Better Trees: An empirical study on hyperparameter tuning of classification decision tree induction algorithms

Rafael Gomes Mantovani¹, Tomáš Horváth²,³, André L. D. Rossi⁴, Ricardo Cerri⁵, Sylvio Barbon Junior⁶, Joaquín Vanschoren⁷ and André C. P. L. F. de Carvalho⁸

¹Federal Technology University, Paraná, Campus of Apucarana, Apucarana, PR, Brazil.
²Pavol Jozef Šafárik University, Faculty of Science, Institute of Computer Science, Košice, Slovakia.
³ELTE Eötvös Loránd University, Faculty of Informatics, Budapest, Hungary.
⁴São Paulo State University (Unesp), Campus of Itapeva, Itapeva, SP, Brazil.
⁵Department of Computer Science, Federal University of São Carlos, São Carlos, SP, Brazil.
⁶University of Trieste (UniTS), Trieste, Italy.
⁷Eindhoven University of Technology (TU/e), Eindhoven, The Netherlands.
⁸Institute of Mathematics and Computer Sciences (ICMC), University of São Paulo (USP), São Carlos, SP, Brazil.

Contributing authors: rafaelmantovani@utfpr.edu.br; tomas.horvath@inf.elte.hu; andre.rossi@unesp.br; cerri@ufscar.br; sylvio.barbonjunior@units.it; j.vanschoren@tue.nl; andre@icmc.usp.br;

Abstract

Machine learning algorithms often contain many hyperparameters whose values affect the predictive performance of the induced models in intricate
Better Trees

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 performance. However, insights into efficiently exploring this vast space of configurations and dealing with the trade-off between predictive and runtime performance remain challenging. Furthermore, there are cases where the default hyperparameters fit the suitable configuration. Additionally, for many reasons, including model validation and attendance to new legislation, there is an increasing interest in interpretable models, such as those created by the Decision Tree (DT) induction algorithms. This paper provides a comprehensive approach for investigating the effects of hyperparameter tuning for the two DT induction algorithms most often used, CART and C4.5. DT induction algorithms present high predictive performance and interpretable classification models, though many hyperparameters need to be adjusted. Experiments were carried out with different tuning strategies to induce models and to evaluate hyperparameters’ relevance using 94 classification datasets from OpenML. The experimental results point out that different hyperparameter profiles for the tuning of each algorithm provide statistically significant improvements in most of the datasets for CART, but only in one-third for C4.5. Although different algorithms may present different tuning scenarios, the tuning techniques generally required few evaluations to find accurate solutions. Furthermore, the best technique for all the algorithms was the Irace. Finally, we found out that tuning a specific small subset of hyperparameters is a good alternative for achieving optimal predictive performance.

**Keywords:** Decision tree induction algorithms, Hyperparameter tuning, Hyperparameter profile, J48, CART

1 Introduction

As a consequence of the growing concerns regarding the development of responsible and ethical Artificial Intelligence (AI) solutions and the attendance of the requirements of new AI-related legislation, such as the General Data Protection Regulation (GDPR) (European Commission, 2016), model interpretability has become an essential issue in the AI research agenda. Thus, when selecting a Machine Learning (ML) algorithm for a new classification task, good predictive performance coupled with easy model interpretation favors the Decision Tree (DT) induction algorithms (Rokach and Maimon, 2014). 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 interpretable than many other model representations, such as an Artificial Neural Network (ANN) (Haykin, 2007) or...
Support Vector Machines (SVMs) (Abe, 2005). As a result, DT induction algorithms are among the most frequently used ML algorithms for classification tasks (Jankowski and Jackowski, 2014; Wu and Kumar, 2009).

**Fig. 1**: Example of a decision tree classification. When unlabeled data is provided to the tree, conditions are applied starting from the root node and following the appropriate branch until a leaf is reached. The class is recommended based on the leaf pointed out. Adapted from Tan et al (2005).

DT algorithms have several other advantages over many ML algorithms, such as robustness to noise, tolerance against missing information, capability to handle various types of attributes, treatment of irrelevant and redundant attributes, and low computational cost (Rokach and Maimon, 2014). Their importance is attested by the wide range of well-known algorithms proposed in the literature, such as Breiman et al.'s Classification and Regression Tree (CART) (Breiman et al, 1984) and Quinlan's C4.5 algorithm (Quinlan, 1993), as well as some hybrid-variants of them, like Naïve-Bayes Tree (NBTree) (Kohavi, 1996), Logistic Model Tree (LMT) (Landwehr et al, 2005) and Conditional Inference Trees (CTree) (Hothorn et al, 2006), to name a few.

Similarly to most ML algorithms, DT induction algorithms might improve their performance through hyperparameters setup. Due to the high number of possible configurations and their significant influence on the predictive performance of the induced models, hyperparameter tuning is often warranted (Bergstra et al, 2011; Massimo et al, 2016; Pilát and Neruda, 2013; Padierna et al, 2017). Moreover, highly accurate DT induction algorithms grounded on pre-prune (e.g., CTree and CHAID) or post-prune (e.g., C4.5,
J48 and CART) strategies demand setting up appropriate hyperparameter settings since inaccurate ones lead to under-fitting or over-fitting problems (Loh, 2014). The tuning task is usually performed to “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 (Barros et al, 2012, 2015), but only a few on hyperparameter tuning (Molina et al, 2012; Reif et al, 2011, 2014).

Alternatively, the default hyperparameter values suggested in the vastest most vast of DT implementations might support effective predictive performance in ordinary classification problems. Furthermore, the tuning execution does not guarantee improvements over the default values at the cost of extra computational effort.

Shedding light on the effects of the hyperparameter tuning, in this paper, we investigated the hyperparameter profile of DT induction algorithms by evaluating their predictive performance and analyzing their convergence during the tuning procedure. We conducted experiments to answer the following research questions:

1. Is HP tuning of DT really necessary?
2. When performing HP tuning, which are the most recommended techniques to perform such a task regarding predictive performance and computational time?
3. Which HPs most impact DT predictive performance?
4. When to tune?

For such, two DT of the most popular decision tree induction algorithms (Wu and Kumar, 2009) were chosen as study cases: the J48 algorithm, a WEKA (Witten and Frank, 2005) implementation for the Quinlan’s C4.5 (Quinlan, 1993); and the Breiman et al (1984)’s CART algorithm Breiman et al (1984). A total of six different hyperparameter tuning techniques (following different learning biases) were benchmarked in the experiments: a simple Random Search (RS), three commonly used meta-heuristics - Genetic Algorithm (GA) (Goldberg, 1989), Particle Swarm Optimization (PSO) (Kennedy and Eberhart, 1995), and Estimation of Distribution Algorithm (EDA) (Hauschild and Pelikan, 2011), Sequential Model-based Optimization (SMBO) (Snoek et al, 2012), and Iterated F-race (Irace) (Birattari et al, 2010)\(^1\). 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 and CART.

In addition, we also assess the relative importance of DT hyperparameters, measured using a recent functional ANOVA framework (Hutter et al, 2014). In all, the main contributions of this study are:

1. Provide further evidence of the need to perform HP tuning for DT for some cases;

\(^1\)These techniques will be described on the following sections.
2. Large-scale comparison of different hyperparameter tuning techniques for DT induction algorithms;
3. Comprehensive analysis of the hyperparameter profile of DT induction algorithms, especially the effect of hyperparameters on the predictive performance of the induced models and the relationship between them;
4. Present simple rules to users to decide when to tune DT HPs.

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 (Vanschoren et al, 2014).

The current study collectively highlights the importance of using DTs for interpretability and explainability in ML models. Literature also reports recent research in this direction. For example, Blanco-Justicia and Domingo-Ferrer (2019); Blanco-Justicia et al (2020) propose using DTs as surrogate models to explain black-box models, achieving a trade-off between comprehensibility and representativeness. Vieira and Digiampietri (2020) focus on understanding the decisions made by SVMs classifiers using DTs as interpretable models. Ribeiro et al (2016) argue for model-agnostic interpretability approaches, treating ML models as black-box functions and providing flexibility in model choice, explanations, and representations. These papers emphasize the need for explainability in critical AI applications and the benefits of DT in achieving interpretability and trust in ML models.

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 7 validates the results of this study. Finally, Section 8 summarizes our findings and highlights future avenues of research.

2 Related work

Many 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 (Gomes et al, 2012) and ANNs (Bergstra and Bengio, 2012); or ensemble algorithms, such as Random Forest (RF) (Reif et al, 2012; Huang and Boutros, 2016) and Boosting Trees (Eggensperger et al, 2015; Wang et al, 2015). They often tune the hyperparameters by using simple techniques, such as Pattern Search (PS) (Eitrich and Lang, 2006) and Random Search (RS) (Bergstra and Bengio, 2012), but also more sophisticated ones, such as meta-heuristics (Gascón-Moreno et al, 2011; Gomes et al, 2012; Nakamura et al, 2014; Ridd and Giraud-Carrier, 2014; Padierna et al, 2017), SMBO (Bergstra et al, 2011; Bardenet et al, 2013), racing algorithms (Lang et al, 2015; Miranda et al, 2014) and Meta-learning (MtL) (Feurer et al, 2015b). However, when considering DT induction algorithms, far fewer studies are available.
Recent work has also used meta-heuristics to design new DT induction algorithms combining components of existing ones (Barros et al., 2015; Podgor- elec et al., 2015). The existing components restrict the algorithms created, 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 3)\(^2\), 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 (2008) presented a benchmark of four different open-source DT induction algorithm implementations, one being J48. This study assessed the algorithm’s 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 ($M$).

Sureka and Indukuri (2008) 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 hyperparameters, ranges, datasets, or evaluation procedures were used to assess the hyperparameter settings. Experiments showed that the algorithm can find good solutions but requires massive computational resources to evaluate all possible models.

Stiglic et al (2012) 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 (Bache and Lichman, 2013) and 30 bioinformatics datasets demonstrated a significant increase in accuracy in visually tuned DTs, when compared with defaults. In contrast to classical ML datasets, bioinformatics datasets had higher gains.

Lin and Chen (2012) 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,

\(^2\)The original J48 nomenclature may also be consulted at [http://weka.sourceforge.net/doc.dev/weka/classifiers/trees/J48.html](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                        | Year | Hyperparameters | Tuning Technique | Datasets Number Source |
|----------------------------------|------|-----------------|------------------|------------------------|
| Schauerhuber et al (2008)        | 2008 | ● ●             | GS               | 18 UCI                 |
| Sureka and Indukuri (2008)       | 2008 |                 | GA               | - -                    |
| Stiglic et al (2012)             | 2012 | ● ● ● ● ●       | VTJ48            | 71 UCI                 |
| Lin and Chen (2012)              | 2012 | ● ●             | SS               | 23 UCI                 |
| Ma (2012)                        | 2012 | ● ●             | GP               | 70 UCI                 |
| Molina et al (2012)              | 2012 | ● ●             | GS               | 14 -                   |
| Sun and Pfahringer (2013)        | 2013 | ●               | PSO              | 466 -                  |
| Reif et al (2014)                | 2014 | ●               | GS               | 54 UCI                 |
| Fernández-Delgado et al (2014)   | 2014 | ● ●             | -                | 121 UCI                |
| Wainberg et al (2016)            | 2016 | ● ●             | -                | -                      |
| Kotthoff et al (2016)            | 2016 | ● ● ● ● ● ● ● ● | SMBO             | 21 -                   |
| Sabharwal et al (2016)           | 2016 | ● ●             | DAUP             | 6 -                    |
| Tantithamthavorn et al (2016)    | 2016 | ●               | caret            | 18 -                   |
### 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                      | Year | cp | min split | Hyperparameter | max bucket | max depth | weights | min leaf | max leaf | max feat | Technique | Number | Source |
|--------------------------------|------|----|-----------|----------------|------------|-----------|---------|----------|----------|----------|-----------|--------|--------|
| Schauerhuber et al (2008)     | 2008 | •  |           |                |            |           |         |          |          |          | GS        | 18     | UCI    |
| Sun and Pfahringer (2013)      | 2013 | •  |           |                |            |           |         |          |          |          | PSO       | 466    | -      |
| Fernández-Delgado et al (2014) | 2014 | •  |           |                |            |           |         |          |          |          | -         | 121    | UCI    |
|                                 | 2016 | •  |           |                |            |           |         |          |          |          | -         |        |        |
| Wainberg et al (2016)          | 2015 | •  |           |                |            |           |         |          |          |          | RS        | 36     | UCI    |
| Bermúdez-Chacón et al (2015)   | 2015 | •  |           |                |            |           |         |          |          |          | SH        |        |        |
| Feurer et al (2015a)           | 2015 | •  |           |                |            |           |         |          |          |          | SMBO      | 140    | OpenML |
| Lévesque et al (2016)          | 2016 | •  |           |                |            |           |         |          |          |          | SMBO      | 18     | UCI    |
| Tantithamthavorn et al (2016)  | 2016 | •  |           |                |            |           |         |          |          |          | caret     | 18     | various |
| Probst et al (2019)            | 2019 | •  |           |                |            |           |         |          |          |          | RS        | 38     | OpenML |
| Bartz et al (2021)             | 2021 | •  |           |                |            |           |         |          |          |          | SMBO      | 1      | OpenML |
were better than those obtained by baselines (defaults, simple GA and a greedy combination of them). When feature selection is considered, most datasets’ classification accuracy rates increase.

Ma (2012) 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 (2016) 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 entire 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 meager computational cost compared to full training of all classifiers.

Tantithamthavorn et al (2016), investigated the performance of prediction models when tuning hyperparameters using “caret”\(^3\) from Jed Wing et al (2016), a ML tool. 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 AUC\(^4\) measure, the tuning produced better results.

Wainberg et al (2016) reproduced the benchmark experiments described in Fernández-Delgado et al (2014). 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 (Molina et al, 2012; Sun and Pfahringer, 2013; Reif et al, 2014; Kotthoff et al, 2016). 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. Molina et al (2012) 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 algorithms and HPs for each problem. The proposed approach, however, did not improve the performance of the DTs with defaults.

Sun and Pfahringer (2013) 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

\(^3\)https://cran.r-project.org/web/packages/caret/index.html

\(^4\)Area under the ROC curve
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 (2014) 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 Thornton et al (2013) as the Auto-WEKA\(^5\) framework, and updated recently in Kottke et al (2016). Auto-WEKA applies SMBO (see Section 3.2) to select an algorithm and its hyperparameters to new problems based on a comprehensive 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. The table presents which hyperparameters, tuning techniques, and the number and source of datasets explored in the experiments for each study.

In Schauerhuber et al (2008), the authors added CART/rpart to their benchmark analysis. They manually tuned only the complexity parameter ‘cp’. Sun et. al. Sun and Pfahringer (2013) 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 (2016), the authors did a similar study but focused on the complexity parameter ‘cp’.

In Bermúdez-Chacón et al (2015), 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 leaves (‘maxleafs’) and the maximum number of features from dataset used in trees (‘maxfeatures’).

\(^5\)http://www.cs.ubc.ca/labs/beta/Projects/autoweka/
In Feurer et al (2015a), the authors used the SMBO approach to select and tune algorithm from the “scikit learn”\(^6\) framework, hence Auto-skLearn\(^7\). The only DT induction algorithm covered here is CART. CART with some hyperparameters manually selected was also experimentally investigated in Fernández-Delgado et al (2014) and Wainberg et al (2016).

Lévesque et al (2016) 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: ‘\texttt{minsplit}’, ‘\texttt{minbucket}’, ‘\texttt{maxdepth}’ and the ‘\texttt{maxleaf}’. The tuning resulted in a significant improvement in generalization accuracy when compared with the Single Best Model Ensemble and Greedy Ensemble Construction techniques.

Probst et al (2019) formalize the problem of tuning from a statistical point of view. They have conducted experiments with 38 datasets from OpenML and six common ML algorithms, one of them is CART, and tuning all of them using a RS technique. Results reported enable users to decide whether conducting a possibly time-consuming tuning strategy is worthwhile. Bartz et al (2021) have performed a similar experiment, but considering a single dataset: CID from OpenML. In this study, the authors’ focus was on providing useful scripts in R that could be used by experts and non-experts when performing tuning of ML algorithms.

2.3 Literature Overview

The literature review indicates that hyperparameter tuning for DT induction algorithm could be more deeply explored. We found eleven studies investigating tuning for the J48 algorithm and nine for CART. 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 seeds\(^8\); and
- some studies did not even describe the experimental methodology used.

Regarding the search space, most studies concerning C4.5/J48 and CART hyperparameter tuning investigated only a small subset of the hyperparameter search spaces (as shown in Tables 1 and 2). 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.

---

\(^6\)http://scikit-learn.org/
\(^7\)https://github.com/automl/auto-sklearn
\(^8\)Since the stochastic nature of the often used tuning algorithms, experimenting with different seeds (for random generator) is desirable.
This paper overcomes these limitations by investigating several techniques for DT hyperparameter tuning using a reproducible and consistent experimental methodology. It also analyzes the importance and relationships between many hyperparameters of the investigated algorithms (C4.5 and CART). These results increase awareness of the importance of tuning DT and provide guidance on performing this task considering two critical criteria: improve predictive performance while minimizing computation cost.

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 mainly depends on using the right hyperparameter values (Feurer et al, 2015a; Thornton et al, 2013). 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 (Bergstra et al, 2011).

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 $\mathcal{H} = \mathcal{H}_1 \times \mathcal{H}_2 \times \cdots \times \mathcal{H}_k$ 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 $a$ ($i \in \{1, \ldots, k\}$) and can be usually defined by a set of constraints. Additionally, let $\mathcal{D}$ be a set of datasets where $D \in \mathcal{D}$ is a dataset from $\mathcal{D}$. The function $f : \mathcal{A} \times \mathcal{D} \times \mathcal{H} \to \mathbb{R}$ measures the predictive performance of the model induced by the algorithm $a \in \mathcal{A}$ on the dataset $D \in \mathcal{D}$ given a hyperparameter configuration $h = (h_1, h_2, \ldots, h_k) \in \mathcal{H}$. Without loss of generality, higher values of $f$ mean higher predictive performance.

Given an algorithm $a \in \mathcal{A}$, its hyperparameter space $\mathcal{H}$ and a dataset $D \in \mathcal{D}$, the goal of hyperparameter tuning is to find $h^* = (h_1^*, h_2^*, \ldots, h_k^*)$ such that

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

(1)

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, such as:

- 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;
hyperparameters often depend on each other (as in the case of SVMs (Benn-Hur and Weston, 2010)). Hence, independent tune of hyperparameters may not lead to good settings; 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 (Bardenet et al, 2013). When applied to tuning, these techniques (iteratively) build a population $\mathcal{P} \subset \mathcal{H}$ of hyperparameter settings for which $f(a, D, h)$ are being computed for each $h \in \mathcal{P}$. 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 a large number of possible settings are being investigated (Andradottir, 2015). 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 $h' \in \mathcal{H}$ in each ($i$th) iteration of the hyperparameter tuning process. RS has obtained efficient results in optimization for Deep Learning (DL) algorithms (Bergstra and Bengio, 2012; Bardenet et al, 2013).

### 3.2 Sequential Model Based Optimization

Sequential Model-based Optimization (SMBO) (Snoek et al, 2012) 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 $h'$, such that the expected value of $f(a, D, h')$ is maximal according to an induced meta-model $\hat{f}$ approximating $f$ on the current population $\mathcal{P}_{i-1}$. In Bergstra et al (2011); Snoek et al (2012); Bergstra et al (2013), 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 (Gomes et al, 2012). In these techniques, the initial population $\mathcal{P}_0 = \{h_1, h_2, \ldots, h_{n_0}\}$, 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 (Simon, 2013). In case of PSO, each particle $h \in P_0$ is associated with its position $h = (h_1, \ldots, h_k) \in H$ in the search space $H$, a velocity $v_h \in \mathbb{R}^k$ and also its so far best found position $b_h \in H$. During iterations, the movements of each particle are changed according to its so far best-found position as well as the so far best-found position $w \in H$ of the entire swarm (recorded through the computation).

3.5 Estimation of Distribution Algorithm

Estimation of Distribution Algorithm (EDA) (Hauschild and Pelikan, 2011) 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) (Birattari et al, 2010) technique was designed for algorithm configuration and optimization problems (Lang et al, 2015; Miranda et al, 2014) based on ‘racing’. One race starts with an initial population $P_0$, iteratively selects the most promising candidates considering the hyperparameter distributions and compares them by statistical tests. Configurations statistically worse than at least one of the 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.

3.7 Other recent techniques

Recently, new optimization/tuning techniques have also been proposed. One that stands out is Hyperband (Li et al, 2018). Hyperband is an early-stopping method that adaptively allocates some predefined resource (iterations, data samples, or features) to randomly sampled configurations. Then, models are trained with each configuration, and the technique stops training configurations that perform poorly while allocating additional resources to promising configurations. The key concept here is the successive halving: half of the configurations are thrown out at each iteration based on performance. The top-best are kept and trained with a new budget. The process is repeated until one configuration remains.

In Falkner et al (2018), the authors proposed a new technique called Bayesian Optimization with HyperBand (BOHB), combining Bayesian Optimization and Hyperband. Unlike Hyperband, which proposes hyperparameter configurations randomly, BOHB uses a model-based approach equivalent to maximizing expected improvement. The authors also showed empirically that
BoHB performs similarly to Hyperband in low-budget executions but outperforms both methods (SMBO and Hyperband) when enough budget are available\textsuperscript{9}.

4 Experimental methodology

The experimental methodology employed to analyze the hyperparameter tuning of DT is illustrated by Figure 2. It follows the nested Cross-validation (CV) (Cawley and Talbot, 2010; Krstajic et al, 2014) resampling procedure. For each dataset, data are split into \( M \) outer-folds. For each iteration, the tuning techniques use \( M - 1 \) folds to find hyperparameter settings that aim to improve the models’ predictive performance, while the remaining fold is used to assess the ‘optimal’ solution found. Internally, the tuning techniques merge the \( M - 1 \) folds and split them to \( N \) inner-folds, used in a simple CV procedure to train the models and assess their predictive performance (fitness) for each 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 Krstajic et al (2014), the authors defined \( M = N = 10 \). However, they argued that there is no rule on choosing the number of folds in the outer and inner CV loops. Here, we have also used \( M = 10 \), but due to time constraints and the size of datasets used in experiments, \( N = 3 \) was adopted. The following subsections detail the sub-components used in the tuning task.

4.1 Hyperparameter spaces

The experiments were performed considering the hyperparameter tuning of two DT induction algorithms: the ‘J48’ algorithm, a \textsc{Weka}\textsuperscript{10} (Witten and Frank, 2005) implementation of the C4.5 algorithm; and the \textsc{rpart} implementation of the CART (Breiman et al, 1984) algorithm. These algorithms were selected due to their wide acceptance and use in many ML applications (Barros et al, 2012; Rokach and Maimon, 2014; Jankowski and Jackowski, 2014). Furthermore, both algorithms are among the most used in ML, especially by non-expert users (Wu and Kumar, 2009). The correspondent hyperparameter spaces investigated are described in Table 3.

Originally, J48 has ten tunable hyperparameters\textsuperscript{11}: all presented at Table 3 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. Regarding CART, all the tunable hyperparameters in \textsc{rpart} were selected.

\textsuperscript{9}For a complete survey on hyperparameter tuning techniques and perspectives, please, consult Bischl et al (2023).
\textsuperscript{10}http://www.cs.waikato.ac.nz/ml/weka/
\textsuperscript{11}http://weka.sourceforge.net/doc.dev/weka/classifiers/trees/J48.html
Fig. 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.
Table 3: Decision Tree hyperparameter spaces explored in the experiments. The J48 nomenclature is based on the `RWeka` package, and the CART terms is based on the `rpart` package.

| Algorithm | Symbol | Hyperparameter | Range     | Type | Default | Conditions |
|-----------|--------|----------------|-----------|------|---------|------------|
| J48       | C      | pruning confidence | (0.001, 0.5) | real | 0.25    | R = False  |
|           | M      | minimum number of instances in a leaf | [1, 50] | integer | 2        |            |
|           | N      | number of folds for reduced error pruning | [2, 10] | integer | 3        | R = True  |
|           | O      | do not collapse the tree | {False, True} | logical | False   |            |
|           | R      | use reduced error pruning | {False, True} | logical | False   |            |
|           | B      | use binary splits only | {False, True} | logical | False   |            |
|           | S      | do not perform subtree raising | {False, True} | logical | False   |            |
|           | A      | Laplace smoothing for predicted probabilities | {False, True} | logical | False   |            |
|           | 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    |            |
|           | minsplit | minimum number of instances in a node for a split to be attempted | [1, 50] | integer | 20      |            |
|           | minbucket | minimum number of instances in a leaf | [1, 50] | integer | 7       |            |
|           | maxdepth | maximum depth of any node of the final tree | [1, 30] | integer | 30      |            |
|           | usesurrogate | how to use surrogates in the splitting process | {0, 1, 2} | factor | 2       |            |
|           | surrogatetstyle | controls the selection of the best surrogate | {0, 1} | factor | 0       |            |
For each hyperparameter, Table 3 shows the allowed range of values, default values provided by the correspondent R packages, and its constraints for setting new values. The range of values for the hyperparameter $M$ is the same used in Reif et al (2011). The pruning confidence ($C$) hyperparameter range was adapted from Reif et al (2014) because the algorithm internally controls the parameter values, not allowing some values near zero or $C \geq 0.5$.

4.2 Datasets

The experiments were carried out using 94 public datasets from the Open Machine Learning (OpenML) (Vanschoren et al, 2014) website, 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 the 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 B1 to B5 at Appendix B.

4.3 Hyperparameter tuning techniques

Six hyperparameter tuning techniques were investigated:

- three different meta-heuristics: a Genetic Algorithm (GA) (Goldberg, 1989), Particle Swarm Optimization (PSO) (Kennedy and Eberhart, 1995) and an Estimation of Distribution Algorithm (EDA) (Hauschild and Pelikan, 2011). These techniques are often used for hyperparameter tuning of ML classification algorithms in general (Gascón-Moreno et al, 2011; Yang et al, 2013);
- a simple Random Search (RS) technique: suggested by Bergstra and Bengio (2012) as a good alternative for hyperparameter tuning replacing Grid Search (GS) technique;
- Iterated F-race (Irace) (Birattari et al, 2010): a racing technique designed for algorithm configuration problems; and
- a Sequential Model-based Optimization (SMBO) (Snoek et al, 2012) technique: a state-of-the-art technique for optimization that employs statistical and/or ML techniques to predict distributions over labels and allows a more direct and faster optimization.

Table 4 summarizes the choices to accomplish the general hyperparameter tuning techniques. Experiments were coded and executed with the R language. Most of the experiments were implemented using the mlr package (Bischl et al, 2016) (measures, resampling strategies, tuning main processes and RS technique). The GA, PSO and EDA meta-heuristics were implemented using

\[ \text{http://www.openml.org/} \]
\[ \text{Initially, there were 100 datasets, but 6 of them spent too much time to finish their tuning jobs. They consumed over 1000 hours when we proceeded with their interruption.} \]
\[ \text{https://github.com/mlr-org/mlr} \]
Table 4: 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       |
| Baseline                       | Default values (DF)           | RWeka       |
|                                |                               | rpart       |
| Decision Trees                 | J48 algorithm                 | RWeka       |
|                                | CART algorithm                | rpart       |
| Resampling                     | Outer: 10-fold CV             | mlr         |
|                                | Inner: 3-fold CV              |             |
| Optimized measure              | {Balanced per class Accuracy (BAC)} |             |
| Evaluation measure             | {Balanced per class Accuracy (BAC), Optimization paths } | mlr |
| Budget                         | 900 evaluations               | -           |
| Repetitions                    | 30 times with different seeds | -           |
|                                | seeds = \{1, \ldots, 30\}   |             |
| Statistical Evaluation         | Wilcoxon \( \alpha = 0.05 \) | stats       |

Since the experiments handle many 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) (Brodersen et al, 2010), is used for model evaluation.

When tuning occurs in real scenarios, time is a crucial aspect to be considered. Sometimes, the tuning process may take many hours to find good settings for a single dataset (Reif et al, 2012; Ridd and Giraud-Carrier, 2014). Thus, this study investigates whether it is possible to find the same good settings

The GA\(^{15}\) (Scrucca, 2013), pso\(^{16}\) (Bendtsen., 2012), and copulaedas\(^{17}\) (Gonzalez-Fernandez and Soto, 2014) packages, respectively. The J48 and CART algorithms were implemented using the RWeka\(^{18}\) (Hornik et al, 2009), and rpart\(^{19}\) (Therneau et al, 2015) packages, respectively, wrapped into the mlr package. The SMBO technique was implemented using the mlrMBO\(^{20}\) package, with its RF surrogate models implemented by the randomForest\(^{21}\) package (Liaw and Wiener, 2002). The Irace technique was implemented using the irace\(^{22}\) (López-Ibáñez et al, 2016) package.
Table 5: Tuning techniques hyperparameters. Excepting the budget-dependent hyperparameters all of them are the defaults provided by each R package implementation.

| Tuning Technique | Hyperparameters                  | Value                                      |
|------------------|----------------------------------|--------------------------------------------|
| RS               | stopping criteria                | budget size                                |
| PSO              | number of particles              | 10                                         |
|                  | maximum number of iterations     | 90                                         |
|                  | stopping criteria                | budget size                                |
|                  | algorithm implementation         | SPSO2007 (Clerc, 2012)                     |
| EDA              | number of individuals            | 10                                         |
|                  | maximum number of iterations     | 90                                         |
|                  | stopping criteria                | budget size                                |
|                  | EDA implementation              | GCEDA                                      |
|                  | copula function                 | normal                                     |
|                  | margin function                 | truncnorm                                  |
| GA               | 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                              |
|                  | infill criteria                 | budget size                                |
|                  | infill criteria                 | expected improvement                       |
| Irace            | number of instances for resampling | 100                                      |
|                  | stopping criteria               | budget size                                |

faster by using a reduced number of evaluations (budget). Based on previous results and analyses (Mantovani et al, 2016), a budget size of 900 evaluations was adopted in the experiments²³.

Since all techniques are stochastic, each one was executed 30 times for each dataset using different seed values. It gives a total of $270,000 = 30$ (replications) $\times 10$ (outer-folds) $\times 900$ (budget) HP-settings generated during the search process for one single dataset. So, we evaluated a total of 25,380,000 hyperparameter configurations, considering all the 94 datasets. Besides, the default hyperparameter values provided by the ‘RWeka’ and ‘rpart’ 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 and the recursive problem of tuning the tuning techniques, the authors decided to use their default values. Each tuning technique has a different set of hyperparameters, which are specific and different considering each technique’s paradigm. In the SMBO, Irace and

²³The budget size choice is discussed with more details in Section 7.
PSO cases, the use of the defaults has been shown robust enough to save time and resources (Zambrano-Bigiarini et al, 2013; López-Ibáñez et al, 2016). For EDA and GA (and evolutionary methods in general), there are no standard values for their parameters (Mills et al, 2015). So, to keep fair comparisons, the default parameter values provided by the correspondent R packages were used. These values may be seen in Table 5.

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

Details of the hyperparameter tuning experiments are publicly available in an OpenML Study (id 50). All datasets, classification tasks, and algorithms/flows are listed on the corresponding pages and available for reproducibility. The code used for the tuning process (HpTuning), running meta-learning (mtlSuite), and performing the graphical analyses (DecisionTreeTuningAnalysis) are hosted at GitHub. These repositories are also listed in Table 6. Instructions to run each project may be found directly at the correspondent websites.

Table 6: Repositories with tools developed by the authors and results generated by experiments.

| Task/Experiment               | Website/Repository                                      |
|-------------------------------|---------------------------------------------------------|
| Hyperparameter tuning code    | https://github.com/rgmantovani/HpTuning                 |
| Hyperparameter tuning tasks   | https://www.openml.org/s/50                             |
| Meta-learning code            | https://github.com/rgmantovani/mtlSuite                 |
| Graphical Analysis            | https://github.com/rgmantovani/DecisionTreeTuningAnalysis |

5 Hyperparameter tuning of decision trees

This section presents the results and analysis of optimizing the hyperparameters of DT algorithms. These empirical findings aim to provide a comprehensive understanding of tuning the hyperparameter values for decision trees and offer guidance on the most effective techniques to perform this task while considering the criteria of improving predictive performance and minimizing computation cost.

The population size = 10 might be small initially, but it proves to be enough to provide good and accurate results as empirically evaluated in Mantovani et al (2016).
5.1 Is hyperparameter tuning necessary for decision trees?

Tuning results for J48 and CART algorithms are depicted in Figure 3 and Figure 4, respectively. These figures show the predictive performance in terms of BAC values averaged over the 30 repetitions (y-axis), for each tuning technique and default values over all datasets (x-axis) presented in decreasing order of the default results. The name of the tuning technique that achieved the best predictive performance is shown above the x-axis for each dataset. 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 (▲) 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 (▼) is presented, the use of defaults was statistically better than the use of tuning techniques.

Tuning the HP values of J48 (Fig. 3) has not led to patent improvements in predictive performance for most of the datasets. In general, the small peaks of improvements due to hyperparameter tuning show that default values are inappropriate for specific cases. This occurred, for instance, for the datasets with the ids = {36, 46, 61, 88}. When the Wilcoxon statistical paired-test is applied, comparing defaults with the best tuning technique, they show that tuned trees were better overall 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). Additionally, all tuning techniques presented similar performances, with few exceptions, since most curves overlap.

On the other hand, the CART algorithm benefits most by hyperparameter tuning. For most of the datasets analyzed, the use of tuned settings improved the predictive performance with statistical significance when compared with the use of default values in 62/94 ($\approx 66\%$) of the cases. Default values were better than tuned ones in 14/94 ($\approx 15\%$) of the cases, while there was no significant statistical in the remaining (18/94) datasets. It must be observed that the Irace and SMBO were the best optimization techniques, regarding just the predictive performance of the induced models.

Figure 5 compares obtained performance of the default HP settings against the optimized ones for both DT induction algorithms. The performance values obtained by the default HPs are projected in the x-axis and the optimized values in the y-axis. Different shapes and colors represent different tuning techniques. The dotted black line represents the reference where defaults and optimized performances would be equal. Thus, points above the line indicate tuning provided improvements, while points below indicate worsening. Comparing both figures, we can see slightly different patterns. J48 points are mostly
Better Trees

**Fig. 3:** Hyperparameter tuning results for the J48 algorithm.

**Fig. 4:** Hyperparameter tuning results for the CART algorithm.

concentrated around the dotted black line (above and below). Some exceptions exist where tuning solutions obtained high improvements, especially for datasets with defaults obtained BAC values higher than 0.5. Conversely, CART points are mostly above the black line, showing that tuning benefits a wider range of datasets.

In addition to evaluating predictive performance, we also analyzed the effect of tuning techniques on tree size, which is given by the number of nodes in the final model. It is important to mention that the tree’s interpretability mostly depends on its size. Thus, larger trees are usually more difficult to understand than smaller ones. The tree sizes for J48 and CART algorithms are shown in Figure 6 and Figure 7, respectively. The order of the datasets in these figures is the same as that of the models’ BAC, and line colors represent the same tuning techniques.

Regarding the J48, in most cases, default values (dotted black line) induced trees larger than those obtained by the hyperparameters suggested by tuning techniques. For most of the multi-class problems (datasets most to the right on the charts), the tuned trees were also smaller than those induced using default values. Conversely, for the CART algorithm, the trees induced with tuned HP settings have similar or larger sizes than those induced by default values. 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.

These results might reflect a biased design related to the origin of the DT induction algorithms. CART (Breiman et al, 1984) was first developed by statisticians, who, at the time, had more interest in interpretable small but maybe underfitting trees. On the other hand, C4.5 (J48) (Quinlan, 1993) was developed by computer scientists mainly concerned with maximum accuracy. Figures 3 to 7 corroborate this bias, showing that default HP values define different hyperparameter profiles for these algorithms: J48 trees tend to be
deeper and more accurate at the same time CART trees are shallower and not so accurate compared with their tuned versions.

The CART hyperparameters’ distributions found by the tuning techniques are presented in Figure C2. Again, unlike 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 Figures C2 (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 Figures C2 (e) and (f), are very uniform, indicating that their choices may not influence the final predictive performance and could even act as “noise” when tuning is performed.

5.2 Which hyperparameter tuning technique should I use?

Considering that hyperparameter tuning may improve predictive performance (mainly for CART) and/or reduce tree size (mainly for J48), the practitioner has to decide which tuning technique to choose. The previous analyses suggest that most of the techniques have a similar behavior. In order to compare them across all datasets, we applied the Friedman test (Demšar, 2006), with significance levels at $\alpha = 0.05$ to evaluate 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 8 presents CD diagrams for the two DT induction algorithms. Techniques are connected when there are no statistically significant differences between them.

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

Fig. 8: Comparison of the BAC values of the hyperparameter tuning techniques according to the Nemenyi test. Groups of techniques that are not significantly different are connected.
Considering $\alpha = 0.05$, Figure 8(a) depicts the comparison for the J48 DT. One may note that there are no statistical differences between the top three best techniques: Irace, PSO, and SMBO. EDA and GA obtained statistically inferior performance. In addition, models induced with the HP found by the best three techniques were not statistically better than those induced by default values. This is in agreement with the analysis of the previous section, i.e., J48 does not generally benefit from performing HP tuning.

For the CART algorithm (Figure 8(b)), the best-ranked technique over all datasets was Irace, followed by RS, but with no statistical significance between them. RS has also no statistical difference with PSO, the third ranked technique here and the second for J48. Finally, DTs induced with default hyperparameter values obtained the worst performance and are statistically comparable only with GA and EDA. It is worth mentioning that Irace was the best tuning technique for both algorithms. At the same time, 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.

We can add another dimension to this analysis examining the performance of various tuning techniques over time (number of evaluations). This is performed through their rankings, which are determined based on the predictive performance achieved using the best hyperparameter settings found by each technique within a specific number of evaluations. Figure 9 shows the correspondent average rank (the smaller, the best) of each tuning technique over the evaluated budget (number of evaluations). Results are aggregated over all the 94 datasets.

Using the average ranking curve (Figure 9) a user may choose different techniques for tuning J48 according to the available budget size. For example, if tuning were performed with at most $b = 150$ evaluations, PSO and SMBO would be the best choices. With more than 200 evaluations ($b > 200$), Irace surpasses all the techniques.

Similar behavior can be observed regarding the average rankings for CART, i.e., different techniques are most suitable according to the budget size. If a tiny budget is provided ($b \leq 50$), PSO is slightly better than the other techniques. From $50 < b \leq 150$, the SMBO would be the best choice. On the other hand, with budgets ($b > 150$) Irace is the technique that best recommends values for CART HPs.

5.3 Which hyperparameters should be adjusted?

Another approach to evaluate how the HP are affecting the performance of the induced models when different tuning techniques are used is the use of fANOVA (Functional ANOVA framework)\textsuperscript{25}, introduced in Hutter et al (2014). In that paper, the authors present a linear-time algorithm for computing marginal predictions and quantify the importance of single

\textsuperscript{25}https://github.com/automl/fanova
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 for both algorithms, it was used to provide the HP to this analysis. The experiments used settings from 3 repetitions, and more memory was allocated to the fANOVA code.

Figure 11 shows the results for both DT algorithms. In the figure, the x-axis shows all datasets while the 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., the more important the hyperparameter is for inducing trees in the dataset (scaled between zero and one).
In the figure, any hyperparameter (or their combination) whose contribution to the performance of the final models was lower than 0.005 was removed. Applying this filter 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 combinations have little contribution to the performance of the induced DTs.

In Figure 11(a), fANOVA indicates that the J48 performance was most influenced by the hyperparameter $M$, alone or in combination with another hyperparameter ($R$, $N$ or $C$). The hyperparameter $M$ defines the minimum number of instances in a leaf, influencing the size of the trees (models). The lower its value, the larger the trees and the better the models. Similar reasoning can be made with the $C$ hyperparameter, which controls the pruning confidence of the pruning procedure. Depending on its value, the induction algorithm will prune the tree more or less, affecting the model’s size. This corroborates the earlier discussion conducted in Subsection 5.1.

Finally, the last two HPs ($R$, $N$) corroborate this hypothesis: $R$ is a HP that enables/disables the Reduced Error Pruning (REP) (Esposito et al, 1999). This post-pruning method finds the smallest version of the most accurate subtree concerning the pruning set. $N$ is its conditional HP that defines the number of inner folds used when post-pruning is enabled.
For CART, we observed the same behavior, but conducted by the ‘\texttt{minbucket}’ and ‘\texttt{minsplit}’ HPs. These HPs are mainly responsible for the performance of the induced DTs, as may be seen in Figure 11(b). The former HP is a counterpart of J48’s \( M \), and affects the size of the trees. The latter determines when a split must occur: the lower its value, the larger the tree since more splits are required. Therefore, \texttt{minsplit} is also related to J48 findings regarding the HP affecting the size of the tree. However, unlike J48, the HP values found by the tuning techniques for CART are substantially different from the default values. These achievements unveil results discussed in the previous subsections, showing that a small subset of hyperparameters seems to influence the final performance of the induced DTs and the models’ size. The major difference is that J48 default settings can generate bigger trees as necessary to improve its predictive performance.

6 In which situations tuning of trees should be required?

Considering that tuning the hyperparameters of DT can significantly improve the predictive performance for some problems, a step forward is to investigate whether it is possible to predict for which problems the tuning should be performed and understand how to make informed decisions. MtL and its “inherent interpretability” could be explored for this aim.

In recent years, Meta-learning (MtL) (Brazdil et al, 2009) has been largely used for algorithm selection (Ali and Smith-Miles, 2006), algorithm ranking (Kanda et al, 2016), prediction of the performance of ML algorithms (Reif et al, 2014), and development of AutoML tools (Feurer et al, 2020; Gijsbers and Vanschoren, 2021). MtL learns from many previous experiences, i.e., applying different learning algorithms to many datasets, inducing a model capable of selecting the most promising algorithm for a new dataset. MtL has also been used to explain the effect of noise filtering techniques (Garcia et al, 2019), data imbalancement (Barella et al, 2021), and when performing HP tuning (Sanders and Giraud-Carrier, 2017; Mantovani et al, 2019). Therefore, we adapted the MtL framework proposed by Mantovani et al (2019) to conduct experiments. The experimental setup is presented in Table 9 and explained as follows.

6.1 Meta-learning framework

Figure 12 depicts the general MtL framework to identify whether HP tuning for DTs is required or not. This framework has four sub-tasks: i) hyperparameter tuning, ii) meta-feature extraction, iii) statistical labeling rule, and iv) meta-learning prediction. Each of them will be explained in sequence.

6.1.1 Hyperparameter tuning task

HP tuning is performed across a collection of datasets. The output of this task is composed of two arrays: an array of the performances obtained through
the tuning and an array of the performances obtained with default HP values. Based on the results presented in Section 5, we enriched the “meta-knowledge” required for the MtL by performing additional hyperparameter tuning experiments. We selected 71 additional datasets, totaling 165 classification problems. The additional HP tuning jobs for J48 and CART were performed with a budget size of $b = 900$ evaluations and, using the Irace technique, executed 30 times with different seeds. It is important to mention that tuning jobs were only required for the datasets not included in previous experiments. Datasets whose results were already available did not need to be tuned again.

### 6.1.2 Meta-feature extraction

The second required sub-task runs some data descriptors to extract likely relevant characteristics (meta-features) from the datasets. These meta-features must be sufficient to describe the main aspects of the dataset necessary to distinguish the predictive performance obtained by defaults and tuned HP settings. Table 7 describes the main categories of the meta-features implemented by the pymfe Python library (Alcobaça et al, 2020). Here, we explored the measures from simple/general (simple) and data complexity (complex) besides the combination of the 80 measures from all categories presented in Table 7.

### 6.1.3 Statistical labeling task

In order to create each instance of the supervised problem at the meta-level, a label must be assigned to every dataset and combined with its respective meta-features. Hence, the third sub-task is a simple procedure that compares

---

**Fig. 12**: Meta-learning recommender system framework to predict when HP tuning is required or not for DTs. Adapted from Mantovani et al (2019).

---

26 These additional datasets are indicated in Appendix B

27 A complete list of the pymfe available meta-features can be found here: https://pymfe.readthedocs.io/en/latest/auto_pages/meta_features_description.html.
Table 7: Categories of meta-features used in meta-learning experiments

| Category                | #  | Description                                                                 |
|-------------------------|----|-----------------------------------------------------------------------------|
| Simple/General          | 17 | General measures about the input dataset, such as the number of (binary/categorical) attributes, examples and classes |
| Statistical             | 7  | Compute statistical descriptors about the input dataset, such as: minimum, maximum, mean and median values from each numerical attribute; skewness, kurtosis, correlation values, and so on. |
| Information-theoretic   | 8  | Information theory descriptors that measure: concentration of distinct attributes; entropy; mutual information; and noisiness of attributes. |
| Model-based (trees)     | 17 | A decision tree is applied to the dataset and statistics of nodes, leaves and branches are extracted. |
| Landmarking             | 8  | The predictive performance and runtime of simple ML algorithms              |
| Data Complexity         | 14 | Measures that analyze the complexity of a problem, such as the attributes values, the separability of the classes, and geometry/topological properties. |
| Complex Networks        | 9  | A complex network (graph) is built with the dataset’s instances and descriptors extracted from this graph: closeness and betweenness centralities, Hub score, average path length, and so on. |

Total 80

performance distributions through statistical tests. The Wilcoxon paired-test is applied with \( \alpha = 0.05 \) to compare models’ predictive performance using tuned and default HP settings. Thus, given a dataset, if its tuned solution was significantly better than the default, its corresponding label assumes class 0 (‘Tuning’), otherwise class 1 (‘Default’).

The labels yielded by this sub-task are concatenated with their corresponding meta-features to create a meta-dataset. Hence, each example (row) in the meta-dataset corresponds to a conventional dataset used in the tuning task and its corresponding label (‘Tuning’ or ‘Default’). Meta-features and labels compose the meta-knowledge of the MtL recommendation problem.

Two meta-datasets were generated, one for each DT algorithm. J48 meta-dataset has the Default class prevailing in two-thirds of the examples (datasets). CART presents the opposite scenario, with two-thirds of examples prevailing in the Tuning class. Table 8 summarizes meta-datasets’ main information, namely the number of meta-examples and meta-features, and the class distribution.

6.1.4 Meta-learning predictions

Finally, the fourth and last sub-task involves meta-learning training. A ML algorithm, referred to as meta-learner, is trained using a meta-dataset to predict whether tuning is required. We selected seven ML algorithms that follow different learning biases so they explore the mapping between meta-features and labels differently. The following algorithms were evaluated as
Table 8: Meta-datasets generated for meta-learning experiments and their class distributions using Wilcoxon paired-test with $\alpha = 0.05$.

| Meta-dataset | Meta examples | Meta features | Class Distribution Tuning | Default |
|--------------|---------------|---------------|---------------------------|---------|
| J48          | 165           | 80            | 57                        | 108     |
| CART         | 165           | 80            | 111                       | 54      |

meta-learners: Classification and Regression Tree (CART), Support Vector Machines (SVMs), Random Forest (RF), k-Nearest Neighbors (kNN), Naïve Bayes (NB), Logistic Regression (LR), and Gaussian Processes (GPs).

For comparison, it is important to mention that two baselines were also evaluated: Random and ZeroR. The former predicts a class by chance, while the latter predicts the majority class. Thus, it is expected that meta-models trained in the meta-datasets outperform them. Otherwise, no learning is happening.

These algorithms were trained in both meta-datasets using a 10-fold CV resampling strategy, repeated 10 times with different seeds, and used their default HP settings. Their predictions were assessed using the Area Under the ROC curve (AUC), a more robust performance measure than BAC for binary classification problems\(^{28}\). The complete MtL setup is detailed in Table 9.

Table 9: Meta-learning experimental setup.

| Element       | Method                                                                 | Package (language) |
|---------------|------------------------------------------------------------------------|--------------------|
| Meta-features | All measures of features categories described in Table 7               | pymfe (Python)      |
| Label definition | Statistical labeling rule Wilcoxon paired-test Significance level $\alpha = 0.05$ | stats (R)          |
| Meta-datasets | J48 tuning recommendation CART tuning recommendation                       | -                  |
| Meta-learner  | Support Vector Machines (SVMs) Classification and Regression Tree (CART) Random Forest (RF) k-Nearest Neighbors (kNN) Naïve Bayes (NB) Logistic Regression (LR) Gaussian Processes (GPs) | e1071 (R) rpart (R) randomForest (R) knn (R) e1071 (R) gbm (R) kernlab (R) |
| Baselines     | Majority (ZeroR) Random                                                 | mlr (R)            |
| Resampling    | 10-fold CV                                                              | mlr (R)            |
| Repetitions   | 10 times with different seeds $\{1, \ldots, 10\}$                       | -                  |
| Evaluation measures | AUC                                                                      | mlr (R)            |

\(^{28}\)The BAC measure was preferred at the tuning level because data collection contains binary and multiclass classification problems.
6.2 Meta-learning results

The predictive performance of the meta-learners when applied to the DTs meta-datasets are summarized in Figure 13. All the meta-learners are listed in the x-axis, while their correspondent AUC values are projected the in y-axis. The colors of the lines represent the meta-features.

![Meta-learners average AUC results on DTs meta-datasets.](image)

**Fig. 13:** Meta-learners average AUC results on DTs meta-datasets. Black dotted lines at $AUC = 0.5$ represent the predictive performance of ZeroR and Random meta-models.

Results for these three sets of meta-features are presented using different colors and line types to distinguish between them. The Wilcoxon paired test with a significance level $\alpha = 0.05$ was applied to assess the statistical significance of the meta-models’ performance obtained by the top two best meta-datasets regarding the meta-feature sets. These differences are indicated in the x-axis. Green triangles identify cases where using “all” the meta-features yielded statistically better results. On the other hand, red triangles indicate where one of the other meta-feature sets (“simple” or “complex”) was significantly better. For the remaining cases, the predictive performance values of the meta-models were equivalent. The baselines (Random and ZeroR) obtained AUC of 0.5 in all meta-datasets, represented by the dotted line at $AUC = 0.5$ in Figure 13.

The best results considering J48 were obtained by the RF, SVM, and GP meta-learners. They obtained their best predictive performances using all the available meta-features (“all” set of meta-features). For the RF meta-learner, using only the simple meta-features also generated accurate meta-models with $AUC > 0.7$. However, the complete meta-feature set generally provided the best results for most algorithms. In addition, these meta-models achieved AUC values $\in [0.67, 0.74]$, which are noticeably better than predictions based on chance.
For the CART algorithm, the best results were also obtained by RF meta-models, but using data complexity meta-features (“complex”). However, there is no significant performance difference to the complete set of meta-features (“all”). These meta-models achieved AUC values near 0.8. These two approaches (“complex” and “all”) performed quite similarly when explored by the meta-learners. In addition to RF, all the algorithms, except for NB and LR, induced meta-models with predictive performance $AUC > 0.75$. It is also noteworthy that the meta-model CART is among the top three meta-learners for the CART algorithm, while this meta-model was one of the worst regarding the J48 algorithm.

Considering these two scenarios, MtL results suggest that it is possible to predict whether tuning is required for DTs. Overall, the best results for J48 and CART were obtained when inducing RF meta-models with all the available meta-features (“all”). Thus, the following analyses for these meta-datasets were performed using the complete set of meta-features.

6.3 Meta-models’ interpretability

Since RF meta-models accurately predicted the tuning necessity of DTs, we can unveil their predictions exploring the relative importance of the meta-features based on the Gini impurity index. Figure 14 shows the average relative importance values for top-15 meta-features in each DT meta-dataset. The y-axis lists meta-features, from best to worst, according to their relative importance, projected in the x-axis. The importance values for the experiments considering all meta-features are shown.

As expected, the figure shows that different meta-features are important for different problems. Some of them contribute to both tasks, such as the absolute correlation of the attributes ($\text{statistical.abs.cor}$) meta-feature, which is the 6th ranked meta-feature in J48 tuning recommendation and the 14th for CART. However, in most cases, the most important meta-features are specific for each problem.

The most crucial meta-feature for the J48 problem was the data complexity measure “f4”. This feature describes the collective attribute efficiency in a dataset. The second most important was “f3”, which describes the maximum individual attribute efficiency. The two data complexity features measure the discriminative power of the dataset’s attributes. The top-3 is completed with a simple measure, “symbols.sd”, which measures the standard deviation of categorical features presented in the dataset. These most important metrics suggest that if a dataset has representative attributes, default HP values are robust enough to solve it. Otherwise, HP tuning is recommended.

For the CART meta-dataset, the two most important meta-features are: “n3” and “nn”. The first is a data complexity meta-feature, and the second is a traditional landmarking. Both measures estimate the error rate of the 1-NN classifier by leave-one-out or cross-validation. They measure how close the examples of different classes are. Low values mean that there is a large gap
in the class boundary. The third most important is a data complexity meta-feature: “n2”, the average intra-class and inter-class distances ratio used by a kNN algorithm to classify data examples. Low values indicate that examples from the same class lay closely in the feature space. This suggests that if the dataset’s examples from the same class are close to each other, the 1-NN will find them closely in the feature space, and CART would also be capable of solving it without tuning. On the other hand, examples would be more overlapped, and the HP tuning would better fit the algorithm’s learning bias.

Fig. 14: Relative importance of the meta-features extracted from RF metamodels.
In general, different aspects are being considered when choosing between tuned or default HP settings for the target algorithms: the discriminative power of the attributes is important to recommend the J48 tuning, and the dispersion of datasets’ examples from different classes to recommend CART tuning. At least for both algorithms, it is important to verify the importance of the dataset’s attributes before doing the HP tuning, which makes sense for a DT induction algorithm.

7 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 of this study are discussed.

7.1 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 can 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 adding datasets will not substantially change the overall tuning behavior of the algorithms investigated.

Regarding the DT induction algorithms, CART and J48 are among the most popular algorithms used in data mining (Wu and Kumar, 2009). Experiments were focused on these algorithms due to the interpretability of their induced models and widespread use. They generate simple models, are robust for specific domains, and allow non-expert users to understand how the classification decision is made. The same experimental methodology and analyses can be applied to any other ML algorithm.

Since a wide variety of datasets compose the data collection, some may be imbalanced. Thus, the BAC performance measure (Brodersen et al, 2010) was used as a 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 main paradigms for HP tuning (black-box optimization) found in the literature (Sureka and Indukuri, 2008; Sun and Pfahringer, 2013; Kotthoff et al, 2016), such that: a swarm method (PSO), an evolutionary method (GA), the standard baseline of random search (RS), and a state-of-the-art Bayesian technique (SMBO). Additionally, we included EDA and Irace because they have been explored recently for HP tuning of other ML algorithms, like
SVMs (Miranda et al, 2014; Padierna et al, 2017), and we had already evaluated them in our previous paper (Mantovani et al, 2019). They are “non-conventional” choices and can be considered novelties in decision tree HP tuning. Hyperband and BOHB would fit in the two different HP tuning paradigms used in the experiments, such as SMBO and RS, since i) Hyperband focuses on speeding up Random Search (RS) “by formulating hyperparameter optimization as a pure-exploration adaptive resource allocation problem addressing how to allocate resources among randomly sampled hyperparameter configurations” (Li et al, 2018), while ii) BOHB is based on the combination of SMBO and Hyperband. It is important to mention that the results reported in Subsection 5.1 are conditioned to the pool of tuning techniques selected in the experimental methodology. Thus, adding more tuning techniques can slightly change the best technique for some of the datasets.

7.2 Internal validity
Krstajic et al (2014) compared different resampling strategies for selecting and assessing the predictive performance of regression/classification models induced by ML algorithms. In Cawley and Talbot (2010) 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 (Thornton et al, 2013; Kotthoff et al, 2016) and Auto-skLearn30 Feurer et al (2015a). 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 (Pérez Cáceres et al, 2014), 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 (Mills et al, 2015), 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.

Using a larger budget, with 5000 evaluations for DT tuning, was investigated in Mantovani et al (2016). The experimental results suggested that all

---

29http://www.cs.ubc.ca/labs/beta/Projects/autoweka/
30https://github.com/automl/auto-sklearn
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 in hyperparameter spaces led to statistically significant improvements in most cases.

7.3 External validity

Section 5.2 presented statistical comparisons between tuning techniques. In Demšar (2006), 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 significant differences. Thus, the Friedman ranking test followed by the Nemenyi post-hoc test was used to evaluate experimental results from this study.

The budget size adopted can directly influence the performance of the meta-heuristics, especially GA and EDA. In Hauschild and Pelikan (2011), the authors recommend to use at least 100 individuals to build a reliable EDA model, a suggestion followed in Mantovani et al (2016). 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 provide good predictive performance values (Mantovani et al, 2016). 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 for space under this budget restriction.

8 Conclusions

This paper investigated the effects of the hyperparameter tuning profile of DT induction algorithms. For this purpose, two of the most popular DT algorithms were chosen as study cases: J48 and CART. 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.
8.1 Tuning of J48

In general, hyperparameter tuning for J48 produced modest improvements when compared to the \texttt{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. Thus, enabling them requires more time to induce and assess trees. 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 that performed some tuning for J48 tried different values for the complexity parameter (C). However, none 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.

None of the related work used the Irace technique: they focused 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 much runtime.

The default hyperparameter values of J48 proved effective for many datasets. This outcome can be because the default settings used by \texttt{RWeka} were chosen to aim to maximize the predictive performance on the UCI ML repository datasets (Bache and Lichman, 2013).

8.2 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 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 setting. 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 '\texttt{minsplit}' and '\texttt{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.

8.3 General scenario

Overall, the general picture showed us that tuning techniques can significantly improve the predictive performance of the DTs. Depending on the dataset, tuning techniques’ performance values can be very small compared to those obtained by default HP settings. Hence, the results indicate that it is better to use the default settings for some optimization problems. Different techniques are more suitable for different budget sizes when comparing tuning techniques. If the user has a large enough budget (time or evaluations), Irace is a good choice. On the other hand, PSO and SMBO are the recommended techniques with faster convergence and faster results.

The fANOVA analysis also indicated that few of the HPs are effectively responsible for the predictive performance of the final trees. Similar results with different ML algorithms were reported in van Rijn and Hutter (2017). In this sense, the fANOVA framework is a powerful tool to reduce the search HP space and time spent with optimization. The last tuning experiment showed that a higher number of statistically significant improvements were obtained when a reduced HP space was used to tune both algorithms.

8.4 When to tune

Lastly, we explored MtL to unveil the tuning process so MtL could explain when to use the tuning approach. We observed that hyperparameter tuning provides the best results for datasets with many classes ($\textit{cls} > 8$), and when there are non-linear decision boundaries. On the other hand, defaults are adequate for simple classification problems, where there is a higher separability between the classes. It can be assumed that the more complex (difficult to classify) a dataset is, the more a DT algorithm will benefit from hyperparameter tuning.

Considering the algorithms investigated in this study, each presented a different behavior under tuning. Generally, it was possible to observe that the default hyperparameter values are suitable for many datasets. However, a fixed value would only suit some data classification tasks. It justifies and motivates the development of recommender systems able to suggest the most appropriate hyperparameter setting for a new problem.
8.5 Future Work

Our findings also point out to some future research directions. The data complexity characteristics provided helpful insight regarding which situations tuning or defaults should be used. However, it would be possible to make more accurate suggestions by 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 a great scientific (and societal) impact. The authors have already begun work in this direction.

Acknowledgements

The authors would like to thank the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for the financial support, the Brazilian National Council for Scientific and Technological Development (CNPq) for the grant #409371/2021-1 (CNPq/MCTI/FNDCT No 18/2021), and specially to the grants #2012/23114-9, #2013/07375-0 and #2015/03986-0 from São Paulo Research Foundation (FAPESP). EFOP-3.6.3-VEKOP-16-2017-00001: Talent Management in Autonomous Vehicle Control Technologies – The Project is supported by the Hungarian Government and co-financed by the European Social Fund.

Declarations

Competing interests: The authors have no competing interests to declare that are relevant to the content of this article.

References

Abe S (2005) Support Vector Machines for Pattern Classification. Springer London, Secaucus, NJ, USA

Alcobaça E, Siqueira F, Rivolli A, et al (2020) MFE: towards reproducible meta-feature extraction. J Mach Learn Res 21:111:1–111:5

Ali S, Smith-Miles KA (2006) A meta-learning approach to automatic kernel selection for support vector machines. Neurocomputing 70(13):173–186

Andradottir S (2015) A review of random search methods. In: Fu MC (ed) Handbook of Simulation Optimization, International Series in Operations Research & Management Science, vol 216. Springer New York, p 277–292
Bache K, Lichman M (2013) UCI machine learning repository. URL http://archive.ics.uci.edu/ml

Bardenet R, Brendel M, Kégl B, et al (2013) Collaborative hyperparameter tuning. In: Dasgupta S, Mcallester D (eds) Proceedings of the 30th International Conference on Machine Learning (ICML-13), vol 28. JMLR Workshop and Conference Proceedings, pp 199–207

Barella VH, Garcia LPF, de Souto MCP, et al (2021) Assessing the data complexity of imbalanced datasets. Inf Sci 553:83–109. https://doi.org/10.1016/j.ins.2020.12.006

Barros R, Basgalupp M, de Carvalho A, et al (2012) A survey of evolutionary algorithms for decision-tree induction. Systems, Man, and Cybernetics, Part C: Applications and Reviews, IEEE Transactions on 42(3):291–312

Barros RC, de Carvalho ACPLF, Freitas AA (2015) Automatic Design of Decision-Tree Induction Algorithms. Springer Briefs in Computer Science, Springer, https://doi.org/10.1007/978-3-319-14231-9

Bartz E, Zaefferer M, Mersmann O, et al (2021) Experimental investigation and evaluation of model-based hyperparameter optimization. CoRR abs/2107.08761. URL https://arxiv.org/abs/2107.08761

Ben-Hur A, Weston J (2010) A user’s guide to support vector machines. In: Data Mining Techniques for the Life Sciences, Methods in Molecular Biology, vol 609. Humana Press, p 223–239

Bendtsen. C (2012) pso: Particle Swarm Optimization. URL https://CRAN.R-project.org/package=pso, r package version 1.0.3

Bergstra J, Bengio Y (2012) Random search for hyper-parameter optimization. J Mach Learn Res 13:281–305

Bergstra J, Yamins D, Cox DD (2013) Making a science of model search: Hyperparameter optimization in hundreds of dimensions for vision architectures. In: Proc. 30th Intern. Conf. on Machine Learning, pp 1–9

Bergstra JS, Bardenet R, Bengio Y, et al (2011) Algorithms for hyperparameter optimization. In: Shawe-Taylor J, Zemel RS, Bartlett PL, et al (eds) Advances in Neural Information Processing Systems 24. Curran Associates, Inc., p 2546–2554

Bermúdez-Chacón R, Gonnet GH, Smith K (2015) Automatic problem-specific hyperparameter optimization and model selection for supervised machine learning: Technical Report. Tech. rep., Zürich
Birattari M, Yuan Z, Balaprakash P, et al (2010) F-Race and Iterated F-Race: An Overview, Springer Berlin Heidelberg, Berlin, Heidelberg, pp 311–336. https://doi.org/10.1007/978-3-642-02538-9_13

Bischl B, Lang M, Kotthoff L, et al (2016) mlr: Machine learning in r. Journal of Machine Learning Research 17(170):1–5. URL http://jmlr.org/papers/v17/15-066.html

Bischl B, Binder M, Lang M, et al (2023) Hyperparameter optimization: Foundations, algorithms, best practices and open challenges. https://doi.org/https://wires.onlinelibrary.wiley.com/doi/10.1002/widm.1484

Blanco-Justicia A, Domingo-Ferrer J (2019) Machine learning explainability through comprehensible decision trees. In: Machine Learning and Knowledge Extraction: Third IFIP TC 5, TC 12, WG 8.4, WG 8.9, WG 12.9 International Cross-Domain Conference, CD-MAKE 2019, Canterbury, UK, August 26–29, 2019, Proceedings. Springer-Verlag, Berlin, Heidelberg, p 15–26, https://doi.org/10.1007/978-3-030-29726-8_2

Blanco-Justicia A, Domingo-Ferrer J, Martínez S, et al (2020) Machine learning explainability via microaggregation and shallow decision trees. Knowledge-Based Systems 194:105,532. https://doi.org/https://doi.org/10.1016/j.knosys.2020.105532

Brazdil P, Giraud-Carrier C, Soares C, et al (2009) Metalearning: Applications to Data Mining, 1st edn. Springer-Verlag Berlin Heidelberg

Breiman L, Friedman J, Olshen R, et al (1984) Classification and Regression Trees. Chapman & Hall (Wadsworth, Inc.)

Brodersen KH, Ong CS, Stephan KE, et al (2010) The balanced accuracy and its posterior distribution. In: Proceedings of the 2010 20th International Conference on Pattern Recognition. IEEE Computer Society, pp 3121–3124

Cawley GC, Talbot NLC (2010) On over-fitting in model selection and subsequent selection bias in performance evaluation. The Journal of Machine Learning Research 11:2079–2107. URL http://www.jmlr.org/papers/v11/cawley10a.html

Clerc M (2012) Standard particle swarm optimization, 15 pages

Demšar J (2006) Statistical comparisons of classifiers over multiple data sets. The Journal of Machine Learning Research 7:1–30

Eggensperger K, Hutter F, Hoos HH, et al (2015) Efficient benchmarking of hyperparameter optimizers via surrogates. In: Proceedings of the Twenty-Ninth AAAI Conference on Artificial Intelligence. AAAI Press, AAAI’15,
pp 1114–1120, URL http://dl.acm.org/citation.cfm?id=2887007.2887162

Eitrich T, Lang B (2006) Efficient optimization of support vector machine learning parameters for unbalanced datasets. Journal of Comp and Applied Mathematics 196(2):425–436

Esposito F, Malerba D, Semeraro G, et al (1999) The effects of pruning methods on the predictive accuracy of induced decision trees. Appl Stochastic Models Bu Ind 15:277–299

European Commission (2016) Regulation (EU) 2016/679 of the European Parliament and of the Council of 27 April 2016 on the protection of natural persons with regard to the processing of personal data and on the free movement of such data, and repealing Directive 95/46/EC (General Data Protection Regulation) (Text with EEA relevance). URL https://eur-lex.europa.eu/eli/reg/2016/679/oj

Falkner S, Klein A, Hutter F (2018) BOHB: Robust and efficient hyperparameter optimization at scale. In: Dy J, Krause A (eds) Proceedings of the 35th International Conference on Machine Learning, Proceedings of Machine Learning Research, vol 80. PMLR, pp 1437–1446

Fernández-Delgado M, Cernadas E, Barro S, et al (2014) Do we need hundreds of classifiers to solve real world classification problems? Journal of Machine Learning Research 15:3133–3181. URL http://jmlr.org/papers/v15/delgado14a.html

Feurer M, Klein A, Eggensperger K, et al (2015a) Efficient and robust automated machine learning. In: Cortes C, Lawrence ND, Lee DD, et al (eds) Advances in Neural Information Processing Systems 28. Curran Associates, Inc., p 2944–2952

Feurer M, Springenberg JT, Hutter F (2015b) Initializing bayesian hyperparameter optimization via meta-learning. In: Proceedings of the Twenty-Ninth AAAI Conference on Artificial Intelligence. AAAI Press, AAAI’15, pp 1128–1135, URL http://dl.acm.org/citation.cfm?id=2887007.2887164

Feurer M, Eggensperger K, Falkner S, et al (2020) Auto-sklearn 2.0: Hands-free automl via meta-learning. arXiv:200704074 [csLG]

García LPF, Lehmann J, de Carvalho ACPLF, et al (2019) New label noise injection methods for the evaluation of noise filters. Knowl Based Syst 163:693–704. https://doi.org/10.1016/j.knosys.2018.09.031

Gascón-Moreno J, Salcedo-Sanz S, Ortiz-García EG, et al (2011) A binary-encoded tabu-list genetic algorithm for fast support vector regression hyperparameters tuning. In: International Conference on Intelligent Systems
Design and Applications, pp 1253–1257

Gijsbers P, Vanschoren J (2021) Gama: A general automated machine learning assistant. In: Dong Y, Ifrim G, Mladenović D, et al (eds) Machine Learning and Knowledge Discovery in Databases. Applied Data Science and Demo Track. Springer International Publishing, Cham, pp 560–564

Goldberg D (1989) Genetic Algorithms in Search, Optimization and Machine Learning. Addison Wesley

Gomes TAF, Prudêncio RBC, Soares C, et al (2012) Combining meta-learning and search techniques to select parameters for support vector machines. Neurocomputing 75(1):3–13

Gonzalez-Fernandez Y, Soto M (2014) copulaedas: An R package for estimation of distribution algorithms based on copulas. Journal of Statistical Software 58(9):1–34. URL http://www.jstatsoft.org/v58/i09/

Hauschild M, Pelikan M (2011) An introduction and survey of estimation of distribution algorithms. Swarm and Evolutionary Computation 1(3):111 – 128

Haykin S (2007) Neural Networks: A Comprehensive Foundation (3rd Edition). Prentice-Hall, Inc., Upper Saddle River, NJ, USA

Hornik K, Buchta C, Zeileis A (2009) Open-source machine learning: R meets Weka. Computational Statistics 24(2):225–232

Hothorn T, Hornik K, Zeileis A (2006) Unbiased recursive partitioning: A conditional inference framework. Journal of Computational and Graphical Statistics 15(3):651–674

Huang BF, Boutros PC (2016) The parameter sensitivity of random forests. BMC Bioinformatics 17(1):331. https://doi.org/10.1186/s12859-016-1228-x, URL http://dx.doi.org/10.1186/s12859-016-1228-x

Hutter F, Hoos H, Leyton-Brown K (2014) An efficient approach for assessing hyperparameter importance. In: Proceedings of the 31th International Conference on Machine Learning, ICML 2014, Beijing, China, 21-26 June 2014, pp 754–762, URL http://jmlr.org/proceedings/papers/v32/hutter14.html

Jankowski D, Jackowski K (2014) Evolutionary algorithm for decision tree induction. In: Saeed K, Snášel V (eds) Computer Information Systems and Industrial Management, Lecture Notes in Computer Science, vol 8838. Springer Berlin Heidelberg, p 23–32
from Jed Wing MKC, Weston S, Williams A, et al (2016) caret: Classification and Regression Training. URL https://CRAN.R-project.org/package=caret, r package version 6.0-71

Kanda J, de Carvalho A, Hruschka E, et al (2016) Meta-learning to select the best meta-heuristic for the traveling salesman problem: A comparison of meta-features. Neurocomputing 205:393–406. https://doi.org/https://doi.org/10.1016/j.neucom.2016.04.027

Kennedy J, Eberhart R (1995) Particle swarm optimization. In: Proceedings of the IEEE International Conference on Neural Networks, Perth, Australia, pp 1942–1948

Kohavi R (1996) Scaling up the accuracy of naive-bayes classifiers: A decision-tree hybrid. In: Second International Conference on Knowledge Discovery and Data Mining, pp 202–207

Kotthoff L, Thornton C, Hoos HH, et al (2016) Auto-weka 2.0: Automatic model selection and hyperparameter optimization in weka. Journal of Machine Learning Research 17:1–5

Krstajic D, Buturovic LJ, Leahy DE, et al (2014) Cross-validation pitfalls when selecting and assessing regression and classification models. Journal of Cheminformatics 6(1):1–15. https://doi.org/10.1186/1758-2946-6-10

Landwehr N, Hall M, Frank E (2005) Logistic model trees. Machine Learning 95(1-2):161–205

Lang M, Kotthaus H, Marwedel P, et al (2015) Automatic model selection for high-dimensional survival analysis. Journal of Statistical Computation and Simulation 85(1):62–76. https://doi.org/10.1080/00949655.2014.929131

Lévesque JC, Gagné C, Sabourin R (2016) Bayesian hyperparameter optimization for ensemble learning. In: Proceedings of the Thirty-Second Conference on Uncertainty in Artificial Intelligence. AUAI Press, Arlington, Virginia, United States, UAI’16, pp 437–446, URL http://dl.acm.org/citation.cfm?id=3020948.3020994

Li L, Jamieson K, DeSalvo G, et al (2018) Hyperband: A novel bandit-based approach to hyperparameter optimization. Journal of Machine Learning Research 18(185):1–52. URL http://jmlr.org/papers/v18/16-558.html

Liaw A, Wiener M (2002) Classification and regression by randomforest. R News 2(3):18–22

Lin SW, Chen SC (2012) Parameter determination and feature selection for c4.5 algorithm using scatter search approach. Soft Computing 16(1):63–75.
Loh WY (2014) Fifty years of classification and regression trees. International Statistical Review 82(3):329–348

López-Ibáñez M, Dubois-Lacoste J, Cáceres LP, et al (2016) The irace package: Iterated racing for automatic algorithm configuration. Operations Research Perspectives 3:43 – 58. https://doi.org/https://doi.org/10.1016/j.orp.2016.09.002

Ma J (2012) Parameter Tuning Using Gaussian Processes. Master’s thesis, University of Waikato, New Zealand

Mantovani RG, Horváth T, Cerri R, et al (2016) Hyper-parameter tuning of a decision tree induction algorithm. In: 5th Brazilian Conference on Intelligent Systems, BRACIS 2016, Recife, Brazil, October 9-12, 2016. IEEE Computer Society, pp 37–42, https://doi.org/10.1109/BRACIS.2016.018, URL http://ieeexplore.ieee.org/xpl/mostRecentIssue.jsp?punumber=7837801

Mantovani RG, Rossi AL, Alcobaça E, et al (2019) A meta-learning recommender system for hyperparameter tuning: predicting when tuning improves svm classifiers. Information Sciences 501:193–221. https://doi.org/https://doi.org/10.1016/j.ins.2019.06.005

Massimo CM, Navarin N, Sperduti A (2016) Hyper-Parameter Tuning for Graph Kernels via Multiple Kernel Learning, Springer International Publishing, Cham, pp 214–223. https://doi.org/10.1007/978-3-319-46672-9_25

Mills KL, Filliben JJ, Haines AL (2015) Determining relative importance and effective settings for genetic algorithm control parameters. Evol Comput 23(2):309–342. https://doi.org/10.1162/EVCO_a_00137

Miranda P, Silva R, Prudência R (2014) Fine-tuning of support vector machine parameters using racing algorithms. In: Proceedings of the 22nd European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning, ESANN 2014, pp 325–330

Molina MM, Luna JM, Romero C, et al (2012) Meta-learning approach for automatic parameter tuning: A case study with educational datasets. In: Proceedings of the 5th International Conference on Educational Data Mining, EDM 2012, pp 180–183

Nakamura M, Otsuka A, Kimura H (2014) Automatic selection of classification algorithms for non-experts using meta-features. China-USA Business Review 13(3):199–205
Better Trees

Padierna LC, Carpio M, Rojas A, et al (2017) Hyper-Parameter Tuning for Support Vector Machines by Estimation of Distribution Algorithms, Springer International Publishing, Cham, pp 787–800

Pérez Cáceres L, López- Ibáñez M, Stützle T (2014) An Analysis of Parameters of irace, Springer Berlin Heidelberg, Berlin, Heidelberg, pp 37–48. https://doi.org/10.1007/978-3-662-44320-0_4

Pilát M, Neruda R (2013) Multi-objectivization and Surrogate Modelling for Neural Network Hyper-parameters Tuning, Springer Berlin Heidelberg, Berlin, Heidelberg, pp 61–66. https://doi.org/10.1007/978-3-642-39678-6_11

Podgorelec V, Karakatic S, Barros RC, et al (2015) Evolving balanced decision trees with a multi-population genetic algorithm. In: IEEE Congress on Evolutionary Computation, CEC 2015, Sendai, Japan, May 25-28, 2015. IEEE, pp 54–61, https://doi.org/10.1109/CEC.2015.7256874, URL http://ieeexplore.ieee.org/xpl/mostRecentIssue.jsp?punumber=7229815

Probst P, Boulesteix A, Bischl B (2019) Tunability: Importance of hyperparameters of machine learning algorithms. J Mach Learn Res 20:53:1–53:32. URL http://jmlr.org/papers/v20/18-444.html

Quinlan JR (1993) C4.5: Programs for Machine Learning. Morgan Kaufmann Publishers Inc., San Francisco, CA, USA

Reif M, Shafait F, Dengel A (2011) Prediction of classifier training time including parameter optimization. In: Bach J, Edelkamp S (eds) KI 2011: Advances in Artificial Intelligence, Lecture Notes in Computer Science, vol 7006. Springer Berlin Heidelberg, p 260–271

Reif M, Shafait F, Dengel A (2012) Meta-learning for evolutionary parameter optimization of classifiers. Machine Learning 87:357–380

Reif M, Shafait F, Goldstein M, et al (2014) Automatic classifier selection for non-experts. Pattern Analysis and Applications 17(1):83–96

Ribeiro MT, Singh S, Guestrin C (2016) Model-agnostic interpretability of machine learning. 1606.05386

Ridd P, Giraud-Carrier C (2014) Using metalearning to predict when parameter optimization is likely to improve classification accuracy. In: Vanschoren J, Brazdil P, Soares C, et al (eds) Meta-learning and Algorithm Selection Workshop at ECAI 2014, pp 18–23

van Rijn JN, Hutter F (2017) An empirical study of hyperparameter importance across datasets. In: Proceedings of the International Workshop on
Automatic Selection, Configuration and Composition of Machine Learning Algorithms co-located with the European Conference on Machine Learning & Principles and Practice of Knowledge Discovery in Databases, AutoML@PKDD/ECML 2017, Skopje, Macedonia, September 22, 2017., pp 91–98, URL http://ceur-ws.org/Vol-1998/paper_09.pdf

Rokach L, Maimon O (2014) Data Mining With Decision Trees: Theory and Applications, 2nd edn. World Scientific Publishing Co., Inc., River Edge, NJ, USA

Sabharwal A, Samulowitz H, Tesauro G (2016) Selecting near-optimal learners via incremental data allocation. In: Proceedings of the Thirtieth AAAI Conference on Artificial Intelligence. AAAI Press, AAAI’16, pp 2007–2015, URL http://dl.acm.org/citation.cfm?id=3016100.3016179

Sanders S, Giraud-Carrier CG (2017) Informing the use of hyperparameter optimization through metalearning. In: 2017 IEEE International Conference on Data Mining, ICDM 2017, New Orleans, LA, USA, November 18-21, 2017, pp 1051–1056

Schauerhuber M, Zeileis A, Meyer D, et al (2008) Benchmarking Open-Source Tree Learners in R/RWeka, Springer Berlin Heidelberg, Berlin, Heidelberg, pp 389–396. https://doi.org/10.1007/978-3-540-78246-9_46

Scrucca L (2013) Ga: A package for genetic algorithms in r. Journal of Statistical Software 53(1):1–37. https://doi.org/10.18637/jss.v053.i04, URL https://www.jstatsoft.org/index.php/jss/article/view/v053i04

Simon D (2013) Evolutionary Optimization Algorithms, 1st edn. Wiley

Snoek J, Larochelle H, Adams RP (2012) Practical bayesian optimization of machine learning algorithms. In: Pereira F, Burges C, Bottou L, et al (eds) Advances in Neural Information Processing Systems 25. Curran Associates, Inc., p 2951–2959

Stiglic G, Kocbek S, Pernek I, et al (2012) Comprehensive decision tree models in bioinformatics. PLOS ONE 7(3):1–13. https://doi.org/10.1371/journal.pone.0033812

Sun Q, Pfahringer B (2013) Pairwise meta-rules for better meta-learning-based algorithm ranking. Mach Learn 93(1):141–161. https://doi.org/10.1007/s10994-013-5387-y

Sureka A, Indukuri KV (2008) Using Genetic Algorithms for Parameter Optimization in Building Predictive Data Mining Models, Springer Berlin Heidelberg, Berlin, Heidelberg, pp 260–271. https://doi.org/10.1007/978-3-540-88192-6_25
Tan PN, Steinbach M, Kumar V (2005) Introduction to Data Mining, (First Edition), 1st edn. Addison-Wesley Longman Publishing Co., Inc., Boston, MA, USA

Tantithamthavorn C, McIntosh S, Hassan AE, et al (2016) Automated parameter optimization of classification techniques for defect prediction models. In: Proceedings of the 38th International Conference on Software Engineering. ACM, New York, NY, USA, ICSE ’16, pp 321–332, https://doi.org/10.1145/2884781.2884857

Therneau T, Atkinson B, Ripley B (2015) rpart: Recursive Partitioning and Regression Trees. URL https://CRAN.R-project.org/package=rpart, r package version 4.1-10

Thornton C, Hutter F, Hoos HH, et al (2013) Auto-WEKA: Combined selection and hyperparameter optimization of classification algorithms. In: Proc. of KDD-2013, pp 847–855

Vanschoren J, van Rijn JN, Bischl B, et al (2014) Openml: Networked science in machine learning. SIGKDD Explor Newsl 15(2):49–60

Vieira CPR, Digiampietri LA (2020) A study about explainable artificial intelligence: using decision tree to explain svm. Revista Brasileira de Computação Aplicada 12(1):113–121. https://doi.org/10.5335/rbca.v12i1.10247

Wainberg M, Alipanahi B, Frey BJ (2016) Are random forests truly the best classifiers? Journal of Machine Learning Research 17(110):1–5. URL http://jmlr.org/papers/v17/15-374.html

Wang L, Feng M, Zhou B, et al (2015) Efficient hyper-parameter optimization for NLP applications. In: Márquez L, Callison-Burch C, Su J, et al (eds) Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing, EMNLP 2015, Lisbon, Portugal, September 17-21, 2015. The Association for Computational Linguistics, pp 2112–2117, URL http://aclweb.org/anthology/D/D15/D15-1253.pdf

Witten IH, Frank E (2005) Data Mining: Practical Machine Learning Tools and Techniques, 2nd edn. Morgan Kaufmann, San Francisco

Wu X, Kumar V (2009) The Top Ten Algorithms in Data Mining, 1st edn. Chapman & Hall/CRC

Yang XS, Cui Z, Xiao R, et al (2013) Swarm Intelligence and Bio-Inspired Computation: Theory and Applications, 1st edn. Elsevier Science Publishers B. V.
Zambrano-Bigiarini M, Clerc M, Rojas R (2013) Standard particle swarm optimisation 2011 at CEC-2013: A baseline for future PSO improvements. In: Proceedings of the IEEE Congress on Evolutionary Computation, CEC 2013, Cancun, Mexico, June 20-23, 2013. IEEE, pp 2337–2344, https://doi.org/10.1109/CEC.2013.6557848
**Appendix A  List of abbreviations used in the paper**

*AI* Artificial Intelligence.
*ANN* Artificial Neural Network.
*AUC* Area Under the ROC curve.
*AutoML* Automated Machine Learning.

*BAC* Balanced per class Accuracy.
*BOHB* Bayesian Optimization with HyperBand.

*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.
*GDPR* General Data Protection Regulation.
*GP* Gaussian Process.
*GS* Grid Search.

*HP* Hyperparameter.

*Irace* Iterated F-race.

*kNN* k-Nearest Neighbors.

*LMT* Logistic Model Tree.
*LR* Logistic Regression.

*ML* Machine Learning.
*MtL* Meta-learning.

*NB* Naïve Bayes.
*NBTree* Naïve-Bayes Tree.

*OpenML* Open Machine Learning.

*PD* Parametric Density.
*PS* Pattern Search.
PSO  Particle Swarm Optimization.

REP  Reduced Error Pruning.
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.
Appendix B  List of OpenML datasets used in experiments

This appendix presents the full table of datasets used in both tuning and meta-learning experiments performed in this paper. 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), the number of examples belonging to the majority and minority classes (nMaj, nMin), the proportion between them (P), and whether the dataset was added to the enrichment step for meta-learning.

Table B1: (Multi-class) classification OpenML datasets (1 to 29) 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), the number of examples belonging to the majority and minority classes (nMaj, nMin), the proportion between them (P), and whether the dataset was added to the enrichment step for meta-learning.

| Nro | OpenML name            | OpenML did | D  | N   | C   | nMaj | nMin | P      | Meta |
|-----|------------------------|------------|----|-----|-----|------|------|--------|------|
| 1   | kr-vs-kp               | 3          | 37 | 3196| 2   | 1669 | 1527 | 0.91   | base |
| 2   | balance-scale          | 11         | 5  | 625 | 3   | 288  | 49   | 0.17   | base |
| 3   | breast-cancer          | 13         | 10 | 286 | 2   | 201  | 85   | 0.42   |       |
| 4   | mfeat-fourier          | 14         | 77 | 2000| 10  | 200  | 200  | 1.00   | base |
| 5   | breast-w               | 15         | 10 | 699 | 2   | 458  | 241  | 0.53   | base |
| 6   | mfeat-karhunen         | 16         | 65 | 2000| 10  | 200  | 200  | 1.00   |       |
| 7   | mfeat-morphological    | 18         | 7  | 2000| 10  | 200  | 200  | 1.00   |       |
| 8   | car                    | 21         | 7  | 1728| 4   | 1210 | 65   | 0.05   | base |
| 9   | mfeat-zernike          | 22         | 48 | 2000| 10  | 200  | 200  | 1.00   |       |
| 10  | colic                  | 25         | 28 | 368 | 2   | 232  | 136  | 0.59   | base |
| 11  | optdigits              | 28         | 65 | 5620| 10  | 572  | 554  | 0.97   | base |
| 12  | credit-g               | 31         | 21 | 1000| 2   | 700  | 300  | 0.43   | base |
| 13  | pendigits              | 32         | 17 | 10992| 10  | 1144 | 1055 | 0.92   |       |
| 14  | dermatology            | 35         | 35 | 366 | 6   | 112  | 20   | 0.18   | base |
| 15  | segment                | 36         | 20 | 2310| 7   | 330  | 330  | 1.00   | base |
| 16  | diabetes               | 37         | 9  | 768 | 2   | 500  | 268  | 0.54   |       |
| 17  | sick                   | 38         | 30 | 3772| 2   | 3541 | 231  | 0.07   |       |
| 18  | sonar                  | 40         | 61 | 208 | 2   | 111  | 97   | 0.87   | base |
| 19  | haberman               | 43         | 4  | 306 | 2   | 225  | 81   | 0.36   | base |
| 20  | spambase               | 44         | 58 | 4601| 2   | 2788 | 1813 | 0.65   |       |
| 21  | tae                    | 48         | 6  | 151 | 3   | 52   | 49   | 0.94   | base |
| 22  | heart-c                | 49         | 14 | 303 | 5   | 165  | 0    | 0.00   | base |
| 23  | tic-tac-toe            | 50         | 10 | 958 | 2   | 626  | 332  | 0.53   |       |
| 24  | heart-statlog          | 53         | 14 | 270 | 2   | 150  | 120  | 0.80   | base |
| 25  | vehicle                | 54         | 19 | 846 | 4   | 218  | 199  | 0.91   | base |
| 26  | hepatitis              | 55         | 20 | 155 | 2   | 123  | 32   | 0.26   | base |
| 27  | vote                   | 56         | 17 | 435 | 2   | 267  | 168  | 0.63   |       |
| 28  | ionosphere             | 59         | 35 | 351 | 2   | 225  | 126  | 0.56   | base |
| 29  | waveform-5000          | 60         | 41 | 5000| 3   | 1692 | 1653 | 0.98   | base |
Table B2: (Multi-class) classification OpenML datasets (30 to 67) 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), the number of examples belonging to the majority and minority classes (nMaj, nMin), the proportion between them (P), and whether the dataset was added to the enrichment step for meta-learning.

| Nro | OpenML name                  | OpenML did | D  | N  | C  | nMaj | nMin | P        | Meta |
|-----|------------------------------|------------|----|----|----|------|------|----------|------|
| 30  | iris                         | 61         | 5  | 150| 3  | 50   | 50   | 1.00     | base |
| 31  | molecular-biology_promoters  | 164        | 59 | 106| 2  | 53   | 53   | 1.00     | base |
| 32  | satimage                     | 182        | 37 | 6430| 6  | 1531 | 625  | 0.41     |      |
| 33  | baseball                     | 185        | 18 | 1340| 3  | 1215 | 57   | 0.05     |      |
| 34  | wine                         | 187        | 14 | 178 | 3  | 71   | 48   | 0.68     | base |
| 35  | eucalyptus                   | 188        | 20 | 736 | 5  | 214  | 105  | 0.49     |      |
| 36  | Australian                   | 292        | 15 | 690 | 2  | 383  | 307  | 0.80     |      |
| 37  | satellite_image              | 294        | 37 | 6435| 6  | 871  | 275  | 0.32     | base |
| 38  | libras_move                  | 299        | 91 | 360 | 11 | 24   | 11   | 0.46     | base |
| 39  | vowel                        | 307        | 13 | 990 | 11 | 90   | 90   | 1.00     |      |
| 40  | mammography                  | 310        | 7  | 11183| 2  | 10923| 260  | 0.02     | base |
| 41  | oil_spill                    | 311        | 50 | 937 | 2  | 896  | 41   | 0.05     |      |
| 42  | yeast_ml8                    | 316        | 117| 2417| 2  | 2383 | 34   | 0.01     | base |
| 43  | hayes-roth                   | 329        | 5  | 160 | 4  | 65   | 0    | 0.01     |      |
| 44  | monks-problems-1             | 333        | 7  | 556 | 2  | 278  | 278  | 1.00     | base |
| 45  | monks-problems-2             | 334        | 7  | 601 | 2  | 395  | 206  | 0.52     | base |
| 46  | monks-problems-3             | 335        | 7  | 554 | 2  | 288  | 266  | 0.92     | base |
| 47  | SPECT                        | 336        | 23 | 267 | 2  | 212  | 55   | 0.26     |      |
| 48  | grub-damage                  | 338        | 9  | 155 | 4  | 49   | 19   | 0.39     |      |
| 49  | synthetic_control            | 377        | 62 | 600 | 6  | 100  | 100  | 1.00     |      |
| 50  | analcatdata_boxing2          | 444        | 4  | 132 | 2  | 71   | 61   | 0.86     | base |
| 51  | analcatdata_boxing1          | 448        | 4  | 120 | 2  | 78   | 42   | 0.54     | base |
| 52  | analcatdata_lawsuit          | 450        | 5  | 264 | 2  | 245  | 19   | 0.08     |      |
| 53  | irish                        | 451        | 6  | 500 | 2  | 278  | 222  | 0.80     |      |
| 54  | analcatdata_broadwaymult     | 452        | 8  | 285 | 7  | 118  | 21   | 0.18     |      |
| 55  | cars                         | 455        | 9  | 406 | 3  | 254  | 73   | 0.29     |      |
| 56  | analcatdata_authorship       | 458        | 71 | 841 | 4  | 317  | 55   | 0.17     | base |
| 57  | analcatdata_creditscore      | 461        | 7  | 100 | 2  | 73   | 27   | 0.37     | base |
| 58  | backache                     | 463        | 33 | 180 | 2  | 155  | 25   | 0.16     |      |
| 59  | prnasyth                     | 464        | 3  | 250 | 2  | 125  | 125  | 1.00     |      |
| 60  | schizo                       | 466        | 15 | 340 | 2  | 177  | 163  | 0.92     |      |
| 61  | analcatdata_dmft             | 469        | 5  | 797 | 6  | 155  | 123  | 0.79     | base |
| 62  | probf                        | 470        | 10 | 672 | 2  | 448  | 224  | 0.50     |      |
| 63  | analcatdata_germanuss        | 475        | 6  | 400 | 4  | 100  | 100  | 1.00     | base |
| 64  | biomed                       | 481        | 9  | 209 | 2  | 134  | 75   | 0.56     |      |
| 65  | rmftsa_sleepdata             | 679        | 3  | 1024| 4  | 404  | 94   | 0.23     |      |
| 66  | visualizing_livestock        | 685        | 3  | 130 | 5  | 26   | 26   | 1.00     |      |
| 67  | diggle_tablea2               | 694        | 9  | 310 | 9  | 41   | 18   | 0.44     |      |
Table B3: (Multi-class) classification OpenML datasets (68 to 104) 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), the number of examples belonging to the majority and minority classes (nMaj, nMin), the proportion between them (P), and whether the dataset was added to the enrichment step for meta-learning.

| Nro | OpenML name           | OpenML did | D   | N   | C   | nMaj | nMin | P       | Meta |
|-----|-----------------------|------------|-----|-----|-----|------|------|---------|------|
| 68  | ada_prior             | 1037       | 15  | 4562| 2   | 3430 | 1132 | 0.33    | •    |
| 69  | ada_agnostic          | 1043       | 49  | 4562| 2   | 3430 | 1132 | 0.33    | •    |
| 70  | jEdit_4.2_4.3         | 1048       | 9   | 369 | 2   | 204  | 165  | 0.81    | •    |
| 71  | pc4                   | 1049       | 38  | 1458| 2   | 1280 | 178  | 0.14    | •    |
| 72  | pc3                   | 1050       | 38  | 1563| 2   | 1403 | 160  | 0.11    | •    |
| 73  | mc2                   | 1054       | 40  | 161 | 2   | 109  | 52   | 0.48    | •    |
| 74  | ml                   | 1056       | 39  | 9466| 2   | 9398 | 68   | 0.01    | •    |
| 75  | ar4                   | 1061       | 30  | 107 | 2   | 87   | 20   | 0.23    | •    |
| 76  | kc2                   | 1063       | 22  | 522 | 2   | 415  | 107  | 0.26    | •    |
| 77  | ar6                   | 1064       | 30  | 101 | 2   | 86   | 15   | 0.17    | •    |
| 78  | kc3                   | 1065       | 40  | 458 | 2   | 415  | 43   | 0.10    | •    |
| 79  | kc1-binary            | 1066       | 95  | 145 | 2   | 85   | 60   | 0.71    | •    |
| 80  | kc1                   | 1067       | 22  | 2109| 2   | 1783 | 326  | 0.18    | •    |
| 81  | pc1                   | 1068       | 22  | 1109| 2   | 1032 | 77   | 0.07    | •    |
| 82  | pc2                   | 1069       | 37  | 5589| 2   | 5566 | 23   | 0.00    | •    |
| 83  | mw1                   | 1071       | 38  | 403 | 2   | 372  | 31   | 0.08    | •    |
| 84  | jEdit_4.0_4.2         | 1073       | 9   | 274 | 2   | 140  | 134  | 0.96    | •    |
| 85  | datatieve             | 1075       | 9   | 130 | 2   | 119  | 11   | 0.09    | •    |
| 86  | PopularKids           | 1100       | 11  | 478 | 3   | 247  | 90   | 0.36    | •    |
| 87  | teachingAssistant     | 1115       | 7   | 151 | 3   | 52   | 49   | 0.94    | •    |
| 88  | musk                  | 1116       | 170 | 6598| 2   | 5581 | 1017 | 0.18    | •    |
| 89  | badges2               | 1121       | 12  | 294 | 2   | 210  | 84   | 0.40    | •    |
| 90  | pc1_req               | 1167       | 9   | 320 | 2   | 213  | 107  | 0.50    | •    |
| 91  | MegaWatt1             | 1442       | 38  | 253 | 2   | 226  | 27   | 0.12    | •    |
| 92  | PizzaCutter1          | 1443       | 38  | 661 | 2   | 609  | 52   | 0.09    | •    |
| 93  | PizzaCutter3          | 1444       | 38  | 1043| 2   | 916  | 127  | 0.14    | •    |
| 94  | CostaMadrel           | 1446       | 38  | 296 | 2   | 258  | 38   | 0.15    | •    |
| 95  | CastMetal1            | 1447       | 38  | 327 | 2   | 285  | 42   | 0.15    | •    |
| 96  | PieChart1             | 1451       | 38  | 705 | 2   | 644  | 61   | 0.09    | •    |
| 97  | PieChart2             | 1452       | 37  | 745 | 2   | 729  | 16   | 0.02    | •    |
| 98  | PieChart3             | 1453       | 38  | 1077| 2   | 943  | 134  | 0.14    | •    |
| 99  | acute-inflammations   | 1455       | 7   | 120 | 2   | 70   | 50   | 0.71    | base |
| 100 | appendicitis          | 1456       | 8   | 106 | 2   | 85   | 21   | 0.25    | base |
| 101 | artificial-characters | 1459       | 8   | 10218| 10 | 1416 | 600  | 0.42    | base |
| 102 | banknote-authentication | 1462 | 5 | 1372 | 2 | 762 | 610 | 0.80    | base |
| 103 | blogger               | 1463       | 6   | 100 | 2   | 68   | 32   | 0.47    | •    |
| 104 | blood-transfusion-service-center | 1464 | 5 | 748 | 2 | 570 | 178 | 0.31    | base |
Table B4: (Multi-class) classification OpenML datasets (105 to 141) 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), the number of examples belonging to the majority and minority classes (nMaj, nMin), the proportion between them (P), and whether the dataset was added to the enrichment step for meta-learning.

| Nro | OpenML name                  | OpenML did | D  | N    | C  | nMaj | nMin | P       | Meta |
|-----|------------------------------|------------|----|------|----|------|------|---------|------|
| 105 | breast-tissue                | 1465       | 10 | 106  | 6  | 22   | 14   | 0.64    | base |
| 106 | cardiotography               | 1466       | 35 | 2126 | 10 | 579  | 53   | 0.091   | base |
| 107 | cnae-9                       | 1468       | 57 | 1080 | 9  | 120  | 120  | 1.00    |      |
| 108 | fertility                    | 1473       | 10 | 100  | 2  | 88   | 12   | 0.14    | base |
| 109 | first-order-theorem-proving  | 1475       | 52 | 6118 | 6  | 2554 | 486  | 0.19    | base |
| 110 | hill-valley                  | 1479       | 101| 1212 | 2  | 606  | 606  | 1.00    | base |
| 111 | ilpd                         | 1480       | 11 | 583  | 2  | 416  | 167  | 0.40    |      |
| 112 | lsvt                         | 1484       | 311| 126  | 2  | 42   | 50   | 0.50    | base |
| 113 | ozone-level-8hr              | 1487       | 73 | 2534 | 2  | 2374 | 160  | 0.07    | base |
| 114 | parkinsons                   | 1488       | 23 | 195  | 2  | 147  | 48   | 0.33    | base |
| 115 | phoneme                      | 1489       | 6  | 5404 | 2  | 3818 | 1586 | 0.42    |      |
| 116 | one-hundred-plants-shape     | 1492       | 65 | 1600 | 100| 16   | 16   | 1.00    | base |
| 117 | qsar-biodeg                  | 1494       | 42 | 1055 | 2  | 699  | 356  | 0.51    |      |
| 118 | qualitative-bankruptcy       | 1495       | 7  | 250  | 2  | 143  | 107  | 0.75    |      |
| 119 | ringnorm                     | 1496       | 21 | 7400 | 4  | 3736 | 3664 | 0.98    |      |
| 120 | wall-robot-navigation        | 1497       | 25 | 5456 | 4  | 2205 | 328  | 0.15    | base |
| 121 | sa-heart                     | 1498       | 10 | 462  | 2  | 302  | 160  | 0.53    |      |
| 122 | steel-plates-fault           | 1504       | 34 | 1941 | 4  | 1268 | 673  | 0.53    | base |
| 123 | thoracic-surgery             | 1506       | 17 | 470  | 4  | 400  | 70   | 0.18    | base |
| 124 | twnorm                       | 1507       | 21 | 7400 | 2  | 3703 | 3097 | 1.00    |      |
| 125 | wdbc                         | 1510       | 31 | 569  | 2  | 357  | 212  | 0.59    |      |
| 126 | wholesale-customers          | 1511       | 9  | 440  | 2  | 298  | 142  | 0.48    |      |
| 127 | heart-long-beach             | 1512       | 14 | 200  | 5  | 56   | 10   | 0.18    | base |
| 128 | robot-failures-lp4           | 1519       | 91 | 117  | 3  | 72   | 21   | 0.29    |      |
| 129 | robot-failures-lp5           | 1520       | 91 | 164  | 5  | 47   | 21   | 0.45    |      |
| 130 | vertebra-column              | 1523       | 7  | 310  | 3  | 150  | 60   | 0.40    | base |
| 131 | volcanoes-a2                 | 1528       | 4  | 1623 | 5  | 1471 | 29   | 0.02    |      |
| 132 | volcanoes-a3                 | 1529       | 4  | 1521 | 5  | 1369 | 29   | 0.02    |      |
| 133 | volcanoes-b1                 | 1531       | 4  | 10176| 5  | 9791 | 26   | 0.00    |      |
| 134 | volcanoes-b3                 | 1533       | 4  | 10386| 5  | 10006| 25   | 0.00    |      |
| 135 | volcanoes-b5                 | 1535       | 4  | 9989 | 5  | 9599 | 26   | 0.00    |      |
| 136 | volcanoes-b6                 | 1536       | 4  | 10130| 5  | 9746 | 26   | 0.00    |      |
| 137 | volcanoes-d2                 | 1539       | 4  | 9172 | 5  | 8670 | 56   | 0.01    |      |
| 138 | volcanoes-d3                 | 1540       | 4  | 9285 | 5  | 8771 | 58   | 0.01    |      |
| 139 | autoUniv-au1-1000            | 1547       | 21 | 1000 | 2  | 741  | 259  | 0.35    | base |
| 140 | autoUniv-au6-750             | 1549       | 41 | 750  | 8  | 165  | 57   | 0.35    | base |
| 141 | autoUniv-au6-400             | 1551       | 41 | 400  | 8  | 111  | 25   | 0.23    | base |
Table B5: (Multi-class) classification OpenML datasets (142 to 182) 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), the number of examples belonging to the majority and minority classes (nMaj, nMin), the proportion between them (P), and whether the dataset was added to the enrichment step for meta-learning.

| Nro | OpenML name                  | OpenML did | D | N    | C   | nMaj | nMin | P    | Meta  |
|-----|------------------------------|------------|---|------|-----|------|------|------|-------|
| 142 | autoUniv-au7-1100            | 1552       | 13| 1100 | 5   | 305  | 153  | 0.50 | base  |
| 143 | autoUniv-au7-500             | 1554       | 13| 500  | 5   | 192  | 43   | 0.22 | base  |
| 144 | acute-inflammations          | 1556       | 7 | 120  | 2   | 61   | 59   | 0.97 | •     |
| 145 | bank-marketing               | 1558       | 17| 4521 | 2   | 4000 | 521  | 0.13 | base  |
| 146 | breast-tissue                | 1559       | 10| 106  | 4   | 49   | 14   | 0.29 | •     |
| 147 | hill-valley                  | 1566       | 101| 1212 | 2   | 612  | 600  | 0.98 | •     |
| 148 | wilt                         | 1570       | 6 | 4839 | 2   | 4578 | 261  | 0.06 | •     |
| 149 | SPECTF                       | 1600       | 45 | 267  | 2   | 212  | 55   | 0.26 | •     |
| 150 | PhishingWebsites             | 4534       | 31 | 11055 | 2   | 6157 | 4898 | 0.80 |        |
| 151 | MiceProtein                  | 4550       | 82 | 1080 | 8   | 150  | 105  | 0.70 | •     |
| 152 | cylinder-bands               | 6332       | 40 | 540  | 2   | 312  | 228  | 0.73 | •     |
| 153 | thyroid-allbp                | 40474      | 27 | 2800 | 5   | 1632 | 31   | 0.02 | base  |
| 154 | thyroid-allhyper             | 40475      | 27 | 2800 | 5   | 1632 | 31   | 0.02 | •     |
| 155 | LED-display-domain-7digit    | 40496      | 8  | 500  | 10  | 57   | 37   | 0.65 | base  |
| 156 | texture                      | 40499      | 41 | 5500 | 11  | 500  | 500  | 1.00 | base  |
| 157 | cmc                          | 23         | 10 | 1473 | 3   | 629  | 333  | 0.53 | base  |
| 158 | credit-a                     | 29         | 16 | 690  | 2   | 383  | 307  | 0.80 | •     |
| 159 | page-blocks                  | 30         | 11 | 5473 | 5   | 4913 | 28   | 0.01 | base  |
| 160 | heart-h                      | 51         | 14 | 294  | 5   | 188  | 0    | 0.00 | base  |
| 161 | banana                       | 1460       | 3  | 5300 | 2   | 2924 | 2376 | 0.81 | base  |
| 162 | planning-relax               | 1490       | 13 | 182  | 2   | 130  | 52   | 0.40 | •     |
| 163 | one-hundred-plants-margin    | 1491       | 65 | 1600 | 100 | 16   | 16   | 1.00 | base  |
| 164 | user-knowledge               | 1508       | 6  | 403  | 5   | 129  | 24   | 0.19 | base  |
| 165 | volcanoes-a1                 | 1527       | 4  | 3252 | 5   | 2952 | 58   | 0.02 | •     |
| 166 | volcanoes-a4                 | 1530       | 4  | 1515 | 5   | 1365 | 29   | 0.02 | •     |
| 167 | autoUniv-au7-700             | 1553       | 13 | 700  | 3   | 245  | 214  | 0.87 | base  |
| 168 | autoUniv-au6-1000            | 1555       | 41 | 1000 | 8   | 240  | 89   | 0.37 | base  |
| 169 | live-disorders               | 8          | 6  | 345  | 2   | 200  | 145  | 0.58 | base  |
| 170 | autoUniv-au4-2500            | 1548       | 100| 2500 | 3   | 1173 | 196  | 0.47 | base  |
| 171 | cardiotocography v.2 (version 2) | 1560   | 35 | 2126 | 3   | 1655 | 176  | 0.78 | base  |
| 172 | cloud                        | 210        | 6  | 108  | 4   | 32   | 10   | 0.30 | base  |
| 173 | solar-flare                  | 173        | 12 | 1066 | 6   | 83   | 24   | 0.29 | base  |
| 174 | heart-h v.3 (version 3)      | 1565       | 13 | 294  | 5   | 188  | 15   | 0.64 | base  |
| 175 | micro-mass                   | 1514       | 1300| 360 | 10  | 36   | 36   | 1.00 | base  |
| 176 | mfeat-factors                | 12         | 217 | 2000 | 10  | 200  | 200  | 1.00 | base  |
| 177 | mushroom                     | 24         | 21 | 8124 | 2   | 4208 | 3916 | 0.52 | base  |
| 178 | nursery (v.3)                | 1568       | 9  | 12958| 4   | 4320 | 4044 | 0.93 | base  |
| 179 | ozone_level v.2              | 40735      | 72 | 2536 | 2   | 2460 | 76   | 0.97 | base  |
| 180 | one-hundred-plants-texture   | 1493       | 65 | 1600 | 100 | 16   | 16   | 1.00 | base  |
| 181 | seeds                        | 1499       | 7  | 210  | 3   | 70   | 70   | 1.00 | base  |
| 182 | semeion                      | 1901       | 257| 1593 | 10  | 161  | 155  | 0.96 | base  |
Appendix C  Hyperparameter distributions of
the best solutions returned by
the Irace tuning technique

Fig. C1: Distribution of the J48 hyperparameters. Default values of the
umerical hyperparameters are identified by black vertical dashed lines.
Fig. C2: Distribution of the CART hyperparameters. Default values of the numerical hyperparameters are identified by black vertical dashed lines.