hyperparameter values often depend on each other (as in the case of SVMs [64]). Hence, independent tune of hyperparameters may not lead to a good set of hyperparameter values;
- the evaluation of a specific hyperparameter configuration, not to mention many configurations, can be subjective and very time-consuming.

In the last decades, population-based optimization techniques have been successfully used for hyperparameter tuning of classification algorithms [12, 41]. When applied to tuning, these techniques (iteratively) build a *population* $\mathcal{P} \subset \mathcal{H}$ of hyperparameter settings for which $f(a, \mathbf{D}, \mathbf{h})$ are being computed for each $\mathbf{h} \in \mathcal{P}$. By doing so, they can simultaneously explore different regions of a search space. There are various population-based hyperparameter tuning strategies, which differ in how they update \mathcal{P} at each iteration. Some of them are briefly described next.

3.1 Random Search

Random Search (RS) is a simple technique that performs random trials in a search space. Its use can reduce the computational cost when there is a large number of possible settings being investigated [65]. Usually, RS performs its search iteratively in a predefined number of iterations. Moreover, \mathcal{P}_i is extended (updated) by a randomly generated hyperparameter setting $\mathbf{h} \in \mathcal{H}$ in each (i th) iteration of the hyperparameter tuning process. RS has obtained efficient results in optimization for Deep Learning (DL) algorithms [32, 41].

3.2 Sequential Model Based Optimization

Sequential Model-based Optimization (SMBO) [26, 66] is a sequential method that starts with a small initial population $\mathcal{P}_0 \neq \emptyset$ which, at each new iteration $i > 0$, is extended by a new hyperparameter configuration \mathbf{h}' , such that the expected value of $f(a, \mathbf{D}, \mathbf{h}')$ is maximal according to an induced meta-model \hat{f} approximating f on the current population \mathcal{P}_{i-1} . In the experiments reported in [12, 26, 67], SMBO performed better than GS and RS and matched or outperformed state-of-the-art techniques in several hyperparameter optimization tasks.

3.3 Genetic Algorithm

Bio-inspired techniques, such as a Genetic Algorithm (GA), based on natural processes, have also been largely used for hyperparameter tuning [31, 68, 69]. In these techniques, the initial population $\mathcal{P}_0 = \{\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_{n_0}\}$, generated randomly or according to background knowledge, is changed in each iteration according to operators based on natural selection and evolution.

3.4 Particle Swarm Optimization

Particle Swarm Optimization (PSO) is a bio-inspired technique relying on the swarming and flocking behaviors of animals [70]. In case of PSO, each particle $\mathbf{h} \in \mathcal{P}_0$ is associated with its position $\mathbf{h} = (h_1, \dots, h_k) \in \mathcal{H}$ in the search space \mathcal{H} , a velocity $\mathbf{v}_h \in \mathbb{R}^k$ and also its so far best found position $\mathbf{b}_h \in \mathcal{H}$. During iterations, the movements of each particle is changed according to its so far best-found position as well as the so far best-found position $\mathbf{w} \in \mathcal{H}$ of the entire swarm (recorded through the computation).

3.5 Estimation of Distribution Algorithm

Estimation of Distribution Algorithm (EDA) [25] lies on the boundary of GA and SMBO by combining the advantages of both approaches such that the search is guided by iteratively updating an explicit probabilistic model of promising candidate solutions. In other words, the implicit crossover and mutation operators used in GA are replaced by an explicit probabilistic model M .

3.6 Iterated F-Race

The Iterated F-race (Irace) [27] technique was designed for algorithm configuration and optimization problems [42, 43] based on ‘racing’. One race starts with an initial population \mathcal{P}_0 , and iteratively selects the most promising candidates considering the hyperparameter distributions, and comparing them by statistical tests. Configurations that are statistically worse than at least one of other configuration candidates are discarded from the racing. Based on the surviving candidates, the distributions are updated. This process is repeated until a stopping criterion is reached.

4 Experimental methodology

The nested Cross-validation (CV) [71, 72] experimental methodology employed is illustrated by Figure 2. For each dataset, data are split into M outer-folds: the training folds are used by the tuning techniques to find good hyperparameter settings, while the test fold is used to assess the ‘optimal’ solution found. Internally, tuning techniques split each of the M training folds into N inner-folds to measure the fitness value of each new hyperparameter setting. At the end of the process, a set of M optimization paths, M settings, and their predictive performances are returned. During the experiments, all the tuning techniques were run on the same data partitions, with the same seeds and data to allow their comparison. In [72], the authors used $M = N = 10$. However, they argued that there is no study suggesting the number of folds in the outer and inner CV loops. Here, the same value used in the original paper was used for $M = 10$. Due to time constraints and the size of datasets used in experiments, $N = 3$ was adopted. Next subsections detail the sub-components used in the tuning task.

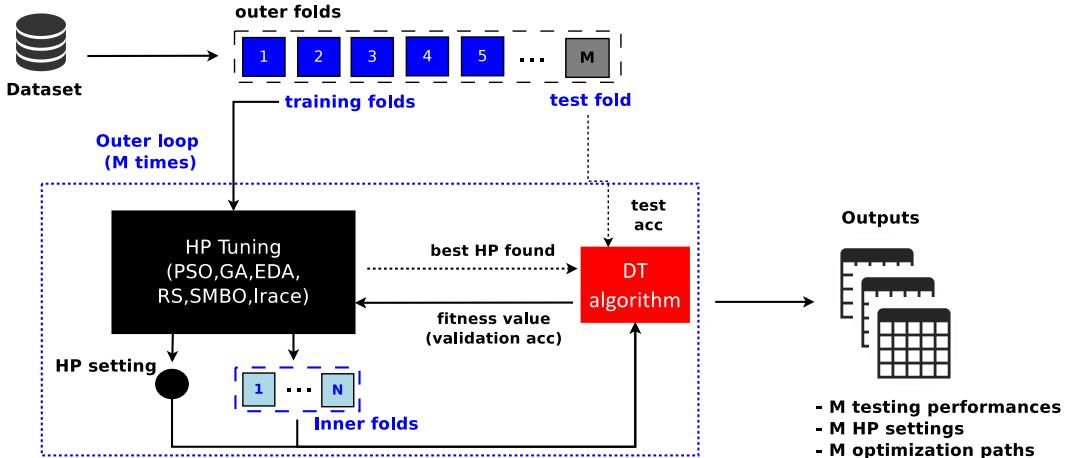


Figure 2: Experimental methodology used to adjust DT hyperparameters. The tuning is conducted via nested cross-validation: 3-fold CV for computing fitness values and 10-fold CV for assessing performances. The outputs are the hyperparameter settings, the predicted performances and the optimization paths of each technique.

4.1 Hyperparameter spaces

The experiments were performed considering the hyperparameter tuning of three DT induction algorithms: the ‘J48’ algorithm, a WEKA⁹ [21] implementation of the C4.5 algorithm; the rpart implementation of the CART [7] algorithm, and the CTree algorithm [11]. These algorithms were selected due to their wide acceptance and use in many ML applications [1, 5, 16]. The first two listed algorithms are among the most used in Machine Learning, specially by non-expert users [4], and the third is a more recent implementation that uses statistical tests for splits, like the classical CHAID algorithm [22]. The correspondent hyperparameter spaces investigated are described in Table 4.

⁹<http://www.cs.waikato.ac.nz/ml/weka/>

Table 4: Decision Tree hyperparameter spaces explored in the experiments. The J48 nomenclature is based on the RWeka package, the CART terms is based on the rpart package, and the CTree terms based on the party package.

Algo	Symbol	hyperparameter	Range	Type	Default	Conditions
J48	C	pruning confidence	(0.001, 0.5)	real	0.25	R = False
J48	M	minimum number of instances in a leaf	[1, 50]	integer	2	-
J48	N	number of folds for reduced error pruning	[2, 10]	integer	3	R = True
J48	O	do not collapse the tree	{False, True}	logical	False	-
J48	R	use reduced error pruning	{False, True}	logical	False	-
J48	B	use binary splits only	{False, True}	logical	False	-
J48	S	do not perform subtree raising	{False, True}	logical	False	-
J48	A	Laplace smoothing for predicted probabilities	{False, True}	logical	False	-
J48	J	do not use MDL correction for info gain on numeric attributes	{False, True}	logical	False	-
CART	cp	complexity parameter	(0.0001, 0.1)	real	0.01	-
CART	minsplit	minimum number of instances in a node for a split to be attempted	[1, 50]	integer	20	-
CART	minbucket	minimum number of instances in a leaf	[1, 50]	integer	7	-
CART	maxdepth	maximum depth of any node of the final tree	[1, 30]	integer	30	-
CART	usesurrogate	how to use surrogates in the splitting process	{0, 1, 2}	factor	2	-
CART	surrogatestyle	controls the selection of the best surrogate	{0, 1}	factor	0	-
CTree	mincriterion	the value of the statistic test ($1 - p$ -value) to be exceed for a split occurrence	(0.9, 0.999)	real	0.95	-
CTree	minsplit	minimum sum of weights in a node for a split occurrence	[1, 50]	integer	20	-
CTree	minbucket	minimum sum of weights in a leaf	[1, 50]	integer	7	-
CTree	mtry	number of input variables randomly sampled as candidates at each node for random forest like algorithms	$[p^{0.1}, p^{0.9}]$	real	0	-
CTree	maxdepth	maximum depth of any node of the final tree	[1, 30]	integer	no restriction	-
CTree	stump	a stump (a tree with three nodes only) is to be computed	{False, True}	logical	False	-

Originally, J48 has ten tunable hyperparameters¹⁰: all presented at Table 4 plus the hyperparameter ‘U’, which enables the induction of unpruned trees. Since pruned trees look for the most interpretable models without loss of predictive performance, this hyperparameter was removed from the experiments, and just pruned trees were considered. For CTree, all the statistically dependent hyperparameters were kept out, since their effects were previously studied and the default choices were robust for a wide range of problems [11], thus the non-statistically dependent hyperparameters were selected. Regarding CART, all the tunable hyperparameters in rpart were selected.

For each hyperparameter, Table 4 shows the allowed range of values, default values provided by the correspondent packages, and its constraints for setting new values. The M hyperparameter values were the same used in Reif et. al. [18]. The range of the pruning confidence (C) hyperparameter was adapted from Reif et. al. [20], because the algorithm internally controls the parameter values, does not allowing some values near zero or $C \geq 0.5$.

¹⁰<http://weka.sourceforge.net/doc.dev/weka/classifiers/trees/J48.html>

4.2 Datasets

The experiments were carried out using 94 public datasets from the Open Machine Learning (OpenML) [30] website¹¹, a free scientific platform for standardization of ML experiments, collaboration and sharing empirical results. Binary and multiclass classification datasets were selected, varying the number of attributes (D) ($3 \leq D \leq 1300$) and examples (N) ($100 \leq N \leq 45000$). In all selected datasets each class (C) has at least 10 examples, to allow the use of the stratified methodology. All datasets, with their main characteristics, are presented in Tables 7 and 8 at B.

4.3 Hyperparameter tuning techniques

Six hyperparameter tuning techniques were investigated:

- three different meta-heuristics: a Genetic Algorithm (GA) [23], Particle Swarm Optimization (PSO) [24] and an Estimation of Distribution Algorithm (EDA) [25]. These techniques are often used for hyperparameter tuning of ML classification algorithms in general [38, 73, 74];
- a simple Random Search (RS) technique: suggested in [32] as a good alternative for hyperparameter tuning replacing Grid Search (GS) technique;
- Iterated F-race (irace) [27]: a *racing* technique designed for algorithm configuration problems; and
- a Sequential Model-based Optimization (SMBO) [26] technique: a state of the art technique for optimization that employs statistical and/or machine learning techniques to predict distributions over labels, and allows a more direct and faster optimization.

Table 5: Setup of the hyperparameter tuning experiments.

Element	Method	R package
HP-tuning techniques	Random Search	mlr
	Genetic Algorithm	GA
	Particle Swarm Optimization	PSO
	Estimation of Distribution Algorithm	copulaedas
	Sequential Model Based Optimization	mlrMBO
	Iterated F-race	irace
Decision Trees	J48 algorithm	RWeka
	CART algorithm	rpart
	CTree algorithm	party
Inner resampling	3-fold cross-validation	mlr
Outer resampling	10-fold cross-validation	mlr
Optimized measure	{Balanced per class accuracy}	mlr
Evaluation measure	{Balanced per class accuracy, Optimization paths }	mlr
Budget	900 iterations	
Repetitions	30 times with different seeds seeds = {1, ..., 30}	-
		-
Baseline	Default values (DF)	RWeka
		rpart
		party

Table 5 summarizes the choices made to accomplish the general hyperparameter tuning techniques. Most of the experiments were implemented using the `mlr` R package¹² [75] (measures, resampling

¹¹<http://www.openml.org/>

¹²<https://github.com/mlr-org/mlr>

strategies, tuning main processes and RS technique). The GA, PSO and EDA meta-heuristics were implemented using the `GA`¹³[76], `pso`¹⁴[77], and `copulaedas`¹⁵[78] R packages, respectively. The J48, CART and CTree algorithms were implemented using the `RWeka`¹⁶[79], `rpart`¹⁷[80] and `party`¹⁸[11] packages, respectively, wrapped into the `mlr` package. The SMBO technique was implemented using the `mlrMBO`¹⁹ [81] R package, with its RF surrogate models implemented by the `randomForest`²⁰ R package [82]. The Irace technique was implemented using the `irace`²¹ [83] R package.

Since the experiments handle a high number of datasets with different characteristics, many datasets may have unbalanced classes. Thus, the same predictive performance measure used during optimization as the fitness value, Balanced per class Accuracy (BAC) [84], is used for model evaluation.

When tuning occurs in real scenarios, time is an important aspect to be considered. Sometimes the tuning process may take many hours to find good settings for a single dataset [33, 40]. Thus, this work investigates whether it is possible to find the same good settings faster by using a reduced number of evaluations (budget). Based on previous results and analyses [29], a budget size of 900 evaluations was adopted in the experiments²².

Since all techniques are stochastic, each one was executed 30 times for each dataset using different seed values. It gives a total of $270.000 = 30$ (repetitions) $\times 10$ (outer-folds) $\times 900$ (budget) HP-settings generated during the search process for one dataset. Besides, the default hyperparameter values provided by the ‘`RWeka`’, ‘`rpart`’ and ‘`party`’ packages were used as baseline for the experimental comparisons.

As this paper evaluates different tuning techniques, to avoid the influence of their hyperparameter values on their performances, the authors decided to use their default values. Each tuning technique has a different set of hyperparameters, and these are specific and different considering each technique’s paradigm. In the SMBO, Irace and PSO cases, the use of the defaults have been shown robust enough to save time and resources[81, 83, 86]. For EDA and GA (and evolutionary methods in general) there is no *standard* values for their parameters [87]. So, to keep fair comparisons, the default parameter values provided by the correspondent R packages were used. All of these values may be seen in Table 6.

The tuning techniques have an initial population with 10 random hyperparameter settings and the same stopping criteria: the budget size. The GA, PSO and EDA techniques use a “real-value” codification for the individuals/particles, thus, they were adapted to handle discrete and Boolean hyperparameters. All of them were executed sequentially in the same cluster environment. Every single job generated was executed in a dedicated core with no concurrency, and scheduled by the cluster system.

4.4 Repositories for the coding used in this study

The code for implementations used in this study are publicly available at:

- Tuning procedures: <https://github.com/rgmantovani/HpTuning>;
- Graphical analysis: <https://github.com/rgmantovani/TuningAnalysis> .

Instructions to run each project may be found directly at the correspondent websites. The experimental results are also available as an OpenML study (<https://www.openml.org/s/50>), where all datasets, classification tasks, algorithms/flows and results of runs for this paper can be listed and downloaded.

¹³<https://github.com/luca-scr/GA>

¹⁴<https://cran.r-project.org/web/packages/pso/index.html>

¹⁵<https://github.com/yasserglez/copulaedas>

¹⁶<https://cran.r-project.org/web/packages/RWeka/index.html>

¹⁷<https://cran.r-project.org/web/packages/rpart/index.html>

¹⁸<https://cran.r-project.org/web/packages/party/index.html>

¹⁹<https://github.com/mlr-org/mlrMBO>

²⁰<https://cran.r-project.org/web/packages/randomForest/index.html>

²¹<http://iridia.ulb.ac.be/irace/>

²²The budget size choice is discussed with more details in Section 6.

Table 6: hyperparameter tuning techniques parameters. Excepting the budget-dependent parameters all of them are the defaults provided by each R package implementation.

Technique	Parameter	Value
RS	stopping criteria	budget size
PSO	number of particles	10
	maximum number of iterations	90
	stopping criteria	budget size
	algorithm implementation	SPSO2007 [85]
EDA	number of individuals	10
	maximum number of iterations	90
	stopping criteria	budget size
	EDA implementation	GCEDA
	copula function	normal
GA	margin function	truncnorm
	number of individuals	10
	maximum number of iterations	90
	stopping criteria	budget size
	selection operator	proportional selection with linear scaling
	crossover operator	local arithmetic crossover
	crossover probability	0.8
	mutation operator	random mutation
	mutation probability	0.05
	elitism rate	0.05
SMBO	points in the initial design	10
	initial design method	Random LHS
	surrogate model	Random Forest
	stopping criteria	budget size
Irace	infill criteria	expected improvement
	number of instances for resampling	100
	stopping criteria	budget size

5 Experimental results

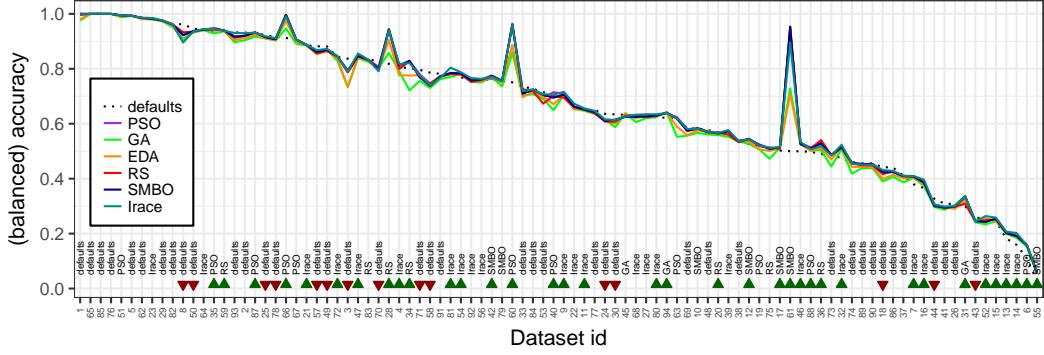
Next subsections present main experimental results regarding the DT implementations.

5.1 Performance analysis regarding J48 algorithm

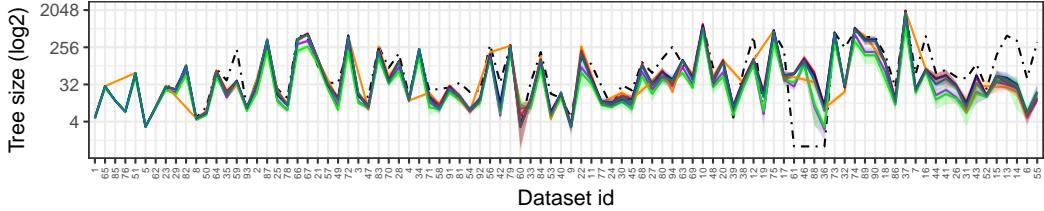
Figure 3 presents the results obtained by the tuning techniques when applied to the J48 DT induction algorithm. Sub-figure 3(a) shows the average *Balanced per class Accuracy (BAC)* values obtained by the tuning techniques and defaults over all datasets. The datasets at the x-axis are placed in decreasing order according to their predictive performances using default hyperparameter values²³.

For each dataset, the name of the tuning technique that resulted in the best predictive performance is shown above the x-axis. The Wilcoxon paired-test was applied to assess the statistical significance of the results obtained by this *best* technique when compared to the results using default values. The test was applied to the solutions obtained from the 30 repetitions (with $\alpha = 0.05$). An upper green triangle (\blacktriangle) at x-axis identifies datasets where statistically significant improvements were detected after applying the hyperparameter tuning technique. On the other hand, every time a red down triangle (\blacktriangledown) is presented, the use of defaults was statistically better than the use of tuning techniques.

²³The corresponding dataset names may be seen in Tables 7 and 8 at B.



(a) Average balanced per class accuracy performance.



(b) Average tree size. X-axis values are in \log_2 scale.

Figure 3: Hyperparameter tuning results for the J48 algorithm.

A first look at the results shows that all tuning techniques have similar performances, with few exceptions, since most of the curves overlap. In general, there is a small difference in predictive performance regarding the default values. Higher improvements may be seen only in a small subset of datasets. When the Wilcoxon statistical paired-test is applied comparing defaults with the best tuning technique, they show that, overall, tuned trees were better than those with default values with statistical significance in 36/94 ($\approx 38\%$) datasets. In most of these situations, the Irace, PSO or SMBO techniques produced the best results. Default values were significantly better in 15/94 of the cases, and the remaining situations (43/94) did not present statistically significant differences (the approaches tied).

Sub-figure 3(b) shows the average tree size of the final J48 induced DTs. The tree size measures the number of nodes in the final tree model. It is important to mention that the interpretability of a tree is mostly dependent on its size. Thus, larger trees are usually more difficult to understand than smaller trees. Regarding the J48 DT size, in most cases, default values (dotted black line) induced trees larger than those obtained by the hyperparameters suggested by tuning techniques. This fact was true whenever default values were the best option with statistical significance. For most of the multi-class tasks with many classes (datasets most to the right at the charts), the tuned trees were also smaller than those induced using default values. Even small concerning performance, the improvements were also significant.

Looking at the peaks of improvements due to the use of hyperparameter tuning, they were reached when the DTs induced using default values were much smaller than those obtained using hyperparameter tuning. This occurred for the datasets with the ids = {36, 46, 61, 88}. When comparing tuning techniques among themselves, significant differences only appear in these datasets. The soft computing techniques tend to produce smaller trees than the SMBO and RS techniques.

To compare default setting with the solutions found during the tuning process, and also get useful insights regarding the defaults effectiveness, the J48 hyperparameter's distributions found by the tuning techniques are presented in Figure 4²⁴. The numerical default values are represented by vertical dashed lines. In the J48 tuning scenario, the largest contrast may be noticed in the 'R' sub-plot: most of the obtained solutions presented 'R=FALSE', which disables the use of the *reduce error pruning* option and the hyperparameter 'N' (like default setting does). The M values obtained also tends to get

²⁴All the hyperparameters were already shown in Table 4

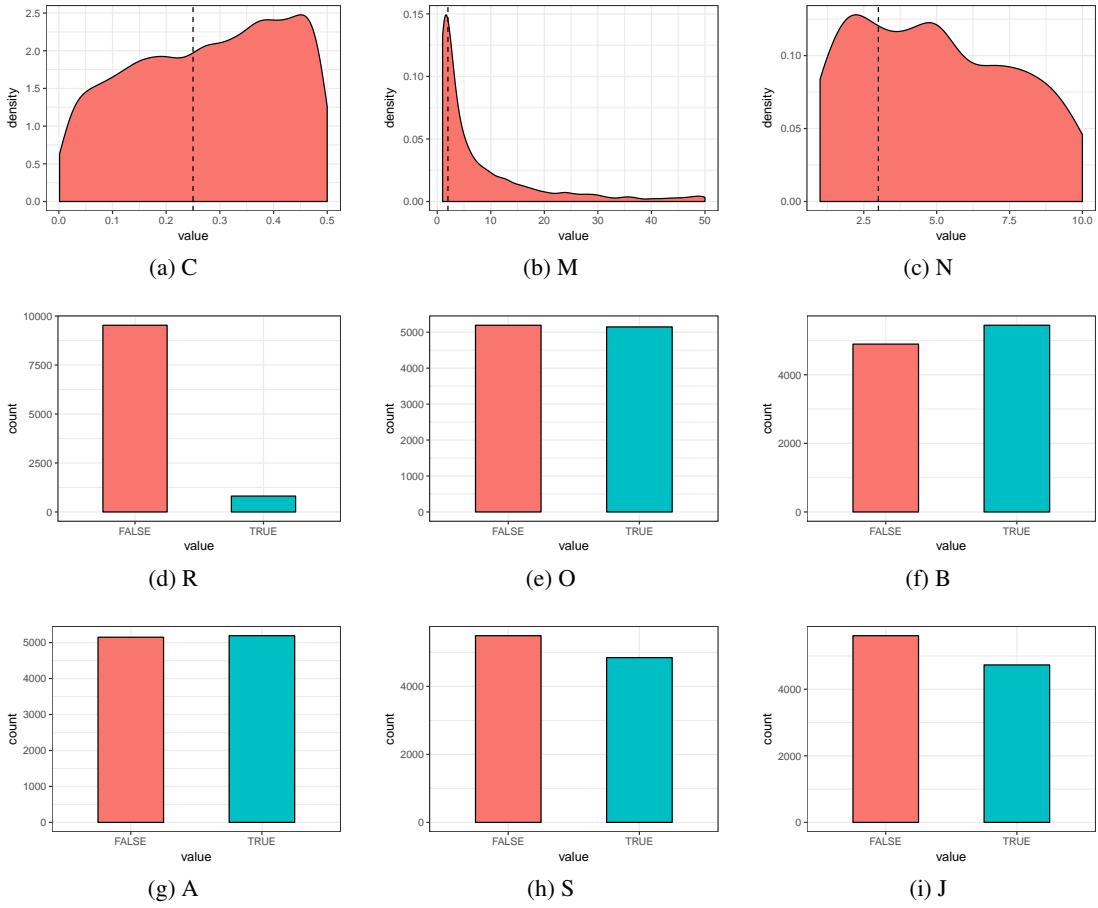


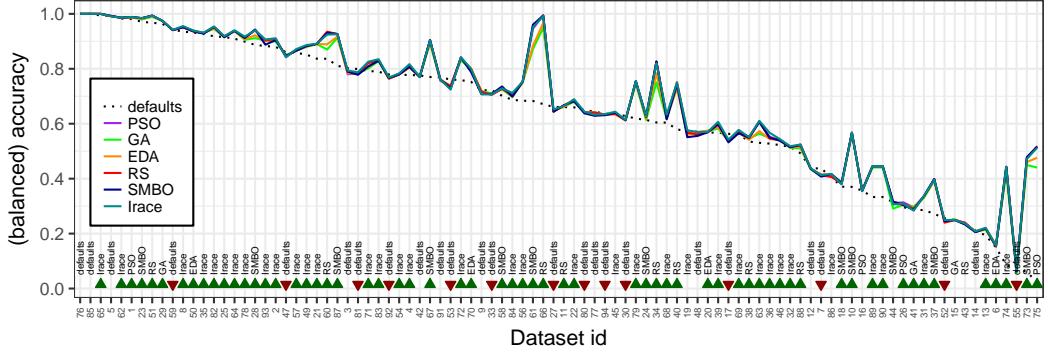
Figure 4: Distribution of the J48 hyperparameters found by the tuning techniques.

close to the default value in most of the cases (close to $m = 2$). The other Boolean hyperparameters seem not to influence the predictive performances reached during the optimization process since they present a very uniform distribution. Overall, the only hyperparameter that may contribute to generate solutions different from the default values is the *confidence pruning* hyperparameter ('C'), as indicated by Sub-figure 4 (a).

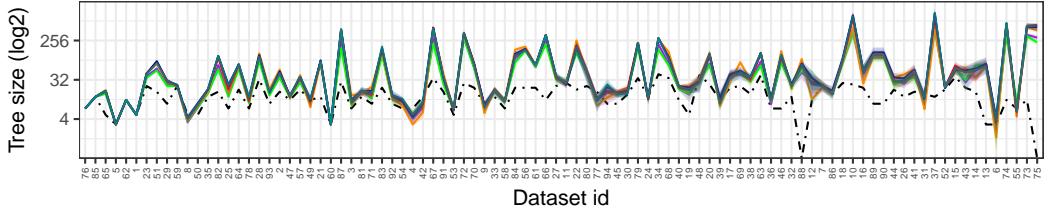
5.2 Performance analysis regarding CART algorithm

Figure 5 presents graphical analysis for the CART results. Different from J48, CART was more affected by hyperparameter tuning. In most of the datasets analyzed, the use of tuned values improved the predictive performance with statistical significance when compared with the use of default values in 62/94 ($\approx 66\%$) of the cases. It must be observed that the Irace and SMBO were the best optimization techniques, regarding just the predictive performance of the induced models. Defaults values were better than tuned ones in 14/94 of the cases. In the remaining 18/94 datasets, there was no significant statistical improvement using optimized values.

Regarding the size of CART DTs, whenever defaults were statistically better, the trees induced by them have similar or lower sizes than the tuned ones. However, in most of the cases, tuned hyperparameter settings induced trees statistically better and much larger than those created using default values. Even 'defaults' trees being simpler, they were incapable of classifying most of the problems properly. The comparison among the tuning techniques showed results different from those obtained for the J48 algorithm. The tuning techniques led to the induction of DTs with similar sizes. However, the DTs induced when Irace was used were slightly larger, and with better predictive performance than those induced using the other optimization techniques.



(a) Average balanced per class accuracy performance.



(b) Average tree size. Results are presented in \log_2 scale.

Figure 5: Hyperparameter tuning results for the CART algorithm.

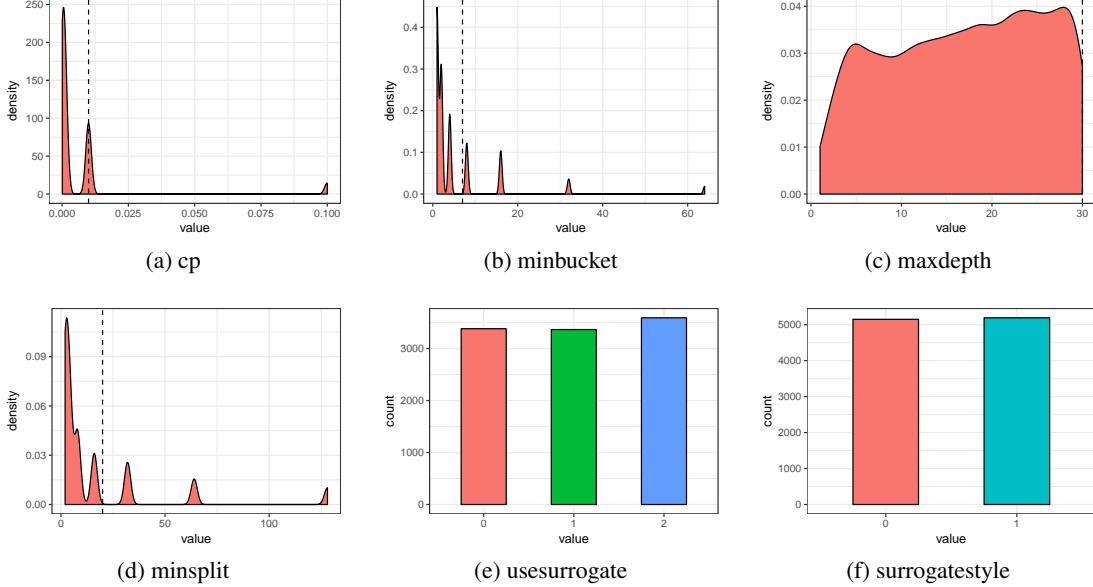


Figure 6: CART hyperparameters' distributions found by the tuning techniques.

TheCART hyperparameters' distributions found by the tuning techniques can be found in Figure 6. Different from J48, CART tuned trees were obtained from values substantially different from the default values. This is more evident for the numerical hyperparameters, as shown in sub-figures 6 (a) to (d). The ‘cp’, ‘minbucket’ and ‘minsplit’ values tend to be smaller than default values. For ‘maxdepth’, a wide range of values is tried, indicating a possible dependence on the input problem (dataset). However, the categorical hyperparameters’ distributions, shown in Sub-figures 6 (e) and (f), are very uniform, indicating that their choices may not influence the final predictive performance.

5.3 Performance analysis regarding CTree algorithm

The results obtained in the experiments with the CTree are illustrated by Figure 7. Most of the tuning techniques presented similar results, with the exception of GA (the green line), which was clearly worse than all the other techniques regarding predictive performance. Unlike the two previous case studies, CTree predictive performance was less influenced by the hyperparameter tuning. Default values generated the best models in 38/94 of the datasets. Tuned values improved the predictive performance of the induced trees in 23/94 ($\approx 25\%$) of the datasets. For the remaining 33/94 there was no statistical difference between the use of default values and values produced by tuning techniques.

Considering the size of the induced trees, tuning techniques did not generate larger or smaller trees than those induced by using default values. There are just a few exceptions, for dataset ids = {79, 57}, were tuned trees are visually larger but improved the predictive performance. Comparing tuning techniques among them, Irace and PSO were the best techniques considering just the predictive performance of the models, followed by the SMBO technique.

Figure 8 presents the CTree hyperparameter values' distributions found during the tuning process. Similarly to the CART scenario, all the numerical hyperparameters presented values different from the default values: some of them produced values smaller than default values ('minbucket', 'minsplit'); another was similar to the default value ('mtry'); and all the others varied in a wide range of values ('maxdepth', 'mincriterion'). The categorical hyperparameter 'stump', which enables the induction of a tree with just one level, is mostly set as `stump = FALSE`, like the default setting, having no real impact on the performance differences.

5.4 Statistical comparisons between techniques

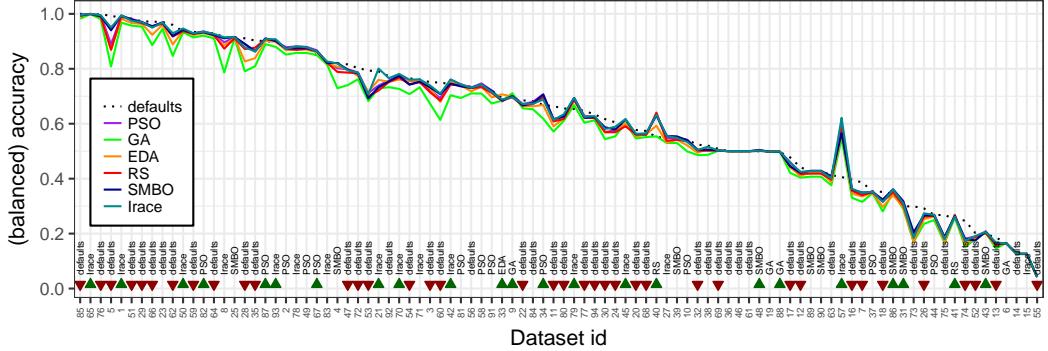
The Friedman test [88], with significance levels at $\alpha = 0.05$ and $\alpha = 0.1$, was also used to compare the hyperparameter tuning techniques, evaluating the statistical significance of the experimental results. The null hypothesis states that all classifiers induced with the hyperparameter settings found by the tuning techniques, and the classifier induced by default values, are equivalent concerning predictive BAC performance. If the null hypothesis was rejected, the Nemenyi post-hoc test was applied, stating that the performances of two different techniques are significantly different if the corresponding average ranks differ by at least a Critical Difference (CD) value.

Figure 9 presents the CD diagram for the three DT induction algorithms. Techniques are connected when there is *no* statistically significant differences between them. Considering $\alpha = 0.05$, Sub-figure 9(a) depicts the comparison in J48 scenario. One may note that there is no statistically differences between the top two best techniques: Irace and PSO. Also, the models induced with default hyperparameter values obtained no statistically better results than Irace, PSO, SMBO and RS. EDA and GA obtained statistically inferior performances.

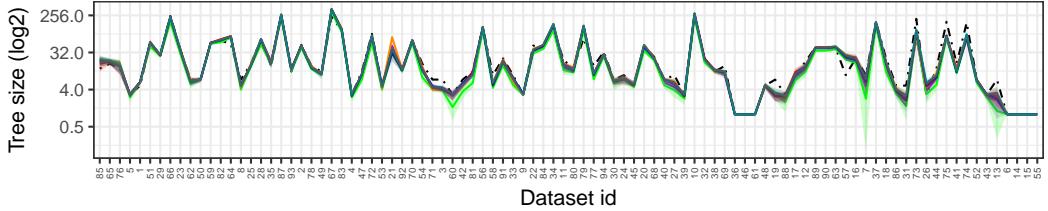
For the CART algorithm (Sub-figure 9(b)), the best ranked technique over all datasets was Irace, followed by RS with no statistically significant results. DTs induced with default hyperparameter values obtained the worst performance, being statistically comparable only with GA and EDA.

CD-diagrams for the CTree results are shown in Sub-figures 9(e) and 9(f). The defaults hyperparameter values were ranked first, followed by the Irace, PSO and SMBO techniques. However, there is no statistical differences between them. The RS and EDA compose the second block of techniques. They do not present statistical differences between them but do in relation to the first group of techniques. Finally, the GA technique was statistically worst than all the other techniques.

It is worth mentioning that Irace was the best tuning technique for all the algorithms. Whereas the statistical test did not show significant differences between Irace and PSO (J48, CTree), and between Irace and RS (CART), it is easy to see that Irace is the preferred technique, presenting the lowest averaging ranking. When a larger $\alpha = 0.1$ value was used (with $CD = 0.848$), there were no changes in J48 and CTree scenarios. However, regarding CART performances, Irace statistically outperformed all the other techniques, as can be seen in Sub-figure 9(d).



(a) Average balanced per class accuracy performance.



(b) Average tree size. Results are presented in \log_2 scale.

Figure 7: Hyperparameter tuning results for the CTree algorithm.

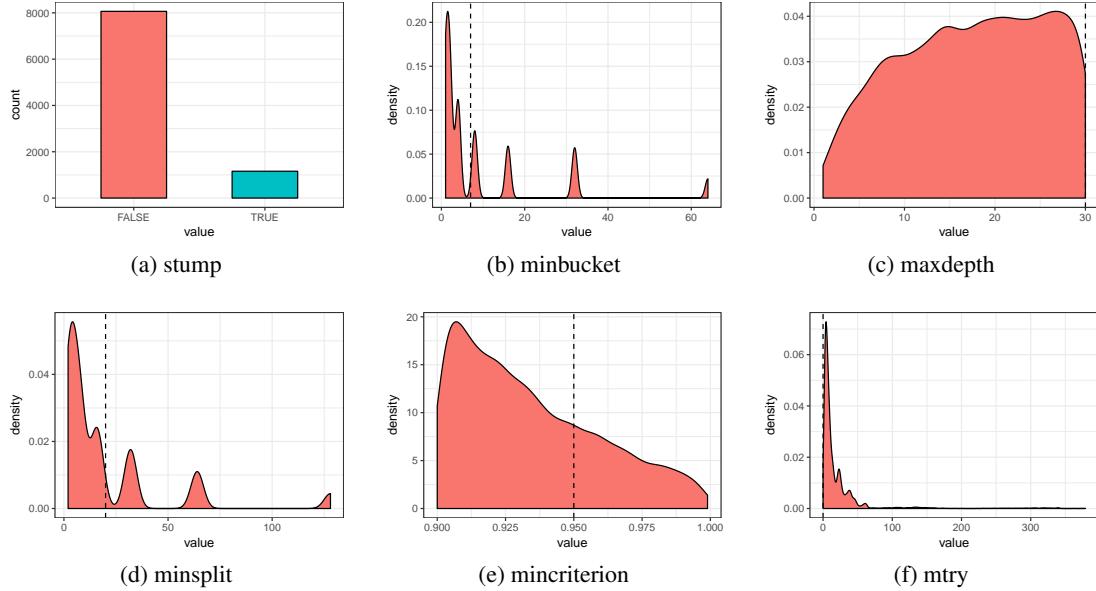
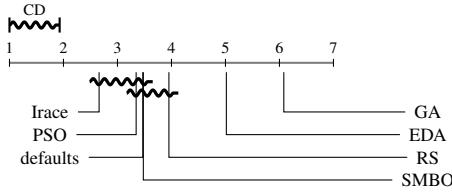


Figure 8: CTree hyperparameters' distributions found by tuning techniques.

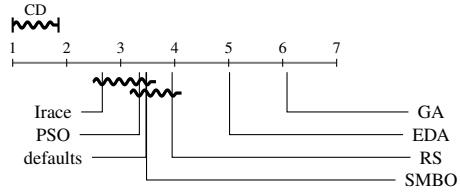
5.5 When to perform tuning?

A set of data complexity [89, 90] measures was used to characterize the datasets, and provide patterns that could explain when it is better to use tuned or default values. From the thirteen measures used, three were able to relate their values with the J48 hyperparameter tuning BAC performances:

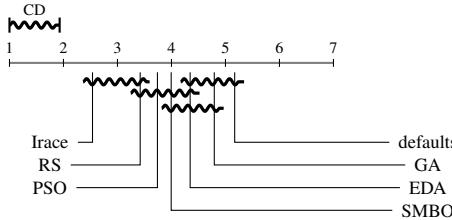
- *Fischer's discriminant ratio* ($f1$, $f1 \in [0, +\infty)$) - selects the attribute that best discriminates the classes: the higher the value, the higher the indicative that at least one of the dataset attributes is able to linearly separate data from different classes;



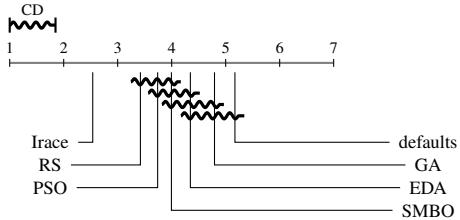
(a) J48 CD diagram with $\alpha = 0.05$.



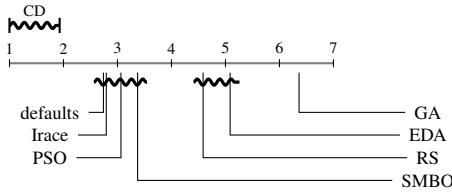
(b) J48 CD diagram with $\alpha = 0.1$.



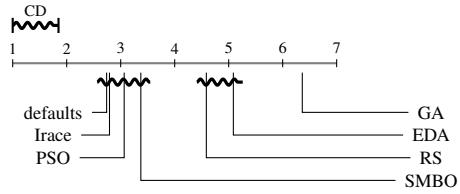
(c) CART CD diagram with $\alpha = 0.05$.



(d) CART CD diagram with $\alpha = 0.1$.



(e) CTree CD diagram with $\alpha = 0.05$.



(f) CTree CD diagram with $\alpha = 0.1$.

Figure 9: Comparison of the Balanced per class Accuracy (BAC) values of the hyperparameter tuning techniques according to the Nemenyi test. Groups of techniques that are not significantly different are connected. Left charts show results with $\alpha = 0.05$, while right charts show comparisons with $\alpha = 0.1$.

- *Collective feature efficiency* ($f4$), $f4 \in [0, +1]$ - considers the discriminative power of all the dataset's attributes;
- *Fraction of points lying on the class boundary* ($n1$), $n1 \in [0, +1]$ - estimates the complexity of the correct hypothesis underlying the data. Higher values indicate the need for more complex boundaries to separate data.

Two of these measures ($f1$ and $n1$) try to identify the existence of at least one dataset attribute that may linearly separate classes, while $f4$ attempts to provide information by taking into account all the attributes available in the dataset. Considering them, some simple rules could also be observed: hyperparameter tuning is commonly recommended for multiclass problems with several classes ($cls > 8$), for datasets with a Fischer's discriminant ratio close to zero ($f1 < 0.06$), and finally, when the average number of instances in the class boundary is $n1 > 0.218$. In cases where a high collective feature efficiency occurs ($f4 > 0.8695$), defaults hyperparameter values induce good models.

For CART, in addition to $n1$, two other measures were important:

- *The maximum individual attribute efficiency* ($f3$), $f3 \in [0, +1]$ - indicates the presence of attributes whose values do not overlap between classes;
- *The non-linearity of the one-nearest neighbor classifier* ($n4$), $n4 \in [0, +1]$ - this measure creates a test set by linear interpolation with random coefficients between pairs of randomly selected instances of the same class. Then, it returns the test error of the 1-NN classifier.

Two of these measures ($n1$, $n4$) evaluate the class separability, while $f3$ measures the overlap in feature space from different classes. Defaults were suggested for few problems when more than $n1 \geq 0.278$ points were placed in the boundaries, there was at least one attribute with a

maximum individual efficiency bigger than $f3 > 0.0125$, and a linear classifier performed quite well ($n4 < 0.2545$). Thus, the analysis suggests that hyperparameter tuning is recommended especially for multiclass problems, and for those without a clear linear decision boundary to separate data instances (they are more *complex*).

Regarding CTree, a different set of measures was considered:

- *Average intra/inter class nearest neighbor distances* ($n2$), $n2 \in [0, +\infty)$ - the average intra-class and inter-class distances ratio used by a k-NN algorithm to classify data examples. Low values indicate that examples from the same class lay closely in the feature space, while high values indicate that examples from the same class are dispersed;
- *Training error of a linear classifier* ($l2$), $l2 \in [0, +1]$ - the predictive performance of a linear classifier for the training data. The lower the value, the closer the problem is to be linearly separable.

The measures $n2$ and $l2$ are also related to the problem classes separability. Tuning is usually recommended when data from the same class are disperse ($n2 > 0.5595$), and when a linear classifier is not able to classify examples with a training error $l2 < 0.129$ (*hard* problems). For the other situations, default values are recommended.

5.6 Runtime analysis

Running time is also an important aspect to be considered when performing experimental analyses. Figures 11 to 13 show the average tuning, training and testing times spent by the techniques when performing the hyperparameter tuning of the DT induction algorithms.

Tuning and testing times are related to the optimization process. The first measures the time required by the techniques to find good hyperparameter settings considering the time budget size. The second calculates the time required for assessing hyperparameter settings recommended by the tuning techniques (illustrated by the outer loop of Figure 2). The training time measures the time required for inducing DTs with the suggested hyperparameters using all the datasets' instances. The idea is to reproduce how models would perform in a practical scenario.

The values in the y-axis of the Figures are in seconds but were scaled with a \log_{10} transformation due to their discrepancy. Each curve with a different color represents a tuning technique. Since there is no tuning with defaults, there is no black dotted curve in the *tuning* sub-charts.

5.6.1 J48 runtime

Figure 11 presents the runtime analysis for J48. Considering the tuning time, the meta-heuristics (PSO, GA, EDA) are the fastest tuning techniques. They are population-based techniques, so they benefit from population coding structure to speed up the convergence of their computation and tend to a common solution. RS and Irace are in the middle. While the former technique simply randomly searches the space, the latter statistically compares many candidates in several rounds. That may explain why they require more running time than population-based techniques.

Finally, the SMBO technique presented the highest optimization/tuning time. The main reason is its inner sub-processes. After evaluating the initial points, the technique fits a RF regression model on the available data. Next, it queries the model to propose a new candidate hyperparameter solution using an acquisition function (or infill criteria). This function searches for a point at the hyperspace which yields the best infill value (the expected improvement) and then adds this value to the model for the next iteration. By checking the technique executions, it was observed that these steps are its main bottleneck, reflected directly in the final runtime.

The test runtime scale is too small, so in practice, there are no significant differences in the processing costs of the optimization techniques. Usually, tuned trees are assessed faster than those induced using default values, because tuning techniques induce smaller trees than the ones induced with default hyperparameter values (see Figure 3). Regarding training costs, training using default settings is faster than using tuned hyperparameter values. It may be due to the Boolean hyperparameters. They enable/disable some transformations that would require more time to handle data. When default hyperparameter settings are used, all of these transformations are disabled.

5.6.2 CART runtime

Figure 12 presents the same analysis for the CART algorithm. In general, running time results using CART provided similar insights to those obtained in the analysis of the J48 results. SMBO was also the technique with the highest processing cost, i.e., it required more time to consume the budget of possible evaluations (as previously discussed). The other techniques have similar cost curves, with oscillating values depending on the dataset characteristics. For J48, for example, Irace and RS required more time than the meta-heuristics.

When evaluating the hyperparameter settings testing the induced DTs, models induced with default hyperparameter values required more time to be assessed than those induced with the recommended tuned settings. This fact occurred every time DTs induced with default values presented a predictive performance statistically better than models induced with tuned hyperparameter settings. Regarding the training time, hyperparameter tuned DTs spent more time to induce the models. Since default hyperparameter values generated smaller trees, the test instances need to follow less internal nodes to be labeled with one of the classes.

5.6.3 CTree runtime

Figure 13 presents the running time analysis for the CTree algorithm. Similarly to scenarios of the previous algorithms, the SMBO technique was the most time-consuming technique to evaluate the defined budget size. The other techniques presented similar behavior, varying slightly depending on the problem under optimization. There are at least five datasets where all the techniques spent a long time to optimize the hyperparameters: they may be observed at data ids = {57, 64, 73, 74, 75}. All of them are multiclass classification tasks with at least 10 classes, implying a difficulty that CTree may have to solve classification tasks with many classes.

Training models with default values required less time than using hyperparameter tuned solutions. By default, CTrees does not apply any random selection of the input features during training ($mtry = 0$). All the other numerical hyperparameters tend to present values smaller than default values, in theory, producing smaller trees. However, this is not seen in practice. Tree sizes are very similar (tuned vs default) and ‘ $mtry$ ’ values might explain the difference. Regarding the test, the runtime scale is too small, so there are no real differences when evaluating settings found by using the tuning.

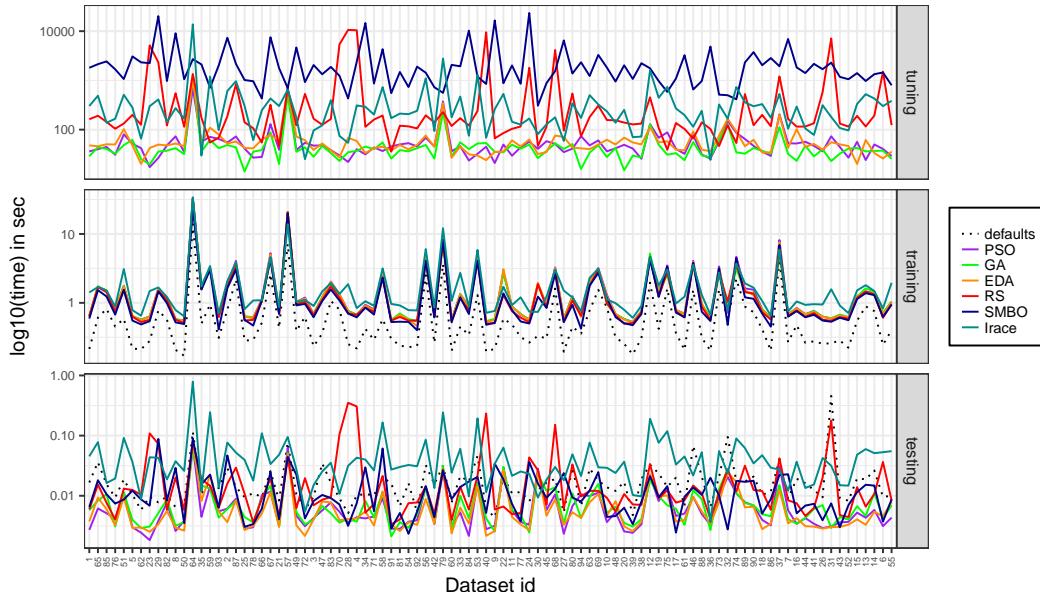


Figure 10: Average processing time required for the tuning, training and test phases of the J48 algorithm.

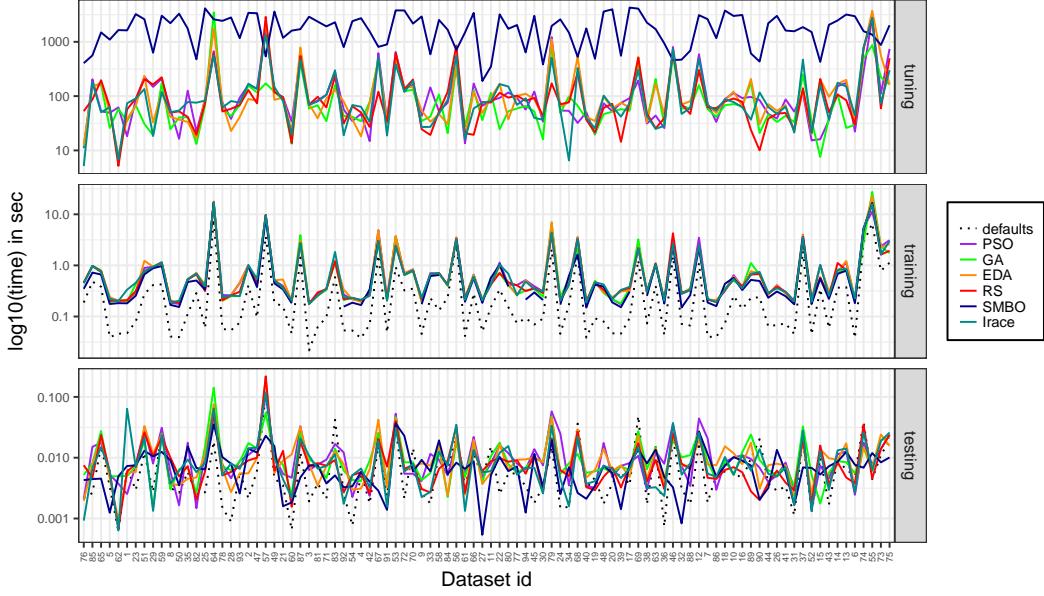


Figure 11: Average processing time required for the tuning, training and test phases of the CART algorithm.

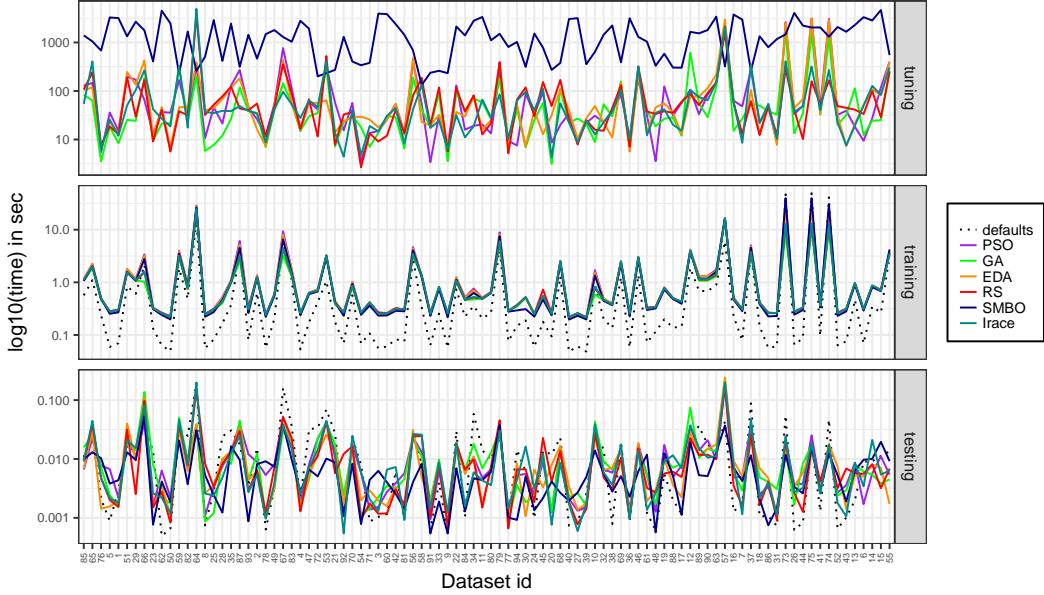


Figure 12: Average processing time required for the tuning, training and test phases of the CTree algorithm.

5.7 Convergence of the tuning techniques

Regarding the convergence of the tuning techniques, the boxplots in Figure 13 show the minimum, maximum and three quartiles for the number of evaluations assessed until the best solution was reached. The y-axis shows the number of evaluations, while the x-axis indicates the tuning techniques. Even using a budget of 900 iterations, all tuning techniques required at most 500 steps in the three case studies. Except for Irace, which required the largest number of candidates to converge, it is still possible to say that most of the good hyperparameter settings were reached between first 300 iterations for CART and J48 (as already observed in [29]).

The *exception* here is the CTree algorithm, since it required more iterations than J48 and CART. Looking back to the tuning results at Figure 7a, default values provided the best solution in almost 40% of the datasets, and the difficulty to find good hyperparameter settings that would outperform them is reflected in Figure 13(c).

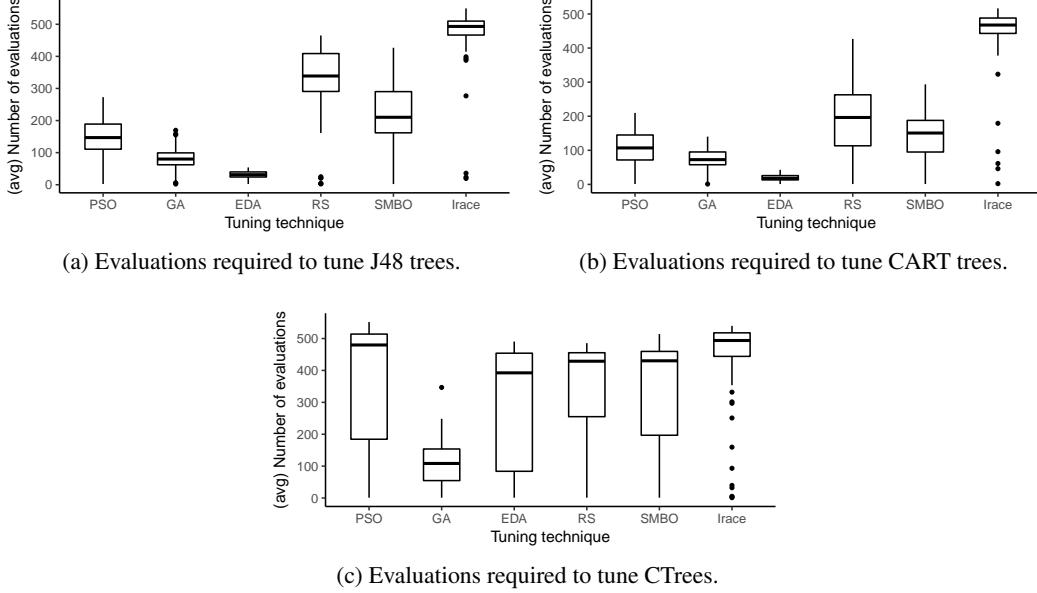


Figure 13: Number of evaluation used by the tuning techniques to reach their best hyperparameter solutions.

Boxplots in Figure 13 also suggest that Irace requires more evaluations than the RS technique. Looking in details, Irace is based on three steps: (1) sampling new hyperparameter configurations according to a particular distribution²⁵; (2) selecting the best set of configurations by means of *racing*, and (3) updating the sampling distributions towards the optimal region [91].

The race procedure starts with a finite set of candidates, and, at each step, discards hyperparameter settings that perform statistically worse than at least another. This process continues with the survivors. In the first iteration, this initial set of candidates is generated from hyperparameter distributions. The authors [91] emphasize that the first elimination process is fundamental, so there are some of instances (T_{First}) that must be seen before performing statistical tests. Therefore, new statistical comparisons are performed after new T_{Each} instances are assessed. By default, Irace suggests $T_{First} = 100$ (as detailed in Table 6) and $T_{Each} = 1$). These values were defined after being tuned and studied for different optimization scenarios [92].

Internally, the technique estimates its racing hyperparameters based on the budget and target hyper-space. The number of races (N_{iter}) depends on the number of hyperparameters, while each race has a proper budget (B_j) limited by the iteration index and a number of evaluations still available²⁶. Thus, Irace works in such a way that the number of candidate settings decreases with the number of iterations, which means more evaluations per configuration will be performed in late iterations.

Therefore, this difference concerning evaluations is better explained by the default value of T_{First} , which increases the minimum number of evaluations required by the technique. The inner racing hyperparameters also influence, since they will control the number of races, requiring more statistical tests (and evaluations) in late iterations. However, even evaluating more hyperparameter candidates than the RS technique, Irace does not require an additional time (as may be seen in Figures 11 to 13, except for some datasets and the J48 algorithm). Moreover, it might be covering different regions of the hyperspace, which is indicated by the results obtained and illustrated by figures 9.

²⁵The distributions are independently for each hyperparameter.

²⁶For further details, please consult the Irace's manual [93].

Considering just the number of hyperparameters assessed during the search, although the runtime analysis showed that SMBO is the most costly, it was able to find good solutions assessing a smaller number of candidates than Irace (the technique that resulted in DTs with the best predictive performance). This occurred for all the algorithms, suggesting that with different stopping criteria (early convergence), even SMBO could be a reliable choice.

The PSO technique was able to find good hyperparameter solutions in J48 and CART scenarios with less than 200 iterations. Based on the statistical results from figure 9, PSO was often among the best techniques for all the three scenarios. In some cases, depending on the statistical test, it was not statistically different from the best technique (Irace). Thus, it may be a good alternative to fast obtain good solutions.

5.8 Hyperparameters' importance analysis

Statistical analysis was also used to understand how different hyperparameters affect each other, and the DT induction algorithm performances. AN approach to evaluate how the hyperparameters are affecting the performance of the induced models when different tuning techniques are performed is the use of fANOVA (Functional ANOVA framework)²⁷, introduced in [28]. In that paper, the authors present a linear-time algorithm for computing marginal predictions and quantify the importance of single hyperparameters and interactions between them. The key idea is to generate regression trees that predict the performance of hyperparameter settings and apply the variance decomposition framework directly to the trees in these forests.

In the source article, the authors ran fANOVA with SMBO hyperparameter settings over some scenarios, but never with more than 13.000 hyperparameter settings. Here, a single execution of Irace generates $30 \times 10 \times 900 = 270.000$ evaluations. Thus, experiments using all techniques would have a high computational cost. Since Irace was the best technique overall in both algorithms, it was used to provide the hyperparameter settings to this analysis. In the experiments, hyperparameter settings from 3 repetitions were used and more memory was allocated to the fANOVA code.

Figure 14 shows the results for DT induction algorithms. In the figure, the x-axis shows all datasets while y-axis presents the hyperparameters importance regarding fANOVA. The larger the importance of a hyperparameter (or pair of them), the darker its corresponding square, i.e., more important is the hyperparameter for inducing trees in the dataset (scaled between zero and one).

In the figure, any single hyperparameter (or combination of them), whose contribution to the performance of the final models was lower than 0.005, was removed. Applying this filter substantially reduced the hyperparameters in focus, but even so, most of the rows in the heatmap are almost white (light red). This analysis shows that most of the combinations have little contribution to the performance of the induced DTs.

In Sub-figure 14(a), fANOVA indicates that most of the J48 performances were influenced by M hyperparameter values: when not alone, in combination with another hyperparameter (R, N, C). For CART, the ‘minbucket’ and ‘minsplit’ hyperparameters are the main responsible for the performance of the induced DTs, as may be seen in Figure 14(b).

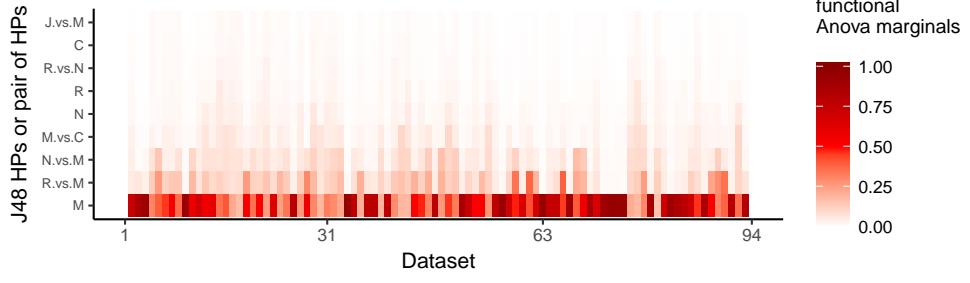
For CTree, seven of the fANOVA’s jobs produced errors when executing. In these situations, a white column is presented at the heatmap. Regarding the analysis, the hyperparameters ‘minbucket’ and ‘minsplit’ are the most important, similarly with the CART’s chart. On the other hand, they have less strength to predict marginal distributions. It reinforces previous findings describing CTree as less sensitive to tuning.

These findings enforce what was discussed in the previous subsection: although each one of the analysis may point out a different important hyperparameter, the same subset of hyperparameters seems to influence the final performance of the induced DTs.

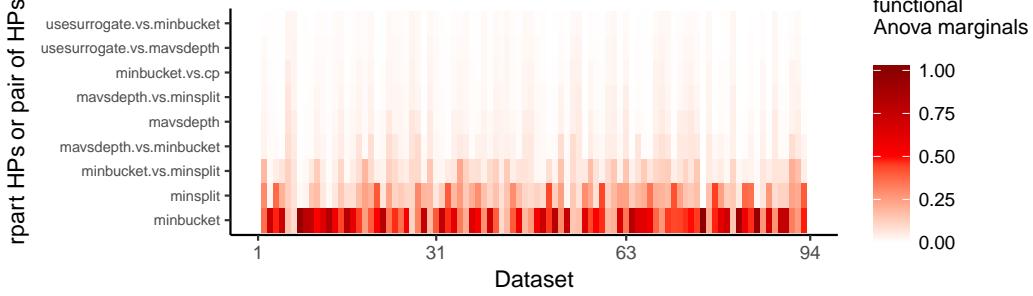
6 Threats to Validity

In an empirical study design, methodological choices may impact the results obtained in the experiments. Next, the threats that may impact the results from this study are discussed.

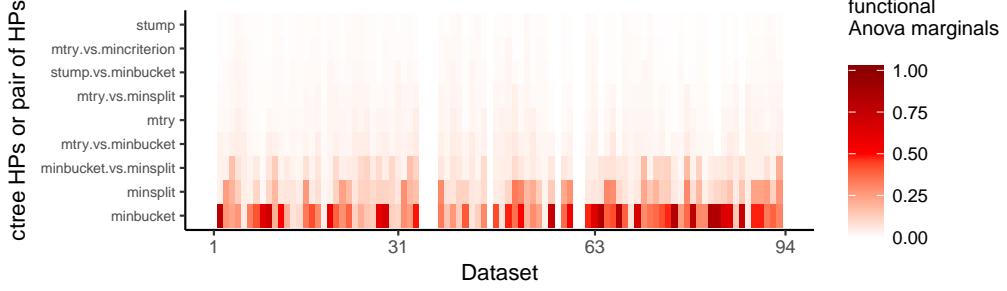
²⁷<https://github.com/automl/fanova>



(a) Functional ANOVA values for J48 hyperparameters.



(b) Functional ANOVA values for CART hyperparameters.



(c) Functional ANOVA values for CTree hyperparameters.

Figure 14: Functional ANOVA hyperparameters marginal predictions for DT algorithms regarding all dataset collection. Marginal predictions are scaled between zero and one.

6.1 Construct validity

The datasets used in the experiments were selected to cover a wide range of classification tasks, with different characteristics. They were used in their original versions, i.e., no preprocessing was required, since DTs are able to handle any missing information or data from different types. The only restriction adopted ensures that all classes in the datasets must have at least 10 observations. Thus, stratification with 10 outer folds can be applied. Of course, other datasets may be used to expand data collection, if they obey the ‘stratified’ criterion. However, the authors believe that addition of datasets will not substantially change the overall behavior of tuning on the algorithms investigated.

Regarding the DT induction algorithms, CART and J48 are among the most popular algorithms used in data mining [4]. The CTree algorithm works similarly to the traditional CHAID algorithm, using statistical tests, but provides a more recent implementation which handles different types of data attributes²⁸. Experiments were focused on these algorithms due to the interpretability of their induced models and widespread use. All of them generate simple models, are robust for specific domains, and allow non-experts users to understand how the classification decision is made. The same experimental methodology and analyses can be applied to any other ML algorithm.

²⁸The CHAID algorithm handles just categorical data attributes.

Since a wide variety of datasets compose the data collection, some of them may be imbalanced. Thus, the BAC performance measure [84] was used as fitness function during the optimization process. Therefore, class distributions are being considered when assessing a candidate solution. The same performance measure is used to evaluate the final solutions returned by the tuning techniques. Other predictive performance measures can generate different results, depending on how they deal with data imbalance.

The experimental methodology described in Section 4 considers the tuning techniques that have been used in related literature [44, 47, 53, 52]. The exceptions are the EDA and Irace techniques, which have been explored recently for hyperparameter tuning of other ML algorithms, like SVMs [15, 43]. Since there is a lack of studies investigating these techniques for DTs (see Section 2.4), they were added to the experimental setup.

6.2 Internal validity

Krstajic et. al. [72] compared different resampling strategies for selecting and assessing the predictive performance of regression/classification models induced by ML algorithms. In Cawley & Talbot [71] the authors also discuss the overfitting in the evaluation methodologies when assessing ML algorithms. They describe a so-called “*unbiased performance evaluation methodology*”, which correctly accounts for any overfitting that may occur in the model selection. The internal protocol described by the authors performs the model’s selection independently within each fold of the resampling procedure. In fact, most of the current studies on hyperparameter tuning have adopted nested-CVs, including important autoML tools, like Auto-WEKA²⁹ [51, 52] and Auto-skLearn³⁰ [44, 61]. Since this paper aims to assess DT induction algorithms optimized by hyperparameter tuning techniques, the nested CV methodology is the best choice and was adopted in the experiments.

In the experiments carried out for this study, all the default settings provided by the implementations of the tuning techniques were used. In fact, most of these default values have been evaluated in benchmark studies and reported to provide good predictive performance [81, 92], while others (like PSO’s) showed to be robust in a high number of datasets. For EDA and GA, there is no standard choice for their parameter values [87], and even adapting both to handle our mixed hyperparameter spaces properly they performed poorly. It suggests that a fine tuning of their parameters would be needed. Since this would considerably increase the cost of experiments by adding a new tuning level (*the tuning of tuning techniques*), and most of the techniques performed well with default values, this additional tuning was not assessed in this study.

The use of a larger budget, with 5000 evaluations for DT tuning, was investigated in [29]. The experimental results suggested that all the considered techniques required only 900 evaluations to converge. The convergence here means the tuning techniques could not improve their predictive performance more than $x = 10^5$ until the budget was consumed. Actually, in most cases, the tuning reached its maximum performance after 300 steps. Thus, a budget size of 900 evaluations was therefore deemed sufficient. Results obtained with this budget value showed that the exploration made in hyperparameter spaces led to statistically significant improvements in most cases.

6.3 External validity

Section 5.4 presented statistical comparisons between tuning techniques. In [88], Demšar discusses the issue of statistical tests for comparisons of several techniques on multiple datasets reviewing several statistical methodologies. The method proposed as more suitable is the non-parametric analog version of ANOVA, i.e. the Friedman test, along with the corresponding Nemenyi post-hoc test. The Friedman test ranks all the methods separately for each dataset and uses the average ranks to test whether all techniques are equivalent. In case of differences, the Nemenyi test performs all the pairwise comparisons between the techniques and identifies the presence of significant differences. Thus, the Friedman ranking test followed by the Nemenyi post-hoc test was used to evaluate experimental results from this study.

Some recent studies raised concerns that a Friedman-Nemenyi test produces overlapping groups [94]. They recommend the use of the Scott-Knott Effect Size Difference test to produce non-overlapping

²⁹<http://www.cs.ubc.ca/labs/beta/Projects/autoweka/>

³⁰<https://github.com/automl/auto-sklearn>

groups. Using the Scott-Knott ESD test, under its assumptions, the analysis of the experimental results did not change. The main effect was to generate clean groups, while in the Friedman test a CD-diagram is required to interpret results. In general, there is no *silver bullet*, and each test will have its pros and cons.

The budget size adopted can directly influence the performance of the meta-heuristics, specially GA and EDA. In [25] the authors recommend to use at least 100 individuals to build a reliable EDA model, suggestion followed in [29]. In this extended version, the budget size was reduced, supported by prior analyses, and tuning techniques adapted to work with the reduced number of evaluations. Increasing the population size would also increase both the number of iterations and the budget size. However, it has already been experimentally shown that just a small number of evaluations provides good predictive performance values [29]. It is important to highlight that even using a small population the PSO technique reached robust results in a wide variety of tasks considering the three DT algorithms investigated. At this point, the poor performance values obtained by GA and EDA can be considered a limitation: they do not search properly space under this budget restriction.

7 Conclusions

This paper investigated the effects of hyperparameter tuning on the predictive performance of DT induction algorithms, as well the impact hyperparameters have on the induced models' performances. For this purpose, three different DT implementations were chosen as study cases: two of the most popular algorithms in ML - the J48 and CART algorithms, and the CTree algorithm, a more recent implementation similar to classical CHAID algorithm. An experimental analysis regarding the sensitivity of their hyperparameters was also presented. Experiments were carried out with 94 public OpenML datasets and six different tuning techniques. The performances of DT induced using these techniques were also compared with DTs generated with the default hyperparameter values (provided by the correspondent R packages). The main findings are summarized below.

7.1 Tuning of J48

In general, hyperparameter tuning for J48 produced modest improvements when compared to the RWeka default values: the trees induced with tuned hyperparameter settings reached performances similar to those obtained by defaults. Statistically significant improvements were detected in only one-third of the datasets, often those datasets where the default values produced very shallow trees.

The J48 Boolean hyperparameters are responsible for enabling/disabling some data transformation processes. In default settings, all of these hyperparameters are disabled. So, enabling them requires more time to induce and assess trees (which can be noted in the runtime analysis and charts in Section 5.6). Furthermore, the relative hyperparameter importance results (via fANOVA analysis) showed that these Boolean hyperparameters are irrelevant for most datasets. Only a subset of hyperparameters (R, C, N, M) contributes actively to the performance of the final DTs.

Most of the related studies which performed some tuning for J48 tried different values for the complexity parameter (C), but none of them tried hyperparameter tuning using reduced error pruning: enabling 'R' and changing 'N' values. The use of 'R' and 'N' options may be a solution when tuning only 'C' does not sufficiently improve performance (as indicated by fANOVA analysis).

None of the related work used the Irace technique: they focused more on SMBO, PSO or another tuning technique. SMBO is often used with an early stopping criterion (a budget) since it is the slowest technique. However, it typically converged after relatively few iterations. If it is desirable to obtain good solutions faster, PSO might be recommended. However, for the J48 algorithm, the best technique concerning performance is Irace: it was better ranked, evaluated more candidates, and did not consume a lot of runtime.

The J48 default hyperparameter values were good for a significant number of datasets. This behavior can be since the defaults used by RWeka were chosen to be the best overall values performing on the UCI ML repository [58] datasets.

7.2 Tuning of CART

Surprisingly, CART was much more sensitive to hyperparameter tuning than J48. Statistically significant improvements were reached in two thirds of the datasets, most of them with a high-performance gain. Most of the hyperparameters control the number of instances in nodes/leaves used for splitting. These hyperparameters directly affect the size and depth of the trees. The experimental analyses showed that default settings induced shallow and small trees for most of the problems. These trees did not obtain good predictive performances. Where the defaults did grow large trees, the performance was similar to the optimized performance. In general, CART's default hyperparameter values induced trees which are on average smaller than those produced by J48 under default settings. One reason that may also explain the poor CART's default performances would be the case that J48 hyperparameters were pre-tuned on UCI datasets while the CART ones were not.

Our relative importance analysis indicated that hyperparameters such as ‘minsplit’ and ‘minbucket’ are the most responsible for the performance of the final trees. In the related literature, just two of the five works investigated the tuning of both. Even so, they used RS and SMBO as tuning techniques. Experiments showed that for CART hyperparameter tuning, the Irace technique significantly outperformed all the other ones (especially with $\alpha = 0.1$). It evaluated a higher number of candidates during the search, and its running time was comparable to that of the meta-heuristics. Thus, Irace would be a good choice and might be further explored in future research.

7.3 Tuning of CTree

The tuning of CTrees was a new task contribution from this study, considering the related results: none of them evaluated more than two hyperparameters before. The algorithm proved to be the least sensitive to the hyperparameter tuning process, setting up a third case distinct from the previous two. Statistically improvements were observed in just a quarter of the datasets. Default values were also statistically better in 40% of the situations.

Similar to CART, most of its hyperparameters control the number of data examples in the node used for splitting (but in a statistical approach). Consequently, they control the size and depth of the induced trees. During the optimization of the hyperparameters, the tuning techniques found a wide range of hyperparameters values that differ from default settings (usually smaller). However, trees sizes did not show any visible difference, with Irace, PSO and SMBO curves almost overlapping for all the datasets. It suggests that different from J48 and CART, another characteristic rather than the tree size could influence the final predictive performances.

The hyperparameter importance analysis also indicated that few of the hyperparameters studied are responsible in some way for the predictive performance of the final trees. Experiments also showed that Irace would be the best hyperparameter tuning technique, being better ranked than other tuning techniques and presenting a running time comparable to the other meta-heuristics.

7.4 General scenario

In this analysis, we hypothesized that dataset complexity could explain when to use each tuning approach. It can be assumed that the more complex (difficult to classify) a dataset is, the more a DT algorithm will benefit from hyperparameter tuning. Thus, to understand when to use each approach, and be able to recommend when to tune the hyperparameter or use the defaults values, each dataset was described by characteristics obtained by extracting a set of complexity measures, which suggest how difficult a dataset is for a classification task.

We observed that hyperparameter tuning provides best results for datasets with many classes ($cls > 8$), and when there are non-linear decision boundaries. On the other hand, defaults seem to be adequate for simple classification problems, where there is a higher separability between the classes.

Considering the algorithms investigated in this study, each one presented a different behavior under tuning. In general, it was possible to observe that the default hyperparameter values are suitable for a large range of datasets, but a fixed value would not be suitable for all the data classification tasks. It justifies and motivates the development of recommender systems able to suggest the most appropriate hyperparameter setting for a new problem.

7.5 Future Work

Our findings also point out to some future research directions. The data complexity characteristics provided some useful insight regarding in which situations tuning or defaults should be used. However, it would be possible to make more accurate suggestions exploring more concepts from the meta-learning field.

It would obviously also be interesting to explore other ML algorithms and their hyperparameters: not only DTs induction algorithms, but many classifiers from different learning paradigms. The code developed in this study, which is publicly available, is easily extendable and may be adapted to cover a wider range of algorithms. The same can be said for the analysis.

All collected hyperparameter information might be leveraged in a recommendation framework to suggest hyperparameter settings. When integrated with OpenML, this framework could have great scientific (and societal) impact. The authors have already begun work in this direction.

Acknowledgments

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A List of abbreviations used in the paper

ANN Artificial Neural Network.

BAC Balanced per class Accuracy.

CART Classification and Regression Tree.

CASH Combined Algorithm Selection and Hyper-parameter Optimization.

CD Critical Difference.

CTree Conditional Inference Trees.

CV Cross-validation.

DL Deep Learning.

DT Decision Tree.

EDA Estimation of Distribution Algorithm.

GA Genetic Algorithm.

GP Gaussian Process.

GS Grid Search.

Irace Iterated F-race.

LMT Logistic Model Tree.

ML Machine Learning.

MtL Meta-learning.

NBTree Naïve-Bayes Tree.

OpenML Open Machine Learning.

PD Parametric Density.

PS Pattern Search.

PSO Particle Swarm Optimization.

RF Random Forest.

RS Random Search.

SH Shrinking Hypercube.

SMBO Sequential Model-based Optimization.

SS Scatter Search.

SVM Support Vector Machine.

UCI University of California Irvine.

VTJ48 Visual Tuning J48.

B List of OpenML datasets used for experiments

Table 7: (Multi-class) classification OpenML datasets (1 to 47) used in experiments. For each dataset it is shown: the OpenML dataset name and id, the number of attributes (D), the number of examples (N), the number of classes (C), and the percentage of examples belonging to the majority class (%MajC).

Nro	OpenML name	OpenML did	D	N	C	%MajC
1	acute-inflammations	1455	6	120	2	0.58
2	analcatdata_authorship	458	70	841	4	0.38
3	analcatdata_boxing1	448	3	120	2	0.65
4	analcatdata_boxing2	444	3	132	2	0.54
5	analcatdata_creditscore	461	6	100	2	0.73
6	analcatdata_dmft	469	4	797	6	0.19
7	analcatdata_germangss	475	5	400	4	0.25
8	analcatdata_lawsuit	450	4	264	2	0.93
9	appendicitis	1456	7	106	2	0.80
10	artificial-characters	1459	7	10218	10	0.14
11	autoUniv-au1-1000	1547	20	1000	2	0.74
12	autoUniv-au4-2500	1548	100	2500	3	0.47
13	autoUniv-au6-1000	1555	40	1000	8	0.24
14	autoUniv-au6-750	1549	40	750	8	0.22
15	autoUniv-au6-400	1551	40	400	8	0.28
16	autoUniv-au7-1100	1552	12	1100	5	0.28
17	autoUniv-au7-700	1553	12	700	3	0.35
18	autoUniv-au7-500	1554	12	500	5	0.38
19	backache	463	31	180	2	0.86
20	balance-scale	11	4	625	3	0.46
21	banana	1460	2	5300	2	0.55
22	bank-marketing	1461	16	45211	2	0.88
23	banknote-authentication	1462	4	1372	2	0.56
24	blood-transfusion-service-center	1464	4	748	2	0.76
25	breast-w	15	9	699	2	0.66
26	breast-tissue	1465	9	106	6	0.21
27	live-disorders	8	6	345	2	0.58
28	car	21	6	1728	4	0.70
29	cardiotocography v.2 (version 2)	1560	35	2126	3	0.78
30	climate-model-simulation-crashes	1467	20	540	2	0.91
31	cloud	210	6	108	4	0.30
32	cmc	23	9	1473	3	0.43
33	sonar	40	60	208	2	0.53
34	vowel	307	13	990	11	0.09
35	dermatology	35	34	366	6	0.31
36	fertility	1473	9	100	2	0.88
37	first-order-theorem-proving	1475	51	6118	6	0.42
38	solar-flare	173	12	1389	6	0.29
39	haberman	43	3	306	2	0.74
40	hayes-roth	329	4	160	3	0.41
41	heart-c	49	13	303	5	0.54
42	heart-h	51	13	294	2	0.64
43	heart-long-beach	1512	13	200	5	0.28
44	heart-h v.3 (version 3)	1565	13	294	5	0.64
45	hepatitis	55	19	155	2	0.79
46	hill-valley	1479	100	1212	2	0.50
47	colic	25	27	300	2	0.64

Table 8: (Multi-class) classification OpenML datasets (48 to 94) used in experiments. For each dataset it is shown: the OpenML dataset name and id, the number of attributes (D), the number of examples (N), the number of classes (C), and the percentage of examples belonging to the majority class (%MajC).

Nro	OpenML name	OpenML did	D	N	C	%MajC
48	ilpd	1480	10	583	2	0.71
49	ionosphere	59	33	351	2	0.64
50	iris	61	4	150	3	0.33
51	kr-vc-kp	3	36	3196	2	0.52
52	LED-display-domain-7digit	40496	7	500	10	0.11
53	lsvt	1484	310	126	2	0.67
54	mammography	310	5	961	2	0.54
55	meta	566	21	528	24	0.04
56	mfeat-fourier	14	76	2000	10	0.10
57	micro-mass	1514	1300	360	10	0.10
58	molecular-biology-promoters	164	57	106	2	0.50
59	splice	46	62	3190	3	0.52
60	monks-problems-1	333	6	556	2	0.50
61	monks-problems-2	334	6	601	2	0.66
62	monks-problems-3	335	6	554	2	0.52
63	libras-move v.2	40736	90	360	15	0.07
64	mfeat-factors	12	217	2000	10	0.10
65	mushroom	24	21	8124	2	0.52
66	nursery (v.3)	1568	9	12958	4	0.33
67	optdigits	28	62	5620	10	0.10
68	ozone-level-8hr	1487	72	2534	2	0.94
69	ozone_level v.2	40735	72	2536	2	0.97
70	page-blocks	30	10	5473	5	0.90
71	parkinsons	1488	22	195	2	0.75
72	phoneme	1489	5	5404	2	0.71
73	one-hundred-plants-margin	1491	65	1600	100	0.01
74	one-hundred-plants-shape	1492	65	1600	100	0.01
75	one-hundred-plants-texture	1493	65	1599	100	0.01
76	wall-robot-navigation v.3 (version 3)	1526	4	5456	4	0.40
77	sa-heart	1498	9	462	2	0.65
78	seeds	1499	7	210	3	0.33
79	semeion	1501	257	1593	10	0.10
80	credit-g	31	20	1000	2	0.70
81	heart-statlog	53	13	270	2	0.56
82	segment	36	18	2310	7	0.14
83	satellite_image v.2	40734	36	2859	6	0.30
84	vehicle	54	18	846	4	0.26
85	steel-plates-fault	1504	33	1941	2	0.65
86	tae	48	5	151	3	0.34
87	texture	40499	40	5500	11	0.09
88	thoracic-surgery	1506	16	470	2	0.85
89	thyroid-allbp	40474	26	2800	5	0.58
90	thyroid-allhyper	40475	26	2800	5	0.58
91	user-knowledge	1508	6	403	5	0.32
92	vertebra-column	1523	6	310	3	0.48
93	wine	187	14	178	3	0.39
94	yeast (version v.7)	40733	8	1484	4	0.36