Robust subgroup discovery

Discovering subgroup lists using MDL

Hugo M. Proença · **Thomas Bäck** · **Matthijs van Leeuwen**

Abstract We introduce the problem of *robust subgroup discovery*, i.e., finding a set of interpretable descriptions of subsets that 1) stand out with respect to one or more target attributes, 2) are statistically robust, and 3) non-redundant. Many attempts have been made to mine either *locally* robust subgroups or to tackle the pattern explosion, but we are the first to address both challenges at the same time from a *global* perspective.

First, we formulate a broad model class of subgroup lists, i.e., ordered sets of subgroups, for univariate and multivariate targets that can consist of nominal or numeric variables. This novel model class allows us to formalize the problem of optimal robust subgroup discovery using the Minimum Description Length (MDL) principle, where we resort to optimal Normalized Maximum Likelihood and Bayesian encodings for nominal and numeric targets, respectively. Notably, we show that our problem definition is equal to mining the top-1 subgroup with an information-theoretic quality measure plus a penalty for complexity.

Second, as finding optimal subgroup lists is NP-hard, we propose RSD, a greedy heuristic that finds good subgroup lists and guarantees that the most significant subgroup found according to the MDL criterion is added in each iteration, which is shown to be equivalent to a Bayesian one-sample proportions, multinomial, or t-test between the subgroup and dataset marginal target distributions plus a multiple hypothesis testing penalty. We empirically show on 54 datasets that RSD outperforms previous subgroup set discovery methods in terms of quality and subgroup list size.

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1 Introduction

Exploratory Data Analysis (EDA)(Tukey, 1977) aims at enhancing its practitioner natural ability to recognize patterns in the data being studied. The more she explores the more she discovers, but also the higher the risk of finding interesting results arising out of coincidences, as, e.g., spurious relations between variables that have no connection in the real world. Intuitively this corresponds to testing multiple hypothesis without realizing it. This duality of EDA requires a thorough analysis of results and highlights the need for statistically robust techniques that allow us to explore the data in a responsible way. While EDA encompasses all techniques referring to data exploration, *Subgroup Discovery* (SD) (Klösgen, 1996; Atzmueller, 2015) is the subfield that is concerned with discovering interpretable descriptions of subsets of the data that stand out with respect to a given target variable, i.e., *subgroups*. This work aims at improving the discovery of subgroup lists, i.e., ordered sets of subsets, that describe different regions of the data, while being statistically robust by themselves and against multiple hypothesis testing. Two simple examples of subgroup lists can be found in Figures 1 and 2.

			$\mathbf{Pr}(\boldsymbol{animaltype} = \cdots \mid \boldsymbol{s})$ in %						
s	**description**	n_s	Mammal	Fish	Invert.	Bug	Reptile	Amph.	Bird
1	backbone = no	18	0	0	56	44	0	0	0
2	breathes = no	14	0	93	0	0	7	0	0
3	feathers = yes	20	0	0	0	0	0	0	100
4	milk = no	8	0	0	0	0	50	50	0
5	feathers = no	41	100	0	0	0	0	0	0
dataset distribution		0*	41	13	10	8	5	4	2

Fig. 1: *Zoo* dataset subgroup list obtained by RSD. *Zoo* contains one nominal target variable with 7 classes, 101 instances, and 15 binary and 1 numeric variables. n_s refers to the number of instances covered by subgroup 's' defined by 'description'. Pr($animaltype = * \mid s$) denotes the estimated probability (in %) of each class label occurring within the subgroup. The bottom row shows the marginal probability distribution of the dataset. $*$ concerns instances not covered by any of the five subgroups. For illustrative purposes the probabilities displayed correspond to the empirical probabilities in the data, not to the probabilities as would be obtained using the appropriate estimator.

			price (K)	
s	**description** of automobile specifications	n_s	$\hat{\mu}$	$\hat{\sigma}$
1	weight = heavy & consumption-city $\leq$ 8 km/L	11	35	8
2	fuel-type = gas & consumption-city $\geq$ 13 km/L	45	7	1
3	weight = light & wheel-base = low	35	9	1
4	length = medium & 13 $\leq$ consumption-city $\leq$ 15 km/L	27	10	2
5	peak-rpm = medium	49	16	3
6	engine-size = medium	12	26	7
	dataset overall distribution	18*	13	8

Fig. 2: *Automobile import 1985* subgroup list obtained with RSD. The dataset contains *price* as numeric target variable, 197 examples, and 17 variables. The dataset was modified, some variables removed and others discretized, for ease of presentation. n_s refers to the number of instances covered by subgroup 's' defined by 'description', $\hat{\mu}$ and $\hat{\sigma}$ its estimated mean and standard deviation for the target variable in thousands of dollars (K). $*$ concerns instances not covered by any of the five subgroups.

Subgroup discovery (SD) can be seen as the exploratory counterpart to rule learning or association rule mining, where the targets/consequent of the rules are fixed and rules are ranked according to quality measures combining subgroup size and deviation of the target variable(s) with respect to the overall distribution in the data. In its traditional form, subgroup discovery is also referred to as top-k subgroup mining (Atzmueller, 2015), which entails mining the k top ranking subgroups according to a *local* quality measure and a number k selected by the user. Since its conception subgroup discovery has been developed for various types of data and targets, e.g., nominal, numeric (Grosskreutz and Rüping, 2009), and multi-label (van Leeuwen, 2010) targets. SD has been applied in a wide range of different domains (Herrera et al., 2011; Atzmueller, 2015), such as identifying the properties of materials (Goldsmith et al., 2017), unusual consumption patterns in smart grids (Jin et al., 2014), identifying the characteristics of delayed flights (Proença et al., 2018), and understanding the influence of pace in long distance running (De Leeuw et al., 2018).

Even though SD appeals to several domains, top-k mining traditionally suffers from three main issues that make it impractical for many applications: 1) poor efficiency of exhaustive search for more relevant quality measures (Boley et al., 2017); 2) *redundancy* of mined subgroups, i.e., the fact that subsets with the highest deviation according to a certain *local* quality measure tend to cover the same region of the dataset with slight variations in their description of the subset (Van Leeuwen and Knobbe, 2012); 3) lack of generalization or statistical robustness of mined subgroups (van Leeuwen and Ukkonen, 2016). In this work we focus on the last two issues together: lowering *redundancy* by finding small lists of subgroups that describe the differences in the data well; and obtaining *statistically robust* subgroups. First, we define what an optimal subgroup list is using the MDL principle and second, we propose a greedy algorithm that finds good subgroup lists using a *local* objective that is equiv-

alent to maximizing a Bayesian one-sample proportions, multinomial or t-test between each subgroup's distribution and the dataset marginal distribution, for binary, nominal or numeric data, respectively, plus a penalty for multiple hypothesis testing.

In recent years both issues have been partially addressed, mostly independent of each other; we next briefly discuss recent advances and limitations.

In terms of *redundancy*, the first main limitation of existing works is their focus on one type of target variables, such as binary targets (Bosc et al., 2018; Belfodil et al., 2019), nominal targets(Lavrač et al., 2004), or numeric targets (Lijffijt et al., 2018), where only DSSD focuses on univariate and multivariate nominal and numeric targets (Van Leeuwen and Knobbe, 2012). The second main limitation is the lack of an optimality criterion for subgroup sets or lists, where the only exception is FSSD (Belfodil et al., 2019). It is important to emphasize that some works aim at finding sequential subgroups or subgroup *lists*, while others aim at finding unordered sets or subgroup *sets*. Subgroup lists are akin to rule lists (Proença and van Leeuwen, 2020) in the sense that each subgroup/rule needs to be interpreted sequentially and they are not allowed to overlap, while subgroup sets are allowed to overlap. In this work we focus solely on subgroup lists, and although previous works often did not use this term we retroactively rename those models that are in fact subgroup lists.

In terms of *statistical robustness*, most existing approaches consider first mining the top-k subgroups and then post-processing them in terms of a statistical test to find if the discovered subgroups are statistically significant (Duivesteijn and Knobbe, 2011; van Leeuwen and Ukkonen, 2016). More recently, Proença et al. (2020) proposed for the first time a global formulation of a subgroup list for numeric targets over the whole dataset. The approach is based on the Minimum Description Length (MDL) principle, taking into account the variance of the subgroup targets distribution to measure their quality. Our present work is an extension of this approach, extending the MDL formulation and algorithm to univariate and multivariate nominal and numeric targets; we discuss the relationship in more detail below.

For an in-depth analysis of related work please refer to Section 2.

Robust subgroup discovery. Informally the problem of robust subgroup discovery is to define and find the *globally* optimal set or list (i.e., an ordered set) of non-redundant subgroups that together explain the most relevant *local* deviations in the data with respect to specified target variables. As finding the optimal set or list will typically be practically infeasible, the secondary problem is to construct an algorithm that efficiently mines 'good' subgroup sets or lists from the data that retains as much from the statistical properties of the *global* formulation as possible.

In this work we restrict our focus to finding *subgroup lists*, because 1) they were one of the first model classes proposed for subgroup set discovery (Lavrač et al., 2004); 2) they allow for an optimal formulation based on the MDL principle due to its property of unambiguously partitioning the data into non-

overlapping parts; and 3) finally, they allow an ordered interpretation of the subgroups, i.e., from most to least relevant discovered subgroup.

Contributions. We aim to bridge the gap in the literature by finding the best non-redundant subgroup list from a *global* dataset perspective, while guaranteeing the *local* quality of the found subgroups, making the approach statistically robust from both perspectives. Two examples of subgroup lists for nominal and numeric targets can be seen in Figures 1 and 2. To solve this problem we propose a formal definition of a *subgroup list* and employ the Minimum Description Length (MDL) (Rissanen, 1978) principle to define its optimality from a global perspective. We provide this formalization for univariate and multivariate nominal and numeric targets, and notably the subgroup that minimizes the MDL-optimal formulation for a subgroup list with one subgroup is the same subgroup that would be found by top-1 subgroup discovery with Weighted Kullback-Leibler divergence (WKL) as quality measure. This makes it the first *global* formulation of subgroup discovery.
To find subgroup lists we propose RSD, a heuristic algorithm that combines beam search to find subgroups with greedy search to iteratively add the best found subgroup to the subgroup list. Maximizing the MDL criterion in each iteration guarantees that each subgroup added to the list adheres to a *local* statistical test equivalent to a Bayesian proportions, multinomial, or t-test (for binary, nominal and numeric targets, respectively) plus a penalty to compensate for multiple hypothesis testing.
This work is an extension of Proença et al. (2020), in which we introduced MDL-based subgroup lists for univariate numeric target variables and SSD++, a heuristic algorithm for finding such subgroup lists. The current manuscript significantly extends our previous work by generalizing theoretical, algorithmic, and empirical results to three new target variable types, namely multivariate numeric targets, and univariate and multivariate nominal targets. Moreover, we provide a new interpretation of the greedy gain as an MDL equivalent to a Bayesian factor.
To summarize, the *primary* contributions presented in this work—including the contributions originally from Proença et al. (2020), which we indicate with a * below—are:

1. **Subgroup list model class** – We define the subgroup list model class* over a tabular dataset in general (Section 4.1), providing a *global* formulation for the problem of sequential subgroup mining, and in particular for univariate and multivariate nominal targets (Section 5), and univariate numeric* and multivariate numeric targets (Section 6).
2. **Robust subgroup lists using MDL** – We define optimal subgroup lists using the MDL principle (Section 4), where we resort to the optimal Normalized Maximum Likelihood (NML) encoding for nominal targets (Section 5) and the Bayesian encoding with non-informative priors for numeric targets* (Section 6). Notably, we show that this problem formalization is equivalent to the standard definition of top-1 subgroup discovery with

WKL as quality measure for the case of a subgroup list with one subgroup (Section 5.4 for nominal targets and Section 6.4 for numeric targets*).
3. **RSD algorithm** – We propose the *Robust Subgroup Discoverer* (RSD) algorithm that combines beam search to find subgroups with greedy search to iteratively add the best found subgroup to the subgroup list* (Section 7). We show that the greedy objective is equivalent to a one-sample Bayes proportions, multinomial, and t-test (for binary, nominal and numeric* targets, respectively) plus a penalty to compensate for multiple hypothesis testing (Section 5.5 for binary and nominal targets, Section 6.5 for numeric targets, and Section 7.3 for the greedy objective of RSD).
4. **Greedy MDL algorithms maximize local statistical test** – We show that the greedy gain commonly used in the MDL for pattern mining literature can be interpreted as an MDL equivalent to a *local* Bayesian hypothesis test, a.k.a. Bayesian factor, on the likelihood of the data being better fitted by the greedy extended model versus the current model plus a penalty for the extra model complexity (Section 7.3).

Moreover, this work includes the following *secondary* contributions, the details of which are all included in the appendices for the interested reader:

5. **Normalized Maximum Likelihood for partition models** – Derivation of the Normalized Maximum Likelihood (NML) optimal encoding, a refined MDL encoding, for model classes that partition the data for nominal target variables—subgroup lists, rule lists, trees, etc. (Appendix A).
6. **Bayesian encoding of normal distributions** – Derivation of a Bayesian optimal encoding of normal distributions with non-informative priors for numeric targets* (Appendix B). It is shown that for large number of instances it converges to the BIC* (Appendix C). Similarly to the NML encoding it can be used by any model class that unambiguously partitions the data, such as subgroup lists, rule lists, trees, etc.
7. **Dispersion-aware Weighted Kullback-Leibler** – We propose the Weighted Kullback-Leibler (WKL) divergence between normal distributions as spread-aware (dispersion-aware) quality measure for numeric targets* (Appendix D for the derivation and formula).
8. **Subgroups discovery versus rule-based prediction** – We demonstrate the difference between the formal objectives for subgroup discovery and predictive rule models, such as classification rule lists, from the perspective of our MDL-based approach (Appendix E).

Structure of this work. In Section 2 the most relevant related work is covered, together with the main differences to our approach. Then, in Section 3 the preliminaries are presented and the problem of subgroup discovery and subgroup set discovery are defined. After that, in Section 4 the Minimum Description Length (MDL) principle is stated, the subgroup lists model class is presented, the model encoding (akin to multiple hypothesis testing) is defined, and the general form of the data encoding is presented. Then, in Sections 5 and 6 the specific data encodings for numeric and nominal target variables

are defined, respectively, together with their respective statistical properties and equivalence to the standard definition of subgroup discovery. After that, in Section 7 the RSD, a heuristic algorithm to mine subgroup lists is defined, as well as its statistical guarantees and time complexity. Then, in Section 8 we show the empirical results of our proposed method when compared against the state-of-the-art algorithms for univariate and multivariate nominal and numeric targets over 54 datasets. After that, in Section 9 we apply robust subgroup discovery to find how descriptions of the socioeconomic background affects the grades of engineering students in Colombia. Finally, in Section 10 the main conclusions are presented.

2 Related work

In this section we cover work related to our proposed MDL subgroup lists, in four categories: *subgroup discovery*; *pattern mining*; *rule lists*; *MDL for pattern mining*; and *algorithmic implementations*. The relevance of each topic is as follows: subgroup discovery directly relates to the task at hand; pattern mining and association rule mining are a generalizations of subgroup discovery; rule lists share the same model structure as subgroup lists; MDL for pattern mining shares the same theory for formalizing the problem; and lastly we go over most of the same works but from an algorithm implementation perspective in order to justify our algorithmic choices.

2.1 Subgroup discovery

In its traditional form, subgroup discovery, also referred to as top-k subgroup mining (Atzmueller, 2015), entails the mining of the k top ranking subgroups according to a quality measure and a number k selected by the user. As mentioned in the introduction, this formulation suffers from three main issues that make it impractical for most applications: 1) poor *efficiency of exhaustive search* for more relevant quality measures (Boley et al., 2017); 2) *redundancy of subgroup sets* mined, i.e., the fact that subsets with the highest deviation according to a certain quality measure tend to cover the same region of the dataset with slight variations in their description of the subset (Van Leeuwen and Knobbe, 2012); 3) lack of *statistical guarantees* and generalization of mined subgroups (van Leeuwen and Ukkonen, 2016). We will now go over the recent contributions for these three issues, with special emphasis for the last two, redundancy and statistical guarantees, which our work proposes to solve.

Efficient exhaustive search. In the last years several developments have been made towards more efficient algorithms for mining the top-k subgroups. Lemmerich et al. (2016) proposed an efficient exhaustive search algorithm for numerical targets, Belfodil et al. (2018) proposed to mine over numeric attributes with guarantees, and Boley et al. (2017) proposed an algorithm that exhaustively mines subgroups that take into account the dispersion (deviation) of the

subgroups target distribution. Subgroup discovery extension from deviations of distributions of target variables to deviations between models is also called Exceptional model mining (Leman et al., 2008; Duivesteijn et al., 2016), and can be applied to models such as Bayesian Networks (Duivesteijn et al., 2010) or non-parametric spatio-temporal patterns (Du et al., 2020). Comparing to our approach these works do not take into account the redundancy of the subgroups found, and thus, the subgroups found tend to overlap in the same region of the dataset.

Redundancy of subgroup sets. To address redundancy among subgroups most previously proposed approaches encompass supervised pattern set mining (Bringmann and Zimmermann, 2007), and methods based on relevance (Großkreutz et al., 2012) and diversity (Van Leeuwen and Knobbe, 2011, 2012). Unlike diversity-based methods, the supervised pattern set mining objective is to find a fixed number of patterns, which has to be chosen in advance, while relevance is limited to non-numeric targets. It is this last group, the diversity based methods that share most similarities to our work, i.e., the area of *Subgroup Set Discovery.*

The main approaches in *Subgroup Set Discovery* are CN2-SD (Lavrač et al., 2004), Diverse Subgroup Set Discovery (DSSD) (Van Leeuwen and Knobbe, 2012), *Skylines* of subgroup sets (Van Leeuwen and Ukkonen, 2013), Monte Carlo Tree Search for Data Mining (MCTS4DM) (Bosc et al., 2018), Subjectively Interesting Subgroup Mining (SISD) (Lijffijt et al., 2018), and FSSD (Belfodil et al., 2019). The differences between Subgroup Set Discovery methods are summarized in Table 1, with RSD representing our approach and where all methods are compared in terms of: if they use a list or a set; the target variables they support; if they have statistical guarantees; if they have an automatic stopping criteria (not defined by the user); and if they have a global definition of a subgroup set or list.
Considering the methods in more detail, CN2-SD (Lavrač et al., 2004) was one of the first methods to deal with redundancy and is a direct adaptation of CN2, a classical rule learner and can be applied to nominal target variables. It uses a sequential approach, where in each iteration it adds one subgroup to the set, and then removes the data covered by that subgroup, until no more data can be covered in this way. DSSD (Van Leeuwen and Knobbe, 2012) developed a technique based on a novel measure of overlap between subgroups, to iteratively find a set of subgroups. It can be applied to single-and-multi-target nominal and numeric variables, with different types of quality measures. Skylines of subgroup sets (Van Leeuwen and Ukkonen, 2013) proposed to directly account for quality-diversity trade-off, to find the Pareto optimal subgroup sets of size k. MCTS4DM (Bosc et al., 2018) uses Monte Carlo tree search to improve the quality of the subgroups found, although it can only be applied to binary target variables, and to attributes of the same type (all numeric or all nominal). Subjectively interesting Subgroup Discovery (Lijffijt et al., 2018) finds the subjectively most interesting subgroup for numeric target variables with

regard to the prior knowledge of the user, based on an information-theoretic framework for formalizing subjective interestingness. By successively updating the prior knowledge based on the found subgroups, it iteratively mines a diverse set of subgroups that are also dispersion-aware. FSSD (Belfodil et al., 2019) is a more recent approach that considers the 'union' of all subgroups as a single pattern by forming a disjunction of subgroups and evaluating its quality and can only be applied to binary target variables. This approach is similar to a sequential approach for mining subgroups although the individual contributions of each subgroup are dissolved in the 'new' subgroup formed by the disjuction of all subgroups. like$^{\text{this}}$

Table 1: Comparison of Subgroup Set Discovery methods in terms of their key properties. From left to right: model class (list or set); types of supported target variables: binary, nominal, numeric and multi-target; *statistical* guarantees of the subgroups mined; automatic *stopping* criterion (not defined by the user); *global* formulation of a subgroup set/list.

		Target variables						
Method	Model	binary	nom.	num.	multi	Statistical	Stopping	Global
RSD	list	✓	✓	✓	✓	✓	✓	✓
CN2-SD	list	✓	✓	-	-	-	-	-
DSSD	set	✓	✓	✓	✓	-	-	-
Skylines	set	✓	✓	-	-	-	-	✓
MCTS4DM	set	✓	-	-	-	-	-	-
SISD	set	-	-	✓	✓	✓	-	-
FSSD	list	✓	-	-	-	-	✓	✓

Statistical guarantees. In terms of statistical guarantees to subgroup discovery, most approaches consider first mining the top-k subgroups and then post-processing them in terms of a test to find subgroups that are statistically significant (Duivesteijn and Knobbe, 2011; van Leeuwen and Ukkonen, 2016). Duivesteijn and Knobbe (2011) proposed to use random permutations of the target variable with respect to a quality measure to evaluate how the discovered subgroups compare against the null hypothesis generated by those permutations. Later, van Leeuwen and Ukkonen (2016) discussed the concept of significance for subgroup discovery, and concluded that p-values should be used with caution as not all false discoveries can be removed in this way, as there will always be random subsets with large effect sizes. An exception to this is the work of Lijffijt et al. (2018) (already mentioned in the last section), which uses the maximum entropy principle to iteratively find subgroups that are subjectively interesting against a user's prior knowledge. Our approach strongly deviates from the first two, as our method tests for statistical guarantees during the mining process, it is parametric, as we use categorical and normal distributions to model the targets, and also, through the use of MDL-based model encoding we take into account the concept of a list of subgroups

and penalize for all the possible subgroup lists that could be discovered in the dataset. Regarding the last approach, even though they also mine subgroups iteratively, they lack a definition of an optimal subgroup set, and their goal is to model the user's subjective knowledge and find regions in the data that the user does not know much about.

2.2 Pattern mining

Pattern mining and association rule mining (Agrawal et al., 1993) are concerned with mining items that co-occur together, i.e., itemsets or patterns, and relationships between itemsets and a target item, e.g., a class, respectively. A key problem is that they suffer from the infamous *pattern explosion*, i.e., they tend to return enormous amounts of patterns/rules. To solve this problem, many approaches were proposed, but two stand out in relation to our work, namely, association rule classifiers and statistical rule mining.

Association rule classifiers. A simple way to reduce the number of rules returned is by aggregating association rules in a set used for classification and using a performance measure to choose the best set. It is relevant to notice that classifiers based on association rule mining have a similar structure to rule lists and subgroup lists, as they tend to order the rules sequentially. The best-known techniques are CBA (Ma and Liu, 1998) and CMAR (Li et al., 2001), but they tend to obtain large numbers of rules. Similar to rule lists, the aim of these methods is to maximize the classification performance, and not to describe the deviations in the data. Another important difference is that these methods tend to return crisp decisions instead of probabilities and can in general only be applied to nominal targets.
A similar class of methods is that of *supervised pattern set mining* (Zimmermann and Nijssen, 2014). The key difference is that these methods do not automatically trade-off model complexity and classification accuracy, requiring the analyst to choose the number of patterns k in advance.

Statistical rule mining. The idea of mining rules with statistical guarantees is appealing as it increases the users trust in the patterns found while at the same time reducing the number of rules returned by a miner (Hämäläinen and Webb, 2019). The concept of statistical rule mining progressed by incrementally adding more statistical guarantees. Webb (2007) proposed for the first time mining of statistically significant patterns, then Hämäläinen (2012) proposed KingFisher, an efficient algorithm to mine dependent rules, i.e., rules that show a dependency with respect to a target in terms a dependency test like Fisher's exact test. After that, Hämäläinen and Webb (2017) added extra procedures to remove spurious relations from the miner findings. Lastly, the criteria under which causal rules can be mined was defined and an efficient algorithm to mine them was proposed (Budhathoki et al., 2020). All these methods focus on mining all the possible *individual* statistically significant (or

causal) rules and not on finding a set that is non-redundant, as is the case of Subgroup Set Discovery. In this paper, we aim to accomplish both at the same time, finding the best *global* subgroup list while assuring *local* statistically robust subgroups.

2.3 Rule lists

Subgroup lists could be regarded as rule lists with a *fixed* default rule, i.e., the last rule that gets activated when no other rule applies is fixed to 'predict' the global distribution of the complete dataset. Sections 5.4 and 6.4 show that fixating the default rule to the overall dataset distribution makes rule discovery theoretically equivalent to sequential subgroup set discovery.
Rule lists have long been successfully applied for classification; RIPPER is one of the best-known algorithms (Cohen, 1995). Similarly, decision trees, which can be easily transformed to rule lists (Quinlan, 1987), have been used extensively; CART (Breiman et al., 1984) and C4.5 (Quinlan, 2014) are probably the best-known representatives. These early approaches represent highly greedy algorithms that use heuristic methods and pruning to find good models.
Although all algorithms mentioned in this section have some resemblance to our approach, their main goal is to make the best predictions—not to find the largest deviations in the data. Even though the two problems are clearly related, we emphasize the theoretical difference between subgroup discovery and prediction in Appendix E, where the former focuses on *local* deviations and the latter on a *globally* homogeneous partition of the data.

Bayesian rule lists and optimal decision lists. Over the past years, rule learning methods that go beyond greedy approaches have been developed for binary classification, i.e., Monte-Carlo search for Bayesian rule lists (Letham et al., 2015; Yang et al., 2017), and branch-and-bound with tight bounds for decision lists (Angelino et al., 2017). Even though in theory these approaches could be easily extended to the multiclass scenario, in practice their algorithms do not scale with the higher dimensionality of those search spaces. Bayesian rule lists (Letham et al., 2015; Yang et al., 2017) are the most similar to our approach, as they not only provide probabilistic predictions but also use a similar formulation based on Bayesian statistics. Nonetheless, their focus is solely on binary targets and on classification rather than subgroup discovery.

MDL Rule lists. More recently, Proença and van Leeuwen (2020) proposed the use of an MDL formulation of rule lists for multiclass classification. The proposed algorithm can be applied to discretized data, and iteratively adds the best rule from a set of premined patterns found by a frequent pattern miner. Our subgroup lists offer an improved encoding for nominal targets by using the Normalized Maximum Likelihood (Shtar'kov, 1987), an encoding that is optimal for fixed number of examples, versus the asymptotic optimality of the prequential plug-in code or Bayesian code. In terms of the algorithm, our new

RSD algorithm uses a beam search to find the rule/subgroup to add at each iteration, which does not require pre-mined rules and also supports numeric attributes. Aoga et al. (2018) also proposed to use to find rule lists using MDL and a set of premined patterns, although its focus was on parsimonious dataset description—versus deviations or even classification—of small transaction datasets through the use of a heavy penalization MDL encoding of data and model.

2.4 MDL in pattern mining

In the past, for models similar to our subgroup lists, the MDL principle has mostly been embedded in small parts of predictive algorithms to solve the problem of overfitting. Prominent examples of this are C4.5 (Quinlan, 2014) and RIPPER (Cohen, 1995), which use the MDL principle to prune overfitting models, and help generalization. Also, Zhang et al. (2000) used the MDL principle to choose the best compressing pattern for prediction.
In data mining, Krimp (Vreeken et al., 2011) was the first method to apply the MDL principle holistically, i.e., for the whole model selection process, unlike previous mentioned approaches that only used it for a subset of the model selection process. This seminal work used a version of crude MDL, i.e., a not completely optimal 'two-part' encoding of the data, to find the pattern list that compressed a transaction dataset best, in order to address the *pattern explosion* issue in pattern mining. Recent works have aimed at improving the encoding through the use of refined MDL for encoding the data, i.e., an encoding that enjoys optimal properties at least in expectation (Grünwald, 2007). The first of such approaches was DiffNorm (Budhathoki and Vreeken, 2015), which used a prequential plug-in code to improve the encoding of transaction data and recently MINT was proposed to mine real-valued patterns sets with a similar encoding(Makhalova et al., 2020). Although Krimp, DiffNorm and MINT are used to describe data, they aim at finding regularities—not deviations—and do not consider a target variable. For an in-depth survey of MDL in pattern mining please refer to the survey by Galbrun (2020).
MDL has been used to find optimal sets of association rules for two-view data (Van Leeuwen and Galbrun, 2015) and for tabular data (Fischer and Vreeken, 2019). The latter is the most related to our work, as it aims to find rule sets that describe the data well. Similar to Krimp it aims at finding all associations in the data though, not at identifying deviations as we do, and no specific target variable(s) are defined.

2.5 Algorithmic comparison in the literature

Our proposed algorithm RSD (presented in Section 7) is based on a combination of beam search for candidate generation and greedy search for iteratively adding subgroups to the subgroup list. Both techniques have been widely employed for similar problems.

Greedy search has been often used for learning decision trees and rule lists (Quinlan, 2014; Cohen, 1995; Fürnkranz et al., 2012; Proença and van Leeuwen, 2020), as well as for pattern-based modeling using the MDL principle (Vreeken et al., 2011; Budhathoki and Vreeken, 2015; Van Leeuwen and Galbrun, 2015). *Beam search* has been commonly used for candidate generation in subgroup discovery (Meeng and Knobbe, 2011), including for finding subgroup sets (Lavrač et al., 2004; Van Leeuwen and Knobbe, 2012). We next provide the motivation for our algorithmic choices, and describe key similarities and differences compared to algorithms in the most related literature: 1) rule list learning; 2) subgroup set discovery; and 3) evolutionary algorithms for rule learning.

Algorithms for finding rule lists. The common way to finding a good rule list is through heuristic search (Cohen, 1995; Fürnkranz et al., 2012; Proença and van Leeuwen, 2020), however recent works have proposed to find optimal models for binary classification under specific conditions (Yang et al., 2017; Angelino et al., 2017). Belong to the former category, Proença and van Leeuwen (2020) uses a Separate and Conquer (SaC) technique to greedily add rules, together with Frequent Pattern Mining for candidate generation. In this paper, the beam search for candidate generation does not require a discretized dataset, is faster, and without large loss in the quality of the subgroups found due to discretization (Meeng and Knobbe, 2020). In the latter category, of optimal rule list discovery, the algorithms were only developed for binary classification, and either require a simplification of the rules in the list to decision rules—with true or false instead of probabilities as consequent—combined with a simple objective function, such as accuracy, that allows for efficient branch-and-bound (Angelino et al., 2017), or it requires the dataset to be sparse and small, with large minimum supports for the rules (above 10%) and using a convergence to an optimal algorithm such as Monte Carlo sampling (Yang et al., 2017). Neither of these approaches can deal with a variety of target variables as our proposed approach can.

Algorithms for subgroup set discovery. Both beam search and greedy search are commonplace in subgroup set discovery (Lavrač et al., 2004; Van Leeuwen and Knobbe, 2012), due to their efficiency and flexibility in being applied to different types of targets. More recently, Monte Carlo Tree Search (MCTS) was proposed for mining sets of subgroups (Bosc et al., 2018), although it can only be applied to binary targets and specific types of explanatory variables. In the classical case of mining top-k subgroups without incorporating diversity, exhaustive search is feasible (Boley et al., 2017), but again it is only efficient for specific types of quality measures or targets, and does not scale well for finding the best set (Van Leeuwen and Knobbe, 2012). Together with the fact that the loss in quality of using beam search is almost negligible (Meeng and Knobbe, 2020), exact algorithms are almost never used in MDL-based data mining, because it is infeasible (Vreeken et al., 2011; Budhathoki and Vreeken, 2015; Fischer and Vreeken, 2019; Proença and van Leeuwen, 2020).

Evolutionary algorithms. Global heuristics, such as evolutionary algorithms, have been applied to fuzzy rule-based model learning (Fernandez et al., 2015), and although they could also be applied here, we found that the arguments in favor of a local search approach were stronger: 1) local heuristics have often been successfully applied for pattern-based modeling using the MDL principle, making it a natural approach to consider; 2) local heuristics are typically faster than global heuristics, as much fewer candidates need to be evaluated; 3) global heuristics typically require substantially more (hyper)parameters that need to be tuned (e.g., population size, selection and mutation operators, etc.), while local heuristics have very few.

3 Subgroup Discovery

In this section we describe the basic notation and concepts of subgroup discovery. Starting from data and target types, we move to subgroups, their interpretation as probabilistic rules, and quality measures for individual subgroups. We pay specific attention to one such quality measure, Weighted Kullback-Leibler divergence (WKL), because it fits our information-theoretic approach well. Next we specify subgroup set discovery, after which we conclude the section with a novel proposal for a quality measure for subgroup sets based on the WKL measure for individual subgroups.

3.1 Data and target types

Consider a dataset $D = (\mathbf{X}, \mathbf{Y}) = \{(\mathbf{x}^1, \mathbf{y}^1), (\mathbf{x}^2, \mathbf{y}^2), ..., (\mathbf{x}^n, \mathbf{y}^n)\}$ of n *i.i.d.* instances. Each instance $(\mathbf{x}, \mathbf{y})$ is composed of a vector of explanatory variable values $\mathbf{x}$ and a vector of target variable values $\mathbf{y}$. Each observed explanatory vector has m values $\mathbf{x} = [x_1, ..., x_m]$, one for each variable $X_1, ..., X_m$. The domain of a variable X_j, denoted $\mathcal{X}_j$, can be one of two types: nominal or numeric. Similarly, each observed target vector is composed of t values $\mathbf{y} = [y_1, ..., y_t]$, one for each target variable $Y_1, ..., Y_t$, with associated domains $\mathcal{Y}_j$. The target variables can be of two types: numeric, or nominal. In the numeric case, the domain is $\mathcal{Y}_j = \mathbb{R}$ and in the nominal it is $\mathcal{Y}_j = \{1, \cdot, k\}$, with $\mathcal{Y}_j$ the set of classes/categories of variable Y_j. For the complete notation used throughout this work please refer to Table 2.
Note that we use subscripts on the dataset variables $(D, \mathbf{X}, \mathbf{Y}, X, Y, x, y)$ to indicate column indices and superscripts for row indices. In the case of other notation, such as number of elements n or statistics μ, σ we will not use the superscript as it could be confused with the exponentiation of that value. Also, X_i (resp. Y_i) refers to both the properties of the i^{th} explanatory (resp. target) variable and to all the values of this variable for a specific column.

Depending on the type and number of targets (one or multiple), the type of problem can be divided into *four* categories: *1) single-nominal*; *2) single-numeric*; *3) multi-nominal*; and *4) multi-numeric*. In machine learning, the

single-numeric case corresponds to regression, the single-nominal to classification, and in the case of more than one variable their multi-target generalizations, respectively.

3.2 Subgroups

A subgroup, denoted by s, consists of a *description* (also intent) that defines a *cover* (also extent), i.e., a subset of dataset D.

Subgroup description: A description a is a Boolean function over all explanatory variables X. Formally, it is a function $a : \mathcal{X}_1 \times \cdots \times \mathcal{X}_m \mapsto \{false, true\}$. In our case, a description a is a conjunction of conditions on $\mathbf{X}$, each specifying a specific value or interval on a variable. The domain of possible conditions depends on the type of a variable: numeric variables support *greater and less than* $\{\geq, \leq\}$; nominal support *equal to* $\{=\}$. The size of a description a, denoted $|a|$, is the number of conditioned variables it contains.

Example 1: In Figure 2, subgroup 1 has a description of size $|a| = 2$, with one condition on a nominal variable: {weigth = heavy}; and another on a numeric variable: {consumption-city $\leq 8km/L$}.

Subgroup cover: The cover is the bag of instances from D where the subgroup description holds true. Formally, it is defined by:

$$D^a = \{(\mathbf{x}, \mathbf{y}) \in D \mid a \sqsubseteq \mathbf{x}\} = \{X_1^a, \cdots, X_m^a, Y_1^a, \cdots, Y_t^a\} = \{\mathbf{X}^a, \mathbf{Y}^a\}, \quad (1)$$

where we use $a \sqsubseteq \mathbf{x}$ to denote $a(\mathbf{x}) = true$. Further, let $n_a = |D^a|$ denote the coverage of the subgroup, i.e., the number of instances it covers.

Example 2 (continuation): In Figure 2, subgroup 1 covers 11 instances in the dataset which can be found by conditions in its description, and thus its coverage is 11.

3.3 Interpretation as probabilistic rule

As D^a encompasses both the explanatory and target variables, the effect of a on the target variables can be interpreted as a probabilistic rule. Regarding the multiple target variables, we assume that they are *independent*. This simplifies the problem and is a common approach in multi-label classification (Herrera et al., 2016). Thus, the general form of the rule is:

$$a \mapsto y_1 \sim Dist(\hat{\Theta}_1^a), \cdots, y_t \sim Dist(\hat{\Theta}_t^a), \quad (2)$$

where y_j is a value of variable Y_j, $Dist$ is a probability distribution (defined later) and $\hat{\Theta}_j^a$ is the shorthand for the maximum likelihood estimation of the

Table 2: Notation table.

Symbol	Definition
$D = \{\mathbf{X}, \mathbf{Y}\}$	Labelled dataset.
$\mathbf{X}$	Dataset of explanatory variables of D.
X	An explanatory variable of $\mathbf{X}$.
$\mathcal{X}$	Domain of X.
$\mathbf{x}$	A explanatory variables sample of $\mathbf{X}$.
x	The value of sample $\mathbf{x}$ for variable X.
$\mathbf{Y}$	Dataset of target variables of D.
Y	An target variable of $\mathbf{Y}$.
$\mathcal{Y}$	Domain of Y.
$\mathbf{y}$	A target variables sample of $\mathbf{Y}$.
y	The value of sample $\mathbf{y}$ for variable Y.
$\lvert \cdot \rvert$	Number of elements in a set, as e.g., $\lvert D \rvert$ for number of samples.
i	Index for subsetting by row.
j	Index for subsetting by column.
v	A generic explanatory variable.
k	Number of classes of a nominal target variable.
n	Number of examples in dataset D.
m	Number of explanatory variables.
t	Number of target variables.
d	Subscript associated with dataset distribution or defaul rule.
M	Subgroup list model (including subgroups S and default rule).
S	Subgroups in model M.
ω	Number of subgroups in M.
s	A subgroup.
a	Description of a subgroup.
a_i	Description of the i^{th} subgroup in model M.
$D^a = \{\mathbf{X}^a, \mathbf{Y}^a\}$	Samples of dataset D covered by description a.
n_a	Number of samples in D^a. $n_a = \lvert D^a \rvert$.
$D^i = \{\mathbf{X}^i, \mathbf{Y}^i\}$	Samples of dataset D covered by the i^{th} subgroup in model M.
n_i	Number of samples in D^i. $n_i = \lvert D^i \rvert$.
$Dist(\Theta)$	Generic probability distribution with parameters Θ.
$\mathcal{N}(\mu; \sigma)$	Normal probability distribution with parameters μ and σ.
$Cat(p_1, \cdots, p_k)$	Categorical probability distribution with p_i probability per category.
$p_{y\lvert c}$	Probability of category y given description a, i.e., $\Pr(y \mid a)$
μ	Mean value parameter.
σ	Standard deviation parameter.
$\hat{\theta}$	Maximum likelihood estimation of parameter θ.
$q(a)$	Subgroup discovery quality measure.
$Q(S)$	Subgroup set discovery quality measure.
$f(\hat{\Theta}^a, \hat{\Theta}^d)$	Function of differences between distribution $\hat{\Theta}^a$ and $\hat{\Theta}^d$.
α	Tradeoff between subgroup coverage and distribution difference.
KL	Kullback-Leibler divergence general form.
KL_{Cat}	Kullback-Leibler divergence for categorical distributions.
KL_{μ}	Kullback-Leibler divergence for location distributions.
$KL_{\mu,\sigma}$	Kullback-Leibler divergence for normal distributions.
WKL	Weighted Kullback-Leibler divergence general form.
SWKL	Sum of Weighted Kullback-Leibler divergences.
$L_{\mathbb{N}}$	Universal code of integers.
$L_{NML}(Y_j^i)$	Normalized Maximum Likelihood length of encoding of data Y_j^i.
$\mathcal{C}(n_a, k)$	Multinomial distribution complexity with n_a points and k categories.
L_{Bayes}	Bayesian length of encoding with improper priors.
$Y^{i\lvert 2}$	The two points that make the Bayesian encoding proper.
$L_{Bayes2.0}$	Bayesian length of encoding made proper with first 2 points.
$\Gamma(n)$	Gamma function, the extension of the factorial to real numbers.
$\Delta_{\beta} L(D, M \oplus s)$	Compression gain of adding subgroup s to model M.
β	Level of normalization of the compression gain.
ζ	Set of all items (possible single conditions) in $\mathbf{X}$.
$stats$	Statistics of a subgroup.
d_{max}	Beam search maximum depth of search.
w_b	Beam search beam width.
n_{cut}	Number of cut points for numeric discretization.

parameters of $Dist$ over values Y_j^a, i.e., $\hat{\Theta}_j^a = \hat{\Theta}_j(Y^a)$. Thus, $y_i \sim Dist(\hat{\Theta}_j^a)$ tells us that the values of variable Y_j are distributed according to a distribution $Dist$ with parameters $\hat{\Theta}_j^a$ estimated over the values Y_j^a. The vector of all parameter values of a rule is denoted by Θ^a. In our case, $Dist$ can be a *categorical* or *normal* distribution in the nominal or numeric target case, respectively. With respect to numeric targets other distributions could have been chosen, however the *normal* distribution incorporates some of the most relevant information of the data through mean and variance of the data, it is well studied for the regression problems (Friedman et al., 2001), and can be solved in a closed form from a Bayesian (Jeffreys, 1998) and MDL (Grünwald, 2007) perspective. For an analysis on the direct use of the numeric empirical distribution in subgroup discovery please refer to Meeng et al. (2020). In the numeric case the normal distribution is represented as: $\mathcal{N}(\hat{\mu}, \hat{\sigma})$. In the nominal case the distribution is $Cat(\hat{p}_1, \cdots, \hat{p}_k)$, where k is the number of classes (or categories) of the corresponding variable and $\hat{p}_c$ the estimated probability for class c.

Example 3 (continuation): Revisiting the *Automobile import* subgroup list in Figure 2, the description and corresponding statistics for the second subgroup are $a = \{$fuel-type = gas & consumption-city $\geq$ 13 km/L $\}$ and $\hat{\Theta}^{a_2} = \{\hat{\mu} = 7; \hat{\sigma} = 1\}$, respectively, where the units are thousands of dollars (K). This corresponds to the following normal probability distribution:

$$\text{price (K)} \sim \mathcal{N}(\hat{\mu} = 7; \hat{\sigma} = 1)$$

Example 4 (continuation): In the case of the *Zoo* subgroup list in Figure 1, the description for the first subgroup is $a = \{\text{feathers} = \text{yes}\}$, and its corresponding statistics are $\hat{\Theta}^{a_1} = \{\hat{p}_1 = 0; \hat{p}_2 = 0; \hat{p}_3 = 0.56; \hat{p}_4 = 0.44; \hat{p}_5 = 0; \hat{p}_6 = 0; \hat{p}_7 = 0\}$, where the class labels $1, ..., 7$ correspond to the animal types in the order of Figure 1. The target variable follows the following categorical distribution:

$$\text{animal\_type} \sim Cat(\hat{p}_1, \hat{p}_2, \hat{p}_5, \hat{p}_6, \hat{p}_7 = 0.00; \hat{p}_3 = 0.56; \hat{p}_4 = 0.44)$$

3.4 Quality measures

To assess the quality (or interestingness) of a subgroup description a, a measure that scores subsets D^a needs to be chosen. The measures used vary depending on the target and task (Atzmueller, 2015), but in general it has two components: 1) representativeness of the subgroup in the data, based on coverage $n_a = |D^a|$; and 2) a function of the difference between statistics of the empirical target distribution of the pattern, $\hat{\Theta}^a = \hat{\Theta}(\mathbf{Y}^a)$, and the overall empirical target distribution of the dataset, $\hat{\Theta}^d = \hat{\Theta}(\mathbf{Y})$. The latter corresponds to the statistics estimated over the whole data, e.g., in the case of the *Automobile import* subgroup list of Figure 2 it is $\hat{\Theta}^d = \{\hat{\mu} = 13; \hat{\sigma} = 8\}$ and it is estimated over all 197 instances of the dataset.

The general form of a quality measure to be maximized is

$$q(a) = (n_a)^{\alpha} f(\hat{\Theta}^a, \hat{\Theta}^d),\ \alpha \in [0,1], \tag{3}$$

where α allows to control the trade-off between coverage and the difference of the distributions, and $f(\hat{\Theta}^a, \hat{\Theta}^d)$ is a function that measures how different the subgroup and dataset distributions are. As an example, the most commonly adopted quality measure for single-numeric targets is Weighted Relative Accuracy (WRAcc)(Lavrač et al., 1999), with $\alpha = 1$ and $f(\hat{\Theta}_a, \hat{\Theta}_d) = \hat{\mu}_a - \hat{\mu}_d$ (the difference between subgroup and dataset averages).

3.5 Weighted Kullback-Leibler divergence

Another commonly adopted measure is the Weighted-Kullback Leibler divergence (WKL) (Van Leeuwen and Knobbe, 2011). This is also the measure that we consider throughout this work because of 1) its flexibility in terms of (number and types of) supported target variables; and 2) its relationship to the MDL principle (see Sections 5.4 and 6.4).
WKL is defined as the Kullback-Leibler (KL) divergence (Kullback and Leibler, 1951) between a subgroup's and dataset target distribution $KL(\hat{\Theta}^a; \hat{\Theta}^d)$ linearly weighted by its coverage. Revisiting Eq. (3) this corresponds to $f(.) = KL(.)$ and $\alpha = 1$. The definition of WKL for a univariate target variable Y is given by:

$$WKL(\hat{\Theta}^a; \hat{\Theta}^d) = n_a KL(\hat{\Theta}^a; \hat{\Theta}^d), \tag{4}$$

where $KL(\hat{\Theta}^a; \hat{\Theta}^d)$ is the Kullback-Leibler divergence between subgroup and dataset for target Y. The KL divergence in Eq. (4) depends on the probabilistic model chosen to describe the target variables. In its general form the KL divergence can be defined as:

$$KL(\hat{\Theta}^a_j; \hat{\Theta}^d_j) = \sum_{y \in Y^a} \Pr(y \mid \hat{\Theta}^a_j) \log \left(\frac{\Pr(y \mid \hat{\Theta}^a_j)}{\Pr(y \mid \hat{\Theta}^d_j)} \right), \tag{5}$$

where the logarithm is to the base two (like all logs in this work). Thus the choice of the distribution used to describe the target is of great importance and should reflect what the analyse would like find in the data. Now, depending of the type of target we will see show how to compute $WKL(\hat{\Theta}^a; \hat{\Theta}^d)$. It is easy to see that for multivariate targets we either use a multivariate distribution, e.g., a multivariate normal distribution, or assume that they are *independent* target variables, where the total WKL turns out to be just the sum the WKL for each target variable.

We will now provide the definitions of WKL for univariate categorical and normal distributions.

Weighted Kullback-Leibler for categorical distributions. In the case of a univariate *nominal target* Y, the distribution can be uniquely described by a categorical distribution with the probability of each category $\hat{\Theta}^a = \{\hat{p}_{1|a}, ..., \hat{p}_{k|a}\}$, so that the $KL(\hat{\Theta}^a; \hat{\Theta}^d)$ of Eq. (4) takes the form of:

$$KL_{Cat}(\hat{\Theta}^a; \hat{\Theta}^d) = \sum_{c \in \mathcal{Y}} \hat{p}_{c|a} \log \left(\frac{\hat{p}_{c|a}}{\hat{p}_c} \right), \tag{6}$$

where $\hat{p}_{c|a} = \Pr(c \mid a)$ is the maximum likelihood estimate of the conditional probability of the target c given the subgroup a, and $\hat{p}_c$ is the marginal probability for that category.

Weighted Kullback-Leibler for normal distributions. In the case of a univariate *numeric* target Y, many distributions could be used for modelling. We resort to the normal distribution for its robustness and analytical properties, as mentioned before. Nonetheless, still two possibilities remain: a location distribution $\hat{\Theta}^a = \{\mu_a\}$ that only accounts for the mean, or a 'complete' normal distribution $\hat{\Theta}^a = \{\mu_a, \sigma_a\}$ that accounts for the mean and the variance. With the location distribution $KL(\hat{\Theta}^a; \hat{\Theta}^d)$ equals[1]:

$$KL_{\mu}(s) = \frac{(\hat{\mu}_d - \hat{\mu}_a)^2}{\hat{\sigma}_d}, \tag{7}$$

while with the normal distribution one obtains:

$$KL_{\mu,\sigma}(s) = \left[\log \frac{\hat{\sigma}_d}{\hat{\sigma}_a} + \frac{\hat{\sigma}_a^2 + (\hat{\mu}_a - \hat{\mu}_d)^2}{2\hat{\sigma}_d^2} \log e - \frac{\log e}{2} \right]. \tag{8}$$

Note that since $\hat{\sigma}_d$ is a constant for each dataset, there is a strong resemblance between $WKL_{\mu}(s)$ and WRAcc, where the only difference is the square of the difference of the means. Also notice that $WKL_{\mu,\sigma}$ directly takes into account the variance of a subgroup and penalizes for a larger variance, while $WKL_{\mu}(s)$ (and also WRAcc) do not take into account the variance, and thus fail to give importance to the spread of subgroup values. This is a key point as this makes a quality measure like $WKL_{\mu,\sigma}(s)$ *dispersion-aware*, while measures like $WKL_{\mu}(s)$ and $WRAcc$ are not.

3.6 Subgroup set discovery

Subgroup set discovery (Van Leeuwen and Knobbe, 2012) is the task of finding a set of high-quality, non-redundant subgroups that together describe all substantial deviations in the target distribution. That is, given a quality function Q for subgroup sets and the set of all possible subgroup sets $\mathcal{S}$, the task is to find that subgroup set $S^* = \{s_1, \ldots, s_k\}$ given by $S^* = \arg\max_{S \in \mathcal{S}} Q(S)$. Note that Q should not only take into account the individual quality of subgroups

[1] The derivations of these formulas can be found in Appendix D.

$q(a)$, but also the overlap of their coverages D^a and quantify the contribution of each instance only once, as opposed to top-k mining where only their individual qualities are taken into account, i.e., $Q(S) = \sum q(a)$.
Ideally a quality measure for subgroup sets Q should: 1) *be global*, i.e., for a given dataset it should be possible to compare subgroup set qualities regardless of subgroup set size or coverage; 2) *maximize the individual qualities* of the subgroups; and 3) *minimize redundancy* of the subgroup set, i.e., the subgroups covers should overlap as little as possible while ensuring the previous point.

3.7 A new measure for subgroup sets: the sum of WKL divergences

Following the previous subsections, we extend the KL-based measure of Eq. (4) for individual subgroups to a measure for subgroup lists. That is, we propose the *Sum of Weighted Kullback-Leibler divergences* (SWKL), which can be interpreted as the sum of weighted KL divergences for the individual subgroups:

$$\text{SWKL}(S) = \frac{\sum_{i=1}^{\omega} n_i KL(\hat{\Theta}_j^i; \hat{\Theta}_j^d)}{|D|}, \tag{9}$$

where i is the index of each subgroup in a subgroup list (as will be formalized in Section 4), ω is the number of subgroups in S, and $|D|$ is the number of instances in D. The latter is used to normalize the measure and make values comparable across datasets. In case of multiple target variables the normalization could also include the number of targets, but we do not use this in this work. The SWKL measure assumes that the data is partitioned per subgroup and is based on the assumption that subgroups can be interpreted sequentially as a list, i.e., the second subgroup is interpreted as: the description of the second subgroup is active, while the one of the first *is not* active.
An advantage of the SWKL measure is that it can be used for any type of target variable(s), as long as they are described by a probabilistic model. Note that computing SWKL is straightforward for subgroup lists, but not for subgroup *sets* as instances can be covered by multiple subgroups. For subgroup sets, it would be necessary to explicitly define the type of probabilistic overlap, e.g., additive or multiplicative mixtures of the individual subgroup models.
It should be noted that this measure only quantifies how well a list of subgroups capture the deviations in a given dataset and is prone to overfitting: the higher the number of subgroups, the easier it is to obtain a higher value as there is no penalty for the number of subgroups (or their individual complexities, for that matter). As such, SWKL can be seen as a measure for 'goodness of fit' for subgroup lists. This turns out to not be an issue for our approach though, as our MDL-based criterion naturally penalizes for multiple hypothesis testing and complexity of the individual subgroups. Further, it is neither an issue in our empirical comparisons in Section 8, as the number of subgroups found was similar for most algorithms, rendering the SWKL-based comparison valid.

4 MDL-based Subgroup Set Discovery

In this section we formalize the task of subgroup set discovery as a model selection problem using the Minimum Description Length (MDL) principle (Rissanen, 1978; Grünwald, 2007; Grünwald and Roos, 2019). To this end we first need to define an appropriate model class $\mathcal{M}$; as we will explain next, we use *subgroup lists* as our models. As we want to find the best model, the model selection problem should then be formalized using a two-part code (Grünwald, 2007), i.e.,

$$M^* = \arg\min_{M \in \mathcal{M}} L(D, M) = \arg\min_{M \in \mathcal{M}} \left[L(\mathbf{Y} \mid \mathbf{X}, M) + L(M) \right], \tag{10}$$

where $L(\mathbf{Y} \mid \mathbf{X}, M)$ is the encoded length, in bits[2], of target variables data $\mathbf{Y}$ given explanatory data $\mathbf{X}$ and model M, $L(M)$ is the encoded length, in bits, of the model, and $L(D, M)$ is the total encoded length and the sum of both terms. Intuitively, the best model M^* is the model that results in the best trade-off between how well the model compresses the target data and the complexity of that model—thus minimizing redundancy and automatically selecting the best subgroup list size. This formulation is similar to those previously used for two-view association discovery and multi-class classification (Van Leeuwen and Galbrun, 2015; Proença and van Leeuwen, 2020).

This section is divided as follows. First, in Section 4.1 we describe the details of the model class. Then, in Section 4.2 the encoding of the model part is shown. Finally, in Section 4.3 the high-level encoding of the data given the model is presented. The specific encoding of the data given the model for categorical and normal distributions is given in Sections 5 and 6, respectively.

4.1 Model Class: Subgroup Lists

Although Eq. (10) provides a *global* criterion that enables the comparison of subgroup sets of different sizes, subgroups are descriptions of *local* phenomena and we require each *individual subgroup to have high quality.*
We accomplish this by using *subgroup lists* as models; see Figure 3. Specifically, as we are only interested in finding subgroups for which the target deviates from the overall distribution, we assume $\mathbf{Y}$ values to be distributed according to $\hat{\Theta}^d$ by default (last line in Figure 3). For each region in the data for which the target distribution deviates from that distribution and a description exists, a subgroup specifying a different distribution $\hat{\Theta}^a$ is added to the list.
We model the empirical distributions $\hat{\Theta}$ of nominal target variables with categorical distributions $Categorical(\hat{p}_1, \cdots, \hat{p}_k)$, and numeric target variables by univariate normal distributions $\mathcal{N}(\hat{\mu}, \hat{\sigma})$. The categorical distribution is a natural choice for describing the probabilities of classes (Letham et al., 2015) and the normal distribution captures two properties of interest in numeric

[2] To obtain code lengths in bits, all logarithms in this paper are to the base 2.

$$
\begin{array}{llllll}
s_1\text{:} & \text{IF} & a_1 \sqsubseteq \mathbf{x} & \text{THEN} & y_1 \sim Dist(\hat{\Theta}_1^1) \quad \cdots & y_t \sim Dist(\hat{\Theta}_t^1) \\
 & & \vdots & & & \\
s_\omega\text{:} & \text{ELSE IF} & a_\omega \sqsubseteq \mathbf{x} & \text{THEN} & y_1 \sim Dist(\hat{\Theta}_1^\omega) \quad \cdots & y_t \sim Dist(\hat{\Theta}_t^\omega) \\
\text{dataset:} & \text{ELSE} & & & y_1 \sim Dist(\hat{\Theta}_1^d) \quad \cdots & y_t \sim Dist(\hat{\Theta}_t^d)
\end{array}
$$

Fig. 3: Generic subgroup list model M with ω subgroups $S = \{s_1, ..., s_\omega\}$ and t (number of target variables) distributions per subgroup.

variables, i.e., center and spread, while being robust to cases where the data violates the normality assumption (Grünwald, 2007).
Ordering the rules formed by subgroups $S = \{s_1, \cdots, s_\omega\}$ and adding the dataset rule at the end (default rule) leads to a subgroup list M of the form of Figure 3. This corresponds to a probabilistic rule list with $\omega = |S|$ subgroups/rules and a last (default) rule that is fixed to the overall empirical distributions for each target variable (Proença and van Leeuwen, 2020). Fixing the distribution of this last 'rule' is crucial and differentiates a subgroup list from a rule list as used in classification and/or regression (Proença and van Leeuwen, 2020), as this enforces the discovery of a set of subgroups whose individual target distributions all substantially deviate from the overall target distribution (dataset rule). It is shown in Section 5.4 for nominal targets and in Section 6.4 for numeric targets that the objective of finding a subgroup list with this format is equivalent to top-k subgroup discovery, when finding subgroup lists with just one subgroup. A theoretical comparison of the difference between the objectives of predictive rule lists and subgroup lists is given in Appendix E.

4.2 Model Encoding

The next step is to define the two length functions; we start with $L(M)$. Following the MDL principle (Grünwald, 2007), we need to ensure that 1) all models in the model class, i.e., all subgroup lists for a given dataset, can be distinguished; and 2) larger code lengths are assigned to more complex models. To accomplish the former we encode all elements of a model that can change, while for the latter we resort to two different codes: when a larger value represents a larger complexity we use the universal code for integers (Rissanen, 1983), denoted[3] $L_\mathbb{N}$, and when we have no prior knowledge but need to encode an element from a set we choose the uniform code.
Specifically, the encoded length of a model M over variables in $\mathbf{X}$ is given by

$$L(M) = L_\mathbb{N}(|S|) + \sum_{a_i \in S} \left[L_\mathbb{N}(|a_i|) + \log \binom{m}{|a_i|} + \sum_{v \in a_i} L(v) \right], \qquad (11)$$

[3] $L_\mathbb{N}(i) = \log k_0 + \log^* i$, where $\log^* i = \log i + \log\log i + \ldots$ and $k_0 \approx 2.865064$.

where we first encode the number of subgroups $|S|$ using the universal code for integers, and then encode each subgroup description individually. For each description, first the number $|a_i|$ of variables used is encoded, then the set of variables using a uniform code over the set of all possible combinations of $|a_i|$ from all explanatory variables, and finally the specific condition for a given variable. As we allow variables of two types, the latter is further specified by

$$L(v) = \begin{cases} \log |\mathcal{X}_v| & \text{if } v \text{ is nominal} \\ L_{\mathbb{N}|2}(|n_{op}|) + \log N(n_{op}, n_{cut}) & \text{if } v \text{ is numeric} \end{cases} \tag{12}$$

where the code for each variable type assigns code lengths proportional to the number of possible parts the variable's domain can partition the dataset. Note that this seems justified, as more parts imply more potential spurious associations with the target that we would like to avoid. For `nominal` variables this is given by the size of the domain, i.e., the number of categories in a nominal variable. For `numeric` variables it equals the number of operators used $L_{\mathbb{N}|2}(|n_{op}|)$[4] plus the possible number of outcomes $N(n_{op}, n_{cut})$ given the operators and n_{cut} cut points. The number of operators for numeric variables can be one or two, as there can be conditions with one (e.g., $x \leq 2$) or two operators (e.g., $1 \leq x \leq 2$), which is a function of the number of possible subsets generated by n_{cut} cut points. Note that we here assume that equal frequency binning is used, which means that knowing X and n_{cut} is sufficient to determine the cut points.

Example 5 (continuation): Let us assume that the subgroup list of the *Automobile* example of Figure 2 is composed of only the first subgroup. In that case the list only has one subgroup with description: {weight = heavy & consumption-city $\leq$ 8 km/L }. Taking into account that the dataset has 17 variables, $|\mathcal{X}_{weight}| = 3$ and only 3 cut points were used for numeric attributes, the expression of the model length is given by:

$$\begin{aligned} L(M) &= L_{\mathbb{N}}(1) + L_{\mathbb{N}}(2) + \log \binom{17}{2} + \log |\mathcal{X}_{weight}| + \left[L_{\mathbb{N}|2}(1) + \log 2n_{cut} \right] \\ &= 1.52 + 2.52 + 7.09 + 1.59 + 0.77 + 2.59 \\ &= 16.08 \text{ bits} \end{aligned}$$

It is important to note that the length of the model can (and should) be a real number, as we are only concerned with the idea of compression, not with materialising and transmitting the actually encoded data (Grünwald, 2007).

[4] $L_{\mathbb{N}|2}$ is the universal code for integers with codes restricted to $n = 1$ or 2. This can be obtained by applying the maximum entropy principle to $L_{\mathbb{N}}$ when it is known that it cannot take values of $n > 2$.

4.3 Data encoding

The remaining length function is that of the target data given the explanatory data and model, $L(\mathbf{Y} \mid \mathbf{X}, M)$. In this section we show how to encode the target data $\mathbf{Y}$ by dividing it into smaller subsets that can be encoded individually and then summed together, and why there are different types of data encoding for each of the subsets. The specifics of encoding nominal and numeric targets are described in Sections 5 and 6, respectively.

Cover of a subgroup in a subgroup list. First, we observe that for any given subgroup list of the form of Figure 3, *any individual instance* $(\mathbf{x}^i, \mathbf{y}^i)$ *can only be 'covered' by one subgroup.* That is, the cover of a subgroup a_i, denoted D^a, depends on the order of the list and is given by the instances where its description occurs minus those instances covered by previous subgroups:

$$D^i = \{\mathbf{X}^i, \mathbf{Y}^i\} = \{(\mathbf{x}, \mathbf{y}) \in D \mid a_i \sqsubseteq \mathbf{x} \wedge \left(\bigwedge_{\forall_{i'<i}} a_{i'} \not\sqsubseteq \mathbf{x} \right)\}. \tag{13}$$

Next, let $n_i = |D^i|$ be the number of instances covered by a subgroup (also known as *usage*). In case an instance $(\mathbf{x}^i, \mathbf{y}^i)$ is not covered by any subgroup $s \in S$ *then it is 'covered' by the default rule.* The instances covered by the default rule D^d are the ones not covered by any subgroup (hence the name default rule) and formally defined as:

$$D^d = \{\mathbf{X}^d, \mathbf{Y}^d\} = \{(\mathbf{x}, \mathbf{y}) \in D \mid \forall_{a_i \in M} a_i \not\sqsubseteq \mathbf{x}\}. \tag{14}$$

Now, given that the subsets for each subgroup or default rule and each target variable are well-defined, one can—for each of the rules and targets—estimate the parameters of its probabilistic distribution using the maximum likelihood estimator.

Note that this shows us that a subgroup $s_i \in M$ is fully defined by its description a_i in a dataset D, and we will interchangeably refer to the subgroup by its description and to its elements (statistics, parameters, distributions, etc.) by its index i when obvious from context.

As the subgroup list induces a *partition of the data*, the total length of the encoded data can be given by the sum of its *non-overlapping parts*:

$$L(\mathbf{Y} \mid \mathbf{X}, M) = L(\mathbf{Y}^d \mid \boldsymbol{\Theta}^d) + \sum_{s_i \in S} L(\mathbf{Y}^i), \tag{15}$$

where $\boldsymbol{\Theta}^d$ is the vector of parameters for each variable $\Theta_1^d, \ldots, \Theta_t^d$. Observe that we dropped $\mathbf{X}^a$ as these are not necessary to encode $\mathbf{Y}^a$ but only to generate the partition of the data, and also dropped the parameters $\boldsymbol{\Theta}^i$ of the subgroups as we do not know what are their parameters until we see the data. This last part will be clarified at the end of this section, where we describe how to encode subsets without knowing the parameters.

As a side-note, note that Eq. (15) concerns the encoding of any supervised partition of the data, which allows to directly quantify the quality of any tree learning method—each such tree induces a partition of the data.

Encoding data of t (assumed) independent target variables. As each target variable is assumed independent from each other the encoding of target data is given by the sum of their individual encodings:

$$L(\mathbf{Y} \mid \mathbf{X}, M) = -\log\left(\prod_{j=1}^{t} \Pr(Y_j \mid \mathbf{X}, M)\right) = \sum_{j=1}^{t} L(Y_j \mid \mathbf{X}, M). \tag{16}$$

Integrating (15) and (16), one obtains:

$$L(\mathbf{Y} \mid \mathbf{X}, M) = \sum_{j=1}^{t}\left(L(Y_j^d \mid \Theta_j^d) + \sum_{s_i \in S} L(Y_j^i)\right) \tag{17}$$

Two types of data encoding: data encoding can be separated in two different categories: 1) with *known parameters*; and 2) with *unknown parameters.*

1*) Known parameters*: when the parameters of a distribution are *known*, one can encode the data points directly using the probability for those points given by the distribution with the known parameters. Thus, the encoding of points Y_j^i (j^{th} variable and i^{th} subgroup) is equal to the negative logarithm of their probability given by known parameters $\hat{\Theta}_j^i$:

$$L(Y_j^i \mid \hat{\Theta}_j^i) = \sum_{y \in Y_j^i} -\log \Pr(y \mid \hat{\Theta}_j^i). \tag{18}$$

This type of code is used in the case of the default rule of a subgroup list, as the parameters $\hat{\Theta}_j^d$ are equal to the marginal distribution of variable Y_j and are constant for each dataset. Note that this is the *key difference between a subgroup list and a predictive rule list*: the last rule of a subgroup list is fixed to the marginal distribution, while in the (predictive) rule list its parameters are unknown and depend on the subset D^d.

2*) Unknown parameters*: when the parameters are *unkown* we need to encode both the parameter values and the data points. We have two possibilities: 1) crude MDL, i.e., encoding the probabilities using a suboptimal probability distribution and then applying the Shannon-Fano code, i.e., the logarithm of the empirical probability (Shannon, 1948); or 2) employ an optimal encoding of both parameters of the distribution and data points together (Grünwald, 2007). In this work, we employ optimal encoding of parameters, as it guarantees optimality in the sense that the encoding is the best possible in the worst case scenario, i.e., in case the sample of the data is not representative of the population. Three types of optimal encodings exist, which are, in increasing

order of optimality guarantees: 1) *prequential plug-in*; 2) *Bayesian*; 3) *Normalized Maximum Likelihood (NML)*. While the first two are asymptotically optimal, the NML encoding is optimal for fixed sample sizes.
Depending on the target type, we employ the best encoding possible while being computationally feasible, i.e., we require adequate run-time for our algorithm. For nominal targets we present a NML encoding for both the probabilities of each class and the data points in Section 5, which is a theoretical improvement over the prequential plug-in code that was recently proposed for classification rule lists by Proença and van Leeuwen (2020). For numeric targets we resort to a Bayesian encoding, as recently proposed by Proença et al. (2020), as the NML code is not computationally feasible for that case.

Difference between subgroup lists and (predictive) rule lists: Although both subgroup lists and rule lists concern a model class of the form of Figure 3, a crucial difference lies in the last rule in the list, the so-called default rule. In case of a subgroup list the default rule is fixed to the marginal distribution of each target, making its parameters *known* and *fixed* for a certain dataset (Proença et al., 2020). In case of a rule list, however, the last rule is 'free' in the sense that it depends on the estimate of its subset $\mathbf{Y}^d$ (Proença and van Leeuwen, 2020). This may seem like a subtle difference, but it allows to find subgroups that always differentiate themselves from the dataset marginal distribution, while it allows to find predictive rules that maximize predictive accuracy. A theoretical proof of their difference from an MDL perspective is given in Appendix E.

5 Data encoding: nominal target variables

When the data have one or more nominal targets, the distributions in the probabilistic rules (2) are categorical distributions $Cat(\Theta)$, each with a set of parameters $\Theta = \{p_1, \cdots, p_k\}$ representing the k classes:

$$\Pr(y = c \mid p_1, \cdots, p_k) = p_c, \text{ subject to } \sum_{c=1}^{k} p_c = 1. \tag{19}$$

This implies a subgroup of the form:

$$a \mapsto y_1 \sim Cat(p_1, \cdots, p_k), \cdots, y_t \sim Cat(p_{1'}, \cdots, p_{k'}),$$

where k and k' are the number of classes Y_1 and Y_t, respectively. To simplify the introduction of concepts we will assume we only have one target variable in $\mathbf{Y}$, and then generalize the results to multiple variables at the end. Thus, throughout this section $\mathbf{Y}$ becomes Y, and the parameters of each subgroup s_i become $\hat{\Theta}^i = \{p_{1|i}, \cdots, p_{k|i}\}$ as there is only one variable with k classes, where $p_{1|i}$ is the probability of class 1 for subgroup i, i.e., $\Pr(c = 1 \mid a_i)$. The general form of a subgroup list with one nominal target takes the form of Figure 4.

$$
\begin{array}{rlll}
s_1\text{:} & \text{IF} & a_1 \sqsubseteq \mathbf{x} & \text{THEN} \quad y \sim Cat(\hat{p}_{1|1}, \cdots, \hat{p}_{k|1}) \\
 & & \vdots & \\
s_\omega\text{:} & \text{ELSE IF} & a_\omega \sqsubseteq \mathbf{x} & \text{THEN} \quad y \sim Cat(\hat{p}_{1|\omega}, \cdots, \hat{p}_{k|\omega}) \\
\text{dataset:} & \text{ELSE} & & \quad y \sim Cat(\hat{p}_{1|d}, \cdots, \hat{p}_{k|d})
\end{array}
$$

Fig. 4: Generic subgroup list model M with ω subgroups $S = \{s_1, ..., s_\omega\}$ and a single nominal target Y with k categories.

In the following sections, we will derive the data encoding for subgroup lists with categorical distributions. First, in Section 5.1 we introduce the maximum likelihood estimators that will be needed to derive the MDL encodings. Then, in Section 5.2, it is shown how to encode a categorical distribution when its parameters are known, which is the case for the default rule of a subgroup list. After that, in Section 5.3 it is shown how to encode a categorical distribution when the parameters of the distribution are unknown. Then, in Section 5.4 the equivalence between subgroup lists with only one subgroup and standard (top-k) subgroup discovery is proven for our MDL-based approach. Finally, in Section 5.5, we show the data encoding is equivalent to a Bayesian test.

5.1 Maximum Likelihood (ML) estimation of the parameters

Each description a_i uniquely defines a subset D^i given by its cover Eq. (13). However in the nominal case for each class label c, we also need to find its subset of the data $D^{c|i}$, formally given by:

$$D^{c|i} = \{(\mathbf{x}, y) \in D^i \mid y = c\}. \tag{20}$$

which allows us to compute the usage over each class $n_{c|i} = |D^{c|i}|$. Now, we are in a position to use the maximum likelihood estimator for the parameters $\hat{\Theta}^i$ of each categorical distribution as:

$$\hat{p}_{c|i} = \frac{n_{c|i}}{n_i}. \tag{21}$$

We can show how to encode each subset of target values with the *known* parameters of the distribution—the default rule of a subgroup list—and *unknown* parameters—all the subgroups.

5.2 Encoding categorical distributions with *known* parameters

To encode target values with *known parameters*—as is the case for the default rule of a subgroup list—we can directly use Eq. (18) with given parameter estimates $\hat{\Theta}^d = \hat{p}_{1|d}, \cdots, \hat{p}_{k|d}$ (marginal distribution over the whole dataset):

$$L(Y^d \mid \hat{p}_{1|d}, \cdots, \hat{p}_{k|d}) = \sum_{c \in \mathcal{Y}} -n_{c|d} \log \hat{p}_{c|d} = -\ell(\hat{\Theta}^d \mid Y^d), \tag{22}$$

where $\ell(\hat{\Theta}^d \mid Y^d)$ is the log-likelihood of the parameter set $\hat{\Theta}^d$, and $n_{c|d}$ denotes the number of points associated with each class c covered by default rule Y^d.

5.3 Encoding categorical distributions with *unknown* parameters

When the parameters are *unknown*—as is the case for each individual subgroup distribution—we will employ the Normalized Maximum Likelihood (NML) code, as it "is optimal in the sense that it achieves the minimax optimal codelength regret" (Grünwald, 2007).
Although the expression of the NML code can be daunting, its intuition is very clear (Kontkanen et al., 2005), i.e., the NML code is equivalent to first encoding all maximum likelihood estimates of sequences Z of n_i points based on their likelihoods, and then encoding data Y^i with its maximum likelihood estimate $\hat{\Theta}^i$ as in Eq. (22). Formally, the NML code length of the subset Y^i is given by[5]:

$$\begin{aligned} L_{NML}(Y^i) &= -\log \frac{\prod_{y \in Y^i} \Pr(y \mid \hat{\Theta}^i)}{\sum_{Z \in \mathcal{Y}^{n_i}} \prod_{z \in Z} \Pr(z \mid \hat{\Theta}^Z)} \\ &= \sum_{c \in \mathcal{Y}} -n_{c|i} \log \hat{p}_{c|i} + \log \sum_{Z \in \mathcal{Y}^{n_i}} \prod_{z \in Z} \Pr(z \mid \hat{\Theta}^Z) \\ &= -\ell(\hat{\Theta}^i \mid Y^i) + \mathcal{C}(n_i, k) \end{aligned} \tag{23}$$

where $\mathcal{Y}^{n_i}$ is the space of all possible sequences of n_i points with cardinality $k = |\mathcal{Y}|$ (possible values per point), $\hat{\Theta}^Z$ is the maximum likelihood estimate over Z, $\mathcal{C}(n_i, k)$ is the complexity—as it is called in MDL literature(Grünwald, 2007)—of the multinomial distribution over n_i points and k categories. Note that this term can be efficiently computed in sub-linear time $\mathcal{O}(\sqrt{dn_i} + k)$ if approximated by a finite floating-point precision of d digits (Mononen and Myllymäki, 2008).

Finally, inserting (22) and (23) in (17) we obtain, for the total data encoding of a **subgroup list**:

$$L(\mathbf{Y} \mid \mathbf{X}, M) = \sum_{j=1}^{t} \left(L(Y_j^d \mid \boldsymbol{\Theta}^d) + \sum_{s_i \in S} L_{NML}(Y_j^i) \right). \tag{24}$$

Example 6 (continuation): Let us revisit the *Zoo* subgroup list example of Figure 1 and compute the length of NML encoding of the first subgroup. To compute it we just need to get the probabilities associated with each category ($\{0; 0; 0.56; 0.44; 0; 0; 0\}$), the number of samples covered by each of them

[5] For details on the derivation of Eq. 23, please see Appendix A.

($\{0; 0; 10; 8; 0; 0; 0\}$), and the total number of categories $k = |\mathcal{Y}| = 7$. Given these, the length of encoding of the data Y^1 is given by:

$$\begin{aligned} L_{NML}(Y^1) &= (-10 \log 0.56 - 8 \log 0.44) + \mathcal{C}(18, 7) \\ &= 17.84 + 10.42 \\ &= 28.26 \text{ bits.} \end{aligned}$$

5.4 Relationship of MDL-optimal subgroup lists to WKL-based SD

We now investigate the relationship between finding a MDL-optimal subgroup list and WKL-based top-k subgroup discovery. Remember that WKL is the weighted Kulback-Leibler (WKL) divergence, an existing subgroup discovery measure (van Leeuwen, 2010) that can be seen as an information-theoretic instance of the general form of a subgroup discovery measure as given in Eq. (3); we described it in more detail in Subsection 3.5.
Assume that we have a single target variable (Y instead of $\mathbf{Y}$) and a subgroup list consisting of just one subgroup s with description a (and the default rule). Next, let us turn the MDL minimization problem into a maximization problem by multiplying Eq. (10) by minus one and adding a constant (for each dataset) $L(Y \mid \boldsymbol{\Theta}^d)$ to obtain:

$$s^* = \arg\max_{s \in \mathcal{M}} \left[L(Y^d \mid \boldsymbol{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(M) \right].$$

In the case of a subgroup list with *one subgroup* and one target, the data encoding of Eq. (24) can be substituted by $L(Y \mid \mathbf{X}, M) = L(Y^d \mid \boldsymbol{\Theta}^d) + L_{NML}(Y^a)$. Also, note that Y^d is actually given by all the points not covered by the subgroup description a, i.e., $Y^{\neg a}$. Thus, we can further develop the maximization problem to:

$$\begin{aligned} &L(Y \mid \hat{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(M) = \\ &\quad = L(Y^a \mid \hat{\Theta}^d) + \cancel{L(Y^{\neg a} \mid \hat{\Theta}^d)} - L_{NML}(Y^a) - \cancel{L(Y^{\neg a} \mid \hat{\Theta}^d)} - L(M) \\ &\quad = \sum_{y \in Y^s} \log \frac{\hat{p}_{y|a}}{\hat{p}_{y|d}} - \mathcal{C}(n_a, k) - L(M) \\ &\quad = n_a \sum_{c \in \mathcal{Y}} \hat{p}_{c|a} \log \left(\frac{\hat{p}_{c|a}}{\hat{p}_{c|d}} \right) - \mathcal{C}(n_a, k) - L(M) \\ &\quad = n_a KL(\hat{\Theta}^a; \hat{\Theta}^d) - \mathcal{C}(n_a, k) - L(M), \end{aligned} \tag{25}$$

where $n_a KL(\hat{\Theta}^a; \hat{\Theta}^d)$ is the Weighted Kulback-Leibler divergence from $\hat{\Theta}^a$ to $\hat{\Theta}^d$. *This result shows that finding the MDL-optimal subgroup is equivalent to finding the subgroup that maximizes WKL, plus two extra terms: one that defines the complexity of the distribution $\mathcal{C}(n_a, k)$, and another that defines the complexity of the subgroup $L(M)$.*

When we consider subgroup lists having more than one subgroup, Eq. (25) simply expands to:

$$L(Y \mid \hat{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(M) = \sum_{a_i \in S} n_i KL(\hat{\Theta}^i; \hat{\Theta}^d) - \sum_{a_i \in S} \mathcal{C}(n_i, k) - L(M)$$
$$= \mathrm{SWKL}(S) - \sum_{a_i \in S} \mathcal{C}(n_i, k) - L(M),$$

where $\mathrm{SWKL}(S)$ is the measure for subgroup set quality that we proposed in Section 3.6, and the other terms penalize the complexity of the subgroup list. The fact that the MDL-based objective for the optimal subgroup list can be formulated as subgroup set quality minus two terms for model complexity clearly demonstrates that our formalization naturally aims for subgroup lists of high quality while penalizing complexity.

5.5 Relationship of MDL-optimal subgroup lists to Bayesian testing

We will now show how our MDL criterion is related to Bayesian testing. The Bayesian alternative to statistical testing is the Bayesian factor, denoted here by K (Jeffreys, 1998; Kass and Raftery, 1995). The Bayesian factor compares two models (hypotheses) through the division of the likelihood of the data given each model $\Pr(D \mid M_1)/\Pr(D \mid M_2)$, where the more likely model dominates. Notice that the form that we arrived at in the term $n_a KL(\hat{\Theta}^a; \hat{\Theta}^d) - \mathcal{C}(n_a, k) - L(M)$ of Eq. (25) (for a list consisting of one subgroup) is very similar to the logarithm of a Bayes factor, and indeed it can be decomposed into:

$$L(Y \mid \hat{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(M) = \log\left(\frac{\Pr(Y \mid \mathbf{X}, M)}{\Pr(Y \mid \hat{\Theta}^d)}\right) L(M)$$
$$= \log K + L(M),$$

where we use the Shannon-Fano code (Shannon, 1948) to transform code length in bits $L(\cdots)$ to probabilities $\Pr(\cdots)$. In practice, taking into account $L(M)$ (or $\Pr(M)$) is equivalent to using the posterior distributions instead of just the Bayes factor, and in our case amounts to a penalty for multiple hypothesis testing. This tells us that when finding the first subgroup we are indeed maximizing an MDL version of a Bayesian factor, and thus, doing an equivalent Bayesian proportions test (with a binary target) or a multinomial test (with a nominal target). When we consider the problem of finding a subgroup beyond the first, it is straightforward to observe that we are testing each subgroup in S against the marginal distribution of the dataset.

6 Data encoding: numeric target variables

When we have one or more numeric target variables, the consequents of probabilistic rules as in Eq. (2) are now normal distributions $\mathcal{N}(\Theta)$ with parameters $\Theta = \{\mu, \sigma\}$, and take the following form:

$$\Pr(y \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right),$$

where we use $\Pr(y \mid \mu, \sigma)$ to denote the probability density function (pdf), which is a slight abuse of notation that we admit to unify the whole work. This translates to a probabilistic rule of the form:

$$a \mapsto y_1 \sim \mathcal{N}(\hat{\mu}_{a1}, \hat{\sigma}_{a1}), \cdots, y_t \sim \mathcal{N}(\hat{\mu}_{at}, \hat{\sigma}_{at}) \tag{26}$$

To simplify the introduction of concepts we will again assume we have only one target variable in $\mathbf{Y}$, and generalize the results to multiple variables at the end. Thus, throughout this section $\mathbf{Y}$ becomes Y, and the parameters of each subgroup s_i become $\Theta^i = \{\mu_i, \sigma_i\}$ as there is only one variable. The general form of a subgroup list with normal target distribution is given in Figure 5.

$$\begin{array}{rllll}
s_1\text{:} & \text{IF} & a_1 \sqsubseteq \mathbf{x} & \text{THEN} & y \sim \mathcal{N}(\hat{\mu}_1, \hat{\sigma}_1) \\
 & & \vdots & & \\
s_\omega\text{:} & \text{ELSE IF} & a_\omega \sqsubseteq \mathbf{x} & \text{THEN} & y \sim \mathcal{N}(\hat{\mu}_\omega, \hat{\sigma}_\omega) \\
\text{dataset:} & \text{ELSE} & & & y \sim \mathcal{N}(\hat{\mu}_d, \hat{\sigma}_d)
\end{array}$$

Fig. 5: Generic subgroup list model M with ω subgroups $S = \{s_1, ..., s_\omega\}$ and a single numeric target Y.

In the following subsections, we will derive the data encoding for subgroup list with normal distributions. First, in Section 6.1 we introduce the maximum likelihood estimators that will be needed to derive the MDL encodings. Then, in Section 6.2 we show how to encode a normal distribution when its parameters μ and σ are known, such as is the case for the default rule of a subgroup list. After that, in Section 6.3 we show how to encode a normal distribution using an uninformative prior when the parameters of the distribution are unknown. Then, in Section 6.4 the equivalence between subgroup lists with only one subgroup and standard (top-k) subgroup discovery is proven for our MDL-based approach. Finally, in Section 6.5, we show the data encoding and corresponding criterion are equivalent to a Bayesian test.

6.1 Maximum Likelihood (ML) estimation of the parameters

Each description a_i uniquely defines a subset D^i given by its cover (13), which allows to estimate the parameters of each normal distribution using the maximum likelihood estimate over Y^i:

$$\hat{\mu}_i = \frac{1}{n_i} \sum_{y \in Y^i} y, \tag{27}$$

$$\hat{\sigma}_i^2 = \frac{1}{n_i} \sum_{y \in Y^i} (y - \hat{\mu}_i)^2, \tag{28}$$

where $\hat{\sigma}_i^2$ is the biased estimator such that the estimate times n_i equals the Residual Sum of Squares, i.e., $n_i \hat{\sigma}_i^2 = \sum_{y \in Y^a} (y - \hat{\mu}_i)^2 = RSS_i$. Note that the parameters of the default rule of Figure 5 are fixed for a dataset and thus correspond to estimates $\hat{\mu}_d$ and $\hat{\sigma}_d$ over all target values Y.
As each subgroup list defines a partition of the data, we can encode each target value part, Y^i or Y^d, separately and sum them to obtain the total encoding of Y. In the case of subgroup lists, the last rule–i.e., default rule—has fixed parameters equal to the overall dataset distribution, while the subgroups parameters are not known in advance, and have thus to be encoded together with the data points.
We start by showing how to encode the subset of target values with the default 'rule'—known parameters of the distribution—and then show how to encode each subgroup subset—unkown parameters of the distribution.

6.2 Encoding normal distributions with *known* parameters

The target values not covered by any subgroup Y^d, as defined in (14), are covered by the default dataset 'rule' and distribution at the end of a subgroup list. As the statistics $\hat{\Theta}_d = \{\hat{\mu}_d, \hat{\sigma}_d\}$ are known and constant for a given dataset, one can simply encode the instances using this (normal) distribution, resulting in encoded length

$$\begin{aligned} L(Y^d \mid \hat{\mu}_d, \hat{\sigma}_d) &= -\log \left[\prod_{y \in Y^d} \frac{1}{\sqrt{2\pi\hat{\sigma}_d^2}} \exp\left(\frac{(y - \hat{\mu}_d)^2}{2\hat{\sigma}_d^2} \right) \right] \\ &= \frac{n_d}{2} \log 2\pi + \frac{n_d}{2} \log \hat{\sigma}_d^2 + \left(\frac{1}{2\hat{\sigma}_d^2} \sum_{y \in Y^d} (y - \hat{\mu}_d)^2 \right) \log e. \end{aligned} \tag{29}$$

The first two terms are normalizing terms of a normal distribution, while the last term represents the Residual Sum of Squares (RSS) normalized by the variance of the data. Note that when $Y_d = Y$, i.e., the whole dataset target, RSS is equal to $n_d \sigma_d$ and the last term reduces to $n_d/2 \log e$.

6.3 Encoding normal distributions with *unknown* parameters

In contrast to the previous case, here *we do not know a priori the statistics defining the probability distribution corresponding to the subgroup*, i.e., $\hat{\mu}$ and

$\hat{\sigma}$ are not given by the model and thus both need to be encoded. For this we resort to the Bayesian encoding of a normal distribution with mean μ and standard deviation σ unknown, which was shown to be asymptotically optimal (Grünwald, 2007). The optimal code length is given by the negative logarithm of a probability, and the optimal Bayesian probability for Y^a is given by

$$L_{Bayes}(Y^i) = \\ -\log \int_{-\infty}^{+\infty} \int_{0}^{+\infty} (2\pi\sigma)^{-\frac{n_i}{2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{y \in Y^i} (y-\mu)^2\right) w(\mu,\sigma)\, \mathrm{d}\mu\, \mathrm{d}\sigma, \tag{30}$$

where $w(\mu, \sigma)$ is the prior on the parameters, which needs to be chosen.

Choosing the prior. The MDL principle requires the encoding to be as unbiased as possible for any values of the parameters, which leads to the use of uninformative priors. The most uninformative prior is Jeffrey's prior, which is $1/\sigma^2$ and therefore constant for any value of μ and σ, but unfortunately its integral is undefined, i.e., $\int\int \sigma^{-2}\, \mathrm{d}\sigma\, \mathrm{d}\mu = \infty$. Thus, we need to 1) constrain the parameter space and 2) make the integral finite, which we will do next in consecutive steps.

One of the best ways to constrain the parameter space without biasing it, is by multiplying Jeffrey's prior by a normal prior on the effect size, i.e., $\rho = \mu/\sigma \sim \mathcal{N}(0, \tau)$ (Rouder et al., 2009). We then still need to describe τ though; the most uninformative choice would be to use an inverse-chi-squared distribution, which would be equivalent to using a Cauchy prior on the effect size (Rouder et al., 2009). Unfortunately, this would lead to an open integral, which would render the approach infeasible for cases—like ours—where many candidates need to be tested. The second best option is to fix $\tau = 1$, which gives a tractable formula that is equivalent to introducing a virtual point and converges[6] to the Bayes Information Criterion (BIC) for large n. This is the best we can do and we proceed with this option.

Now, given the prior defined by $\rho = \mu/\sigma \sim \mathcal{N}(0, 1)$, the remaining question is how we can make the integral over the prior finite. The most common solution, which we also employ, is to use k data points from Y^i, denoted $Y^{i|k}$, to create a proper conditional prior $w(\mu, \sigma \mid Y^{i|k})$. As there are only two unknown parameters, we only need two points hence $k = 2$ (Grünwald, 2007); for more on the interpretation of such "priors conditional on initial data points", see Grünwald and Roos (2019). Consequently, we first encode $Y^{i|2}$ with a non-optimal code that is readily available—i.e., the dataset distribution of Eq. (29)—and then use the Bayesian rule to derive the total encoded length of Y^i as

$$\begin{aligned} L_{Bayes2.0}(Y^i) &= -\log \frac{P_{Bayes}(Y^i)}{P_{Bayes}(Y^{i|2})} P(Y^{i|2} \mid \mu_d, \sigma_d) \\ &= L_{Bayes}(Y^i) + L_{cost}(Y^{i|2}), \end{aligned} \tag{31}$$

[6] See proof in Appendix C.

where $L_{cost}(Y^{i|2}) = L(Y^{i|2} \mid \mu_d, \sigma_d) - L_{Bayes}(Y^{i|2})$ is the extra cost incurred by encoding two points non-optimally. After some re-writing[7] we obtain the encoded length of the y values covered by a subgroup Y^i as

$$\begin{aligned} L_{Bayes2.0}(Y^i) &= L_{Bayes}(Y^i) + L_{cost}(Y^{i|2}) \\ &= 1 + \frac{n_i}{2}\log\pi - \log\Gamma\left(\frac{n_i}{2}\right) + \frac{1}{2}\log(n_i+1) + \frac{n_i}{2}\log n_i\hat{\sigma}_i^2 + L_{cost}(Y^{i|2}), \end{aligned} \tag{32}$$

where Γ is the Gamma function that extends the factorial to the real numbers ($\Gamma(n) = (n-1)!$ for integer n) and $\hat{\mu}_i$ and $\hat{\sigma}_i$ are the statistics of Eqs. (27) and (28), respectively. Note that for $Y^{i|2}$ any two unequal values (otherwise $\hat{\sigma}_2 = 0$ and $L_{Bayes}(Y^{i|2}) = \infty$) can be chosen from Y^a, thus we choose them such that they minimize $L_{cost}(Y^{i|2})$. Finally, inserting (29) and (32) in (17) we obtain for the total data encoding for a **subgroup list**:

$$L(\mathbf{Y} \mid \mathbf{X}, M) = \sum_{j=1}^{t}\left(L(Y_j^d \mid \boldsymbol{\Theta}^d) + \sum_{s_i \in S} L_{Bayes2.0}(Y_j^i)\right).$$

Example 7 (continuation): We revisit the *Automobile* subgroup list of Figure 2 and find the length of the *Bayes*2.0 encoding (Eq. (32)) of the first subgroup. To compute it we need to get the statistics of the subgroup ($\hat{\Theta}^1 = \{\hat{\mu}_1 = 35; \hat{\sigma}_1 = 8\}$), the number of samples it covers ($n_1 = 11$), the dataset statistics ($\hat{\Theta}^d = \{\hat{\mu}_d = 13; \hat{\sigma}_d = 8\}$), and the two points closest to the dataset mean $Y^{1|2} = \{14; 31\}$ that makes the encoding proper (and which are not available in the example information). Assuming that $L_{cost}(Y^{i|2}) = 0.69$ bits for simplicity, the length of the encoding of Y^1 is given by:

$$\begin{aligned} L_{Bayes2.0}(Y^1) =& 1 + \frac{11}{2}\log\pi - \log\Gamma\left(\frac{11}{2}\right) + \frac{1}{2}\log(11+1) + \frac{11}{2}\log 11\cdot 8^2 \\ &+ L_{cost}(Y^{i|2}) \\ =& 58.19 + 0.69 \\ =& 58.88 \text{ bits}. \end{aligned}$$

6.4 Relationship of MDL-optimal subgroup lists to WKL-based SD

As in Section 5 we next investigate the relationship between finding a MDL-optimal subgroup list and WKL-based top-k subgroup discovery, but now for the numeric case.

[7] The full derivation of the Bayesian encoding and an in-depth explanation are given in Appendix B.

First, we show that Eq. (32)—with mean and variance unknown— converges, for large n, to Eq. (29)—with mean and variance known—plus an additional term. Using the Stirling approximation of $\Gamma(n+1) \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$ leads to[8]

$$L_{Bayes2.0}(Y^a) \sim \frac{n_a}{2}\log 2\pi + \frac{n_a}{2}\log \hat{\sigma}_a^2 + \frac{n_a}{2}\log e + \log \frac{n_a}{e}, \tag{33}$$

where $\log \frac{n}{e}$ is equal to the penalty term of BIC and similar to the usual MDL complexity of a distribution (Grünwald, 2007).
Now, we can show that minimizing our MDL criterion is equivalent to maximizing a subgroup discovery quality function of the form of Eq (3). Focusing on the case where $M = \{s\}$ contains only one subgroup with description a and statistics $\hat{\Theta}^a = \{\hat{\mu}_a, \hat{\sigma}_a\}$, we start with $L(Y \mid X, M)$ (Eq. (10)), multiply it by minus one to make it a maximization problem, and add a constant $L(Y \mid \hat{\mu}_d, \hat{\sigma}_d)$, i.e., the encoded size of the whole target Y using the overall distribution dataset. We then get

$$s^* = \arg\max_{s \in \mathcal{M}} \left[L(Y^d \mid \boldsymbol{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(M) \right].$$

Developing this further, the subgroup s that maximizes this expression is equivalent to the one that maximizes

$$\begin{aligned}
&L(Y \mid \hat{\Theta}^d) - L(Y \mid X, M) \\
&= L(Y^a \mid \hat{\Theta}^d) - L_{Bayes2.0}(Y^a \mid \mathbf{X}^a) - L(M) \\
&\sim \frac{n_a}{2}\log\frac{\hat{\sigma}_d^2}{\hat{\sigma}_a^2} + \left[\frac{1}{2\hat{\sigma}_d^2}\sum_{y^i \in Y^a}(y^i - \hat{\mu}_d)^2\right]\log e - \frac{n_a}{2}\log e - \log n_a - L(M) \\
&= \frac{n_a}{2}\log\frac{\hat{\sigma}_d^2}{\hat{\sigma}_a^2} + \left[\frac{\sum_{y^i \in Y^a}(y^i)^2 - n\hat{\mu}_a^2 + n\hat{\mu}_a^2 - 2n\hat{\mu}_a\hat{\mu}_d - \hat{\mu}_d)^2}{2\hat{\sigma}_d^2}\right]\log e \\
&\quad - \frac{n_a}{2}\log e - \log n_a - L(M) \\
&= n_a\left[\log\frac{\hat{\sigma}_d}{\hat{\sigma}_a} + \frac{\hat{\sigma}_a^2 + (\mu_a - \mu_d)^2}{2\hat{\sigma}_d^2}\log e - \frac{\log e}{2}\right] - \log(n_a) - L(M) \\
&= n_a KL(\hat{\Theta}^a; \hat{\Theta}^d) - \log n_a - L(M),
\end{aligned} \tag{34}$$

where $n_a KL(\hat{\Theta}^a; \hat{\Theta}^d)$ is the usage-weighted Kullback-Leibler divergence between the normal distributions specified by the respective parameter vectors. Similar to the result for the nominal target in Section 5.4, this shows that *finding the MDL-optimal subgroup is equivalent to finding the subgroup that maximizes the weighted Kullback-Leibler (WKL) divergence*, an existing subgroup discovery quality measure (van Leeuwen, 2010), *plus two terms*. The

[8] The complete derivation can be found in the Appendix C

first defines the complexity of the subgroup distribution with two parameters, the second compensates for multiple hypothesis testing (i.e., the number of possible subgroups). When we have a list with multiple subgroups, Eq. (25) expands to

$$\begin{aligned} L(Y \mid \hat{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(M) &\sim \sum_{a_i \in S} n_i KL(\hat{\Theta}^i; \hat{\Theta}^d) - \sum_{a_i \in S} \log(n_i) - L(M) \\ &= \mathrm{SWKL}(S) - \sum_{a_i \in S} \log(n_i) - L(M), \end{aligned}$$

where $\mathrm{SWKL}(S)$ is the measure of subgroup set qualities that we proposed in Section 3.6, and the other terms penalize the complexity of the subgroup list.

Dispersion-correction quality measure. Importantly, we can observe from Eq. (25) that the measure based on the Kullback-Leibler divergence of normal distributions is part of the family of *dispersion-corrected* subgroup quality measures, as it takes into account both the centrality and the spread of the target values (Boley et al., 2017).

6.5 Relationship of MDL-optimal subgroup lists to Bayesian testing

When we have only one subgroup s in a subgroup list, the data encoding for numeric targets of Eq. (6.3) is equivalent to the negative logarithm of a Bayes factor (Gönen et al., 2005; Rouder et al., 2009). Indeed, the choice of the prior was based on the Bayesian one-sample t-test by Gönen et al. (2005), and we effectively perform a one-sample t-test (including two extra terms) for each subgroup. Formally—and similar to the nominal case as described in Section 5.5—a Bayes factor K (Jeffreys, 1998; Kass and Raftery, 1995) is given by the division of the likelihoods of the data given each hypothesis: $\Pr(D \mid M_1) / \Pr(D \mid M_2)$. If we use the maximization equivalent of Eq. (34),

$$\begin{aligned} L(Y \mid \hat{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(M) &= \log \left(\frac{\Pr(Y \mid \mathbf{X}, M)}{\Pr(Y \mid \hat{\Theta}^d)} \right) L(M) \\ &= \log K + L(M), \end{aligned}$$

we can see that we have the Bayes factor plus the model encoding. To transform code lengths in bits $L(\cdots)$ to probabilities $\Pr(\cdots)$ we used the Shannon-Fano code (Shannon, 1948), which states that the best encoding is given by the negative logarithm of its probability for an event A, i.e., $L(A) = -\log \Pr(A)$. Our MDL-based criterion aims at maximizing a one-sample t-test for numeric targets between the subgroup distribution and the marginal distribution of the dataset, while taking into account $L(M)$, which is equivalent to using the posterior distribution and penalizes for multiple hypothesis testing. When we aim to find subgroups beyond the first, it is trivial to see that we are testing each subgroup in S against the marginal distribution of the dataset.

7 The RSD Algorithm

In this section we propose the *Robust Subgroup Discoverer* (RSD), a heuristic algorithm to find good subgroup lists based on the proposed MDL formulation. As the problem of finding a optimal subgroup list is NP-hard (Mielikäinen and Mannila, 2003) we propose a heuristic based on the Separate-and-Conquer (SaC) (Fürnkranz, 1999) strategy of iteratively adding the local best subgroup to the list, combined with beam search for candidate subgroup generation.
The use of greedy heuristic approaches is common practice in MDL-based pattern mining (Vreeken et al., 2011; Proença and van Leeuwen, 2020) and rule-based learning (Fürnkranz et al., 2012), and beam-search is widely adopted for its efficient generation of subgroups in subgroup discovery(Lavrač et al., 2004; Meeng and Knobbe, 2011; Van Leeuwen and Knobbe, 2012).

This section is divided as follows. First, in Section 7.1 we give a high-level description of our proposed algorithm and motivate our choices. After that, in Section 7.2 the quality measure used to iteratively add rules—compression gain—is presented, together with its relationship with subgroup discovery quality measures. Then, in Section 7.3 the statistical testing interpretation of the compression gain is given. After that, in Section 7.4 the beam search for candidate subgroup generation is presented in detail. Then, in Section 7.5 the Separate-and-Conquer RSD algorithm is presented. Finally, in Section 7.6 the time and space complexity of the overall algorithm is given.

7.1 Algorithm high-level description

The algorithm we propose is a heuristic composed of two parts: we greedily add one subgroup at a time to the subgroup list, for which candidates are generated using beam search. More specifically, the greedy search algorithm starts from an empty list, with just a default rule equal to the priors in the data, and adds subgroups according to the well-known *separate-and-conquer* strategy (Fürnkranz et al., 2012): 1) iteratively find and add the subgroup that gives the largest improvement in compression; 2) remove the data covered by that rule; and 3) repeat steps 1-2 until compression cannot be improved. This implies that *we always add subgroups at the end of the list, but before the default rule*. Beam search is used for candidate generation at each iteration to find the best candidate to add. Given a beam width w_b and maximum search depth d_{max} it consists of: 1) find all items, i.e., all conditioned variables such as $x_1 < 5$ or $x_2 = category$, and add the best w_b items according to compression gain (Eq. (7.2)) as subgroups of size 1 to the beam; 2) refine all subgroups in the beam with all items and add the best w_b to a new empty beam; 3) repeat 2 and 3 until the maximum depth d_{max} of the beam is reached and return the best subgroup—according to the compression score—found in all iterations. The beam search algorithm is described in detail in Section 7.4 and the greedy

search algorithm RSD in Section 7.5.

The main reasons for using greedy search and adding one subgroup at a time are its computational simplicity and transparency, as it adds at each iteration the locally best and most statistically significant subgroup found by the beam search. Further, in the context of subgroup discovery beam search was empirically shown to be very competitive in terms of quality when compared to a complete search, while it demonstrates a considerable speed-up (Meeng and Knobbe, 2020). Also, its straightforward implementation allows flexibility to easily extend this framework to other types of targets in the future.

7.2 Compression gain

To quantify the quality of annexing a subgroup s at the end (after all the other subgroups and before the default rule) of model M, denoted $M \oplus s$, we employ the *compression gain*:

$$s = \arg\max_{s \in \mathcal{S}} \Delta_\beta L(D, M \oplus s) = \arg\max_{s \in \mathcal{S}} \left[\frac{L(D, M) - L(D, M \oplus s)}{(n_s)^\beta} \right], \ \beta \in [0, 1] \tag{35}$$

where β weighs the level of the normalization, and $\Delta_\beta L(D, M \oplus s)$ should be greater than zero for a decrease in the encoded length from $L(D, M)$ to $L(D, M \oplus s)$. Considering the extremes, with $\beta = 1$ we have the *normalized gain* first introduced for the classification setting by Proença and van Leeuwen (2020), and for $\beta = 0$ we have the *absolute gain* which is just the regular gain used in greedy search in previous MDL-based pattern mining (Vreeken et al., 2011).

Developing Eq. (35) further shows that the compression gain only depends on the added subgroup s, as in the specific case of a subgroup list the default rule is fixed and it is the same for M and $M \oplus s$:

$$\begin{aligned} \Delta_\beta L(D, M \oplus s) &= \frac{L(\mathbf{Y} \mid \mathbf{X}, M) - L(\mathbf{Y} \mid \mathbf{X}, M \oplus s)}{(n_s)^\beta} + \frac{L(M) - L(M \oplus s)}{(n_s)^\beta} \\ &= \Delta_\beta L(\mathbf{Y} \mid \mathbf{X}, M \oplus s) + \Delta_\beta L(M \oplus s), \end{aligned}$$

where $\Delta_\beta L(\mathbf{Y} \mid \mathbf{X}, M \oplus s)$ and $\Delta_\beta L(M \oplus s)$ are the data and model compression gain, respectively.

Furthermore, if we note that maximizing the gain in Eq. (35) is equivalent to maximizing the subgroup discovery equivalent objective of Eq. (25) for nominal targets and Eq. (34) for numeric targets, this means that finding the subgroup that maximizes the compression gain is the same as finding the subgroup that

maximizes the subgroup discovery equivalent objective:

$$
\begin{aligned}
s &= \arg\max_{s \in \mathcal{J}} \Delta_\beta L(M \oplus s) \\
&= \arg\max_{s \in \mathcal{J}} \frac{n_s KL(\hat{\Theta}_s; \hat{\Theta}_d)}{(n_s)^\beta} - \frac{\texttt{COMP}(n_s, \#param)}{(n_s)^\beta} + \Delta_\beta L(M \oplus s)
\end{aligned}
$$

where $n_s KL(\hat{\Theta}_s; \hat{\Theta}_d)$ has the general form of a subgroup discovery measure of Eq. (3), $\texttt{COMP}(n_s, \#param)$ is the complexity associated with each target probability distribution (normal or categorical), and $\Delta_\beta L(M \oplus s)$ the added model complexity of adding s.

Interpretation of hyperparameter β. The hyperparameter β represents a trade-off between finding many subgroups that cover few instances or few subgroups that cover many instances[9]. In the general form of a subgroup quality measure of Eq. (3), β is just given by $\beta = 1 - \alpha$. We empirically show later that the *normalized gain* ($\beta = 1$) usually achieves a better MDL score than other β values; this was already known for other measures from rule learning theory (Fürnkranz et al., 2012). Nonetheless, the main objective of subgroup discovery is to *locally* describe regions in the data that strongly deviate from a certain target. Thus, it is up to the user to specify what one is looking for in the data: either a more granular and detailed perspective (β close to one) or a more general and high-level one (β close to zero). Note that, for comparison to other algorithms *we will always use the normalized gain* ($\beta = 1$) except when explicitly stated.

7.3 Statistical testing interpretation of compression gain

The gain of Eq. (7.2) shares the same expression of the weighted Kullback Leibler divergence that was shown in Sections 5.4 and 6.4 to be equivalent to a Bayesian one-sample proportions/multinominal test and t-test, respectively. Thus, it too guarantees individual "significance" for each subgroup according to these tests. We will now look at this in more detail.
A Bayesian factor is an alternative to frequentist statistical testing and is given by the likelihood of both hypotheses generating the data (Kass and Raftery, 1995):

$$\log K = \log \frac{\Pr(D \mid M_1)}{\Pr(D \mid M_2)},$$

where M_1 and M_2 are two models that we are comparing. Values of $\log K$ above zero tell us that there is more evidence in favour of model M_1, while negative values tell us the opposite (Kass and Raftery, 1995). If we look back at the expression of the greedy gain in Eq. (35), and convert the encoding $L(\cdots)$ to

[9] For details on the empirical analysis of different β values please refer to Appendix H

probabilities $\Pr(\cdots)$ using the Shannon-Fano code: $L(A) = -\log \Pr(A)$ (Shannon, 1948); we can see that it takes exactly the same form plus some extra terms:

$$\Delta_\beta L(M \oplus s) = \log\left(\frac{\Pr(\mathbf{Y} \mid \mathbf{X}, M \oplus s)}{\Pr(\mathbf{Y} \mid \mathbf{X}, M)} \frac{\Pr(M \oplus s)}{\Pr(M)}\right) \frac{1}{(n_s)^\beta} = \frac{\log\left(K \cdot K_M\right)}{(n_s)^\beta},$$

where $K_M = \Pr(M \oplus s)/\Pr(M)$ represents the division of the model's likelihood (called a prior in Bayesian statistics). Thus, we obtain an expression with three terms: the first, K, gives us an MDL equivalent to a Bayesian factor that weighs how likely the data is given each model (M or $M \oplus s$); the second, K_M, gives the likelihood of each model; and the third is a normalizing term to be able to compare the contribution of different subgroups given how much data they cover.

The first conclusion that we can draw from this is that the subgroup that maximizes the compression gain is the one that *locally* maximizes this statistical test, i.e., it is the *mode* of this distribution. In the specific case of subgroup lists, the factor term K of the compression gain corresponds to a proportion/multinomial or t-test depending on the type of target variable. Second, the term K_M can be seen as a multiple hypothesis testing correction, as the way in which $L(M)$ was developed puts more weight on model structures that can generate more variants. Also, it should be noted that the encoding of $L(M)$ is more subjective than $L(D \mid M)$, but it will be an upper-bound on the perfect encoding for M, and can be taken as a more 'conservative' test. Third, if the compression gain is positive for a subgroup, it means that there is more evidence in favor of adding that subgroup than not. Fourth, the normalizing term allows us to adjust the weight that is given to the data covered by each subgroup.

In summary, we can say that the greedy gain based on the compression gain, a common heuristic for MDL in pattern mining, is in fact maximizing the test statistic of a hypothesis test and only adds that subgroup for which most evidence is available.

7.4 Beam search for subgroup generation

The *beam search algorithm* for subgroup generation is shown in Algorithm 1. It starts by discretizing all variables depending on their subsets, i.e., nominal with the operator *equal to* (=) and numeric by generating all subsets with n_{cut} points. At each iteration the w_b subgroups that maximize the selected gain (Eq. (35)) are chosen and will be expanded with all discretized variables until the maximum depth d_{max} of the description is achieved.

The algorithm accepts as inputs the dataset $D = (\mathbf{X}, \mathbf{Y})$, the number of cut points n_{cut} used for equal frequency binning of numeric variables, the beam width w_b, the maximum depth of search or number of variables in a subgroup description d_{max}, and the indexes of the data already covered by the subgroups

already present in the subgroup list, $coverage_S$. The algorithm is initialized by filling the *beam* and *subgroup* with an empty subgroup of size zero (Ln 2 and Ln 3, respectively). The algorithm is composed of three nested loops. In short, the first (outer) loop goes over each depth of subgroups generated, the second loop goes over each candidate to extend for a fixed depth, and the third (interior) loop goes over each item used to extend the candidates. Now we will go into more detail over each loop.
In the *first loop* the depth is increased by one (Ln 6), *candidates* is initialized with the *patterns* of the *beam* from the previous iteration (Ln 7), and after that all *patterns* are removed from the *beam* (Ln 8). The *second loop* iterates over all *candidates* (Ln 9) and expands each of them in the third loop with all the *items* generated from the explanatory variables $\mathbf{X}$ (Ln 11). An *item* is a subgroup of size one that can be generated by logical conditions on one variable $X_j \in \mathbf{X}$. If variable X_j is `nominal`, each item is a condition given by the equality operator ($=$) on each category, e.g., $feathers = yes$ from Figure 1. If the variable is `numeric`, equal frequency binning with open and closed intervals is used to generate all possible items (further explained at the end of this paragraph). Expanding a candidate *cand* to generate a *subgroup_new* (Ln 15) requires computing three properties: 1) its coverage of the data through a bitwise AND (Ln 12); 2) its description (Ln 15); and 3) its statistics Θ_{new} (Ln 15). Its score is computed according to Eq. (35) (Ln 16). Then if the score is higher than the pattern with minimum score in the *beam*, the latter is replaced by the higher scoring one. Finally, if the score is higher than the score of *subgroup*, this is replaced. The algorithm terminates when the maximum search depth of the subgroups is reached and *subgroup* is returned, to be added to the subgroup list (Ln 21).

Numeric discretization. Suppose a numeric variable X_j, and a number of cut points n_{cut}. The *items* generated from this numeric variable are all valid subsets (they must cover at least one instance) given by equal frequency discretization with open and closed intervals for n_{cut} cut points. Open intervals require one operator ($\geq$ or $\leq$), while closed intervals require two ($\geq$ and $\leq$). As an example, in the case of a generic variable X_j and $n_{cut} = 2$, with $cut\_point_1 = 10$ and $cut\_point_2 = 20$ it generates four *items* with one operator, i.e., $items_{1op} = \{\ x_j \geq 10,\ x_j \leq 10, x_j \geq 20,\ x_j \leq 20\}$, and one *item* with two operators, i.e., $items_{2op} = \{10 \leq x_j \leq 20\}$.

7.5 The Robust Subgroup Discoverer

Algorithm 2 presents RSD[10], for *Robust Subgroup Discoverer*, a greedy algorithm that starts with an empty subgroup list and iteratively adds subgroups until no more compression can be gained, where compression is measured in terms of compression gain (Eq. 35) of adding a subgroup s.

[10] Our implementation uses the rulelist package (`https://pypi.org/project/rulelist/`) and can be found on GitHub: `https://github.com/HMProenca/RuleList`

Algorithm 1 Beam search for subgroup generation

Input: Dataset D, number of cut points n_{cut}, beam width w_b, depth max. d_{max}, and data already covered by other subgroups in M $coverage_S$.
Output: *subgroup*

1: $(\mathbf{X}, \mathbf{Y}) \leftarrow D$
2: $beam \leftarrow [\varnothing]$
3: $subgroup \leftarrow \varnothing$
4: $d \leftarrow 1$
5: **while** $d \leq d_{max}$ **do**
6: $\quad d \leftarrow d + 1$
7: $\quad candidates \leftarrow beam$
8: $\quad beam \leftarrow empty\_list(size = w_b)$
9: $\quad$ **for** $(cand, coverage\_cand) \in candidates$ **do**
10: $\quad\quad coverage\_cand \leftarrow coverage\_pattern \;\&\; coverage_S$
11: $\quad\quad$ **for** $(item, bitset\_item) \in items(\mathbf{X})$ **do**
12: $\quad\quad\quad coverage\_new \leftarrow coverage\_item \;\&\; coverage\_cand$
13: $\quad\quad\quad cand\_new \leftarrow cand \oplus item$
14: $\quad\quad\quad \Theta_{new} \leftarrow statistics(\mathbf{Y}, coverage\_new)$
15: $\quad\quad\quad subgroup\_new \leftarrow (cand\_new, \Theta_{new})$
16: $\quad\quad\quad score \leftarrow \Delta_\beta L(D, M \oplus subgroup\_new)$
17: $\quad\quad\quad$ **if** $score > min\_score(beam)$ **then**
18: $\quad\quad\quad\quad beam \leftarrow replace(beam, subgroup\_new, min\_score)$
19: $\quad\quad\quad$ **if** $score > \Delta_\beta L(D, M \oplus subgroup)$ **then**
20: $\quad\quad\quad\quad subgroup \leftarrow replace(subgroup, subgroup\_new)$
21: **return** *subgroup*

The algorithm starts by taking as input a dataset D and the beam search parameters, namely the number of cut points n_{cut}, the width of the beam w_b, and the maximum depth of search d_{max}. It initializes the rule list with the default rule, based on the dataset empirical distribution (Ln 1). Then, while the beam search algorithm returns subgroups that improve compression (Ln 3), it keeps iterating over two steps: 1) finding the best subgroup from all candidates generated in the beam search (Ln 4); and 2) adding that subgroup to the end of the model, i.e., after all the existing subgroups in the model (Ln 5). The beam search returns the best subgroup on the data not covered by any subgroup already in model M. When there is no subgroup that improves compression (non-positive gain) the while loop stops and the subgroup list is returned. Note that beam search is used at each iteration, instead of only once at the beginning, as it can converge to local optima, and running the candidate search once would thus bias our search to the top-k subgroups instead of the best at each iteration.

7.6 Time and Space Complexity

In this section we analyze the time and space complexity of RSD as given in Algorithm 2. The algorithm can be divided in three parts: 1) preprocessing of the data; 2) the Separate and Conquer (SaC) algorithm; and 3) the beam search. Note that depending on the type of target we have different complexities as each statistic requires different computations.

Algorithm 2 RSD algorithm

Input: Dataset D, number of cut points n_{cut}, beam width w_b, depth max. d_{max} and normalization β
Output: Subgroup list S
1: $M \leftarrow [\Theta_d(Y)]$
2: $subgroup \leftarrow BeamSearch(M, D, w_b, n_{cut}, d_{max})$
3: **while** $\Delta_\beta L(D, M \oplus subgroup) > 0$ **do**
4: $\quad subgroup \leftarrow BeamSearch(M, D, w_b, n_{cut}, d_{max})$
5: $\quad M \leftarrow M \oplus subgroup$
6: **return** $S \in M$

1) Preprocessing phase. In the preprocessing phase all the coverage bitsets of the items are generated, i.e., the indexes of the instances covered by each item generated from numerical and nominal variables. The set of all items is ζ and its size is given by $|\zeta|$. Thus, we go over the data a maximum of $|\zeta|$ times, obtaining a time complexity of $\mathcal{O}(|\zeta|n)$, and the results are stored in a dictionary for $\mathcal{O}(1)$ access. Also, there are some constants that are cached for a fixed amount the first time they are computed, such as the universal code of integers $L_{\mathbb{N}}(i)$, and $\Gamma(i)$ for the numeric target case, and $\mathcal{C}(i)$ in the categorical case.

2) SaC phase. For the SaC phase, it is clear that the algorithm runs the beam search $|S|$ times, and will thus multiply the time complexity of the beam search by $|S|$.

3) Beam search phase. For the last $d_{max} - 1$ iterations of the loop, each of w_b candidates in the beam is refined with all $|\zeta|$ items, which gives a time complexity by itself of $\mathcal{O}(d_{max} w_b |\zeta|)$. Then, for each refinement, the algorithm computes its coverage, statistics and score, where the last two depend on the number and type of target.
The *coverage* of the refinement is the logical conjunction of two bitsets, i.e., the bitset of the candidate b_{cand} and that of the item b_{item}. The computation of this new coverage has a time complexity of $\mathcal{O}(|b_{cand}| + |b_{item}|)$, which in a worst case equals a run over the dataset $\mathcal{O}(n + n) = \mathcal{O}(n)$. Thus the time complexity of the algorithm is given by

$$\mathcal{O}\left(|S| d_{max} w_b |\zeta| stats\right),$$

where *stats* is the time complexity associated to computing the statistics for one candidate. Now, we will analyse the specific *stats* complexity depending on the type of target.

Nominal target variables. The *statistics for categorical distributions* require the computation of the usage for each class for each target of each subgroup rule and the new default rule. Assuming a maximum number of classes k (for all target variables) and t target variables, then the worst case for the coverage gives $\mathcal{O}(tnk)$ from which the likelihood can be directly computed.

The *nominal score* requires the computation of the data and model encoding, from which the data encoding dominates. The data encoding entails the computation of the NML complexity and likelihood for each refinement. In general the values of the NML complexity are just computed once and then cached, thus in a worst case where one requires to compute n values for $\mathcal{C}(n_i), \forall_{n_i=1,\ldots,n}$. Using the approximation of Mononen and Myllymäki (2008) for its computation, with $\mathcal{O}(\sqrt{10n_i}+k)$, gives a worst case complexity of $\mathcal{O}(tn(\sqrt{n}+k))$. This does not depend on the parameters of the beam, as the lookup of these values is $\mathcal{O}(1)$. The likelihood in general dominates over this term as it is computed for each refinement.
Thus the total time complexity for **nominal targets** is given by:

$$\mathcal{O}\left(|S|d_{max}w_b|\zeta|tnk + tn(\sqrt{n}+k)\right)$$

Numeric target variables. The *statistics for normal distributions* require the computation of the mean and variance (or residual sum of squares) for the refined subgroup and for the default rule. The mean can be computed in $\mathcal{O}(n)$ and given this the variance can also be computed in $\mathcal{O}(n)$. Thus, for all the targets one obtains $\mathcal{O}(tn)$.
The *numeric score* requires the computation of the data and model encoding, from which the data encoding dominates. The data encoding entails the computation of the gamma function and the direct use of the statistics. Similar to the NML complexity, we compute the values of the gamma function as needed and cache them afterwards. In general, the computation of the gamma function is dominated by the other terms as we only compute it at most n times.
Thus the total time complexity for **numeric targets** is given by:

$$\mathcal{O}\left(|S|d_{max}w_b|\zeta|tn\right).$$

Notice that this represents a worst case scenario and that in practice the direct use of bitsets for the computation of the class usages in the nominal case makes it faster than its numeric counterpart for the same dataset size.

Space Complexity. The main memory consumption resources of the algorithm are: 1) the items storage ζ; 2) the beam; and 3) the cached constants. The item storage requires at most the storage of $|\zeta|$ bitsets, with each bitset taking $\mathcal{O}(n)$, thus it totals $\mathcal{O}(|\zeta|n)$. The beam saves w_b bitsets at a time, thus having a space complexity of $\mathcal{O}(w_b n)$. The cached values make up a total of n values being dominated by the items or beam part. Thus, depending of which part dominates, the space complexity of the algorithm is

$$\mathcal{O}(w_b n + |\zeta|n).$$

8 Empirical evaluation

In this section we will empirically validate our proposed problem formulation and the RSD[11] algorithm. To do this, we will test how varying the hyperaparameters of RSD affects the subgroups found, and then we will compare RSD against state-of-the-art algorithms in subgroup set discovery.

This section is divided as follows. In Section 8.1 we evaluate the effect of changing the different hyperparameters of RSD. Then, in Section 8.2 we present the setup for validating our approach, based on algorithms compared against, and datasets and measures used to evaluate them. After that, in Section 8.3, the results for univariate and multivariate nominal targets are presented. Then, in Section 8.4 the results for univariate and multivariate numeric targets are shown. Finally, in Section 8.5 the runtimes of the algorithms are compared. For replication of the experiments in this paper please refer to: `https://github.com/HMProenca/RobustSubgroupDiscovery`.

8.1 Influence of RSD hyperparameters

Here we study the effect of RSD hyperparameters on the discovered subgroup lists. In order to not overfit our hyperparameters to the datasets and for this reason obtain a better performance than other methods, the values of RSD hyperparameters for the remaining of the experiments (besides this section) are fixed at the standard values of the DSSD implementation for the beam search, i.e., beam width $w_b = 100$, number of cut points $n_{cut} = 5$, and maximum search depth $d_{max} = 5$, and to the compression gain normalization term $\beta = 1$ (normalized gain). These values are assumed to be enough to achieve convergence and to obtain good subgroup lists, and are thus taken as the *standard values* of RSD.
Now, to evaluate hyperparameter influence, we vary one hyperparameter value at the time while others remain fixed at their *standard values*. The results of varying the compression gain normalization hyperparameter β can be seen in Appendix H; the results of varying the beam search hyperparameters w_b, n_{cut}, and d_{max} can be found in Appendix I.

Normalization term β. The results are evaluated in terms of compression ratio, SWKL, and number of rules. For compression gain the results (as shown in Appendix H) are similar for a small number of samples but $\beta = 1$ and 0.5 clearly obtain better results for larger datasets. In terms of SWKL, normalized gain ($\beta = 1$) is clearly better. On the other hand, in terms of the number of rules $\beta = 1$ can obtain one order of magnitude more rules than the others, especially for larger datasets.

[11] Our implementation uses the rulelist package (`https://pypi.org/project/rulelist/`) and can be found on GitHub: `https://github.com/HMProenca/RuleList`

Beam search hyperparameters w_b, d_{max} and n_{cut}. The results are evaluated in terms of compression ratio and average number of conditions per subgroup (for d_{max}). In general increasing any of the three values results in better models according to relative compression. It is also interesting to note that for maximum depths above 5 it is rare to have an average number of conditions above 4, backing up our decision for the standard value $d_{max} = 5$.

8.2 Setup of the subgroup quality performance comparisons

In this section we evaluate the quality of our proposed method by comparing it to the state-of-the-art approaches in subgroup set discovery, which may vary depending on the type of target variable(s). The comparison takes three dimensions: 1) the *algorithms* used to compare against; 2) *measures* used to evaluate the quality of the subgroups found by each algorithm; 3) the *datasets* in which the algorithms are evaluated. We now discuss the details of each dimension.

1) Algorithms. The algorithms we compared to and their relevant characteristic are listed in Table 3. A short description of each is as follows:

1. top-k[12] - standard subgroup discovery miner used as benchmark.
2. seq-cover[12] - sequential covering as implemented in the DSSD implementation.
3. CN2-SD[13] - the classical sequential covering subgroup discovery algorithm, which is only implemented for nominal targets, and only removes the examples of the class of interest already covered (not all examples covered, as seq-cover does).
4. Diverse Subgroup Set Discovery (DSSD)[12] - diverse beam search for diverse sets of subgroups (Van Leeuwen and Knobbe, 2012).
5. Monte Carlo Tree Search for Data Mining (MCTS4DM) - an approach to improve on beam search to find better subgroups without getting stuck in local optima (Bosc et al., 2018).
6. FSSD - a sequential approach for subgroup set discovery that defines a set as a disjunction of subgroups (Belfodil et al., 2019).

As can be seen in Table 3 most algorithms can only be applied to single-target binary problems, and besides RSD only top-k, seq-cover and CN2-SD support the use of Sum of Weighted Kullback-Leibler (SWKL) divergence to measure the quality of the found subgroup set. Thus we only compare against seq-cover and CN2-SD, algorithms that output a subgroup list and can be applied to many target types, and with top-k as reference of a non-diverse subgroup discovery algorithm. The algorithms that output sets do not have a stopping criterion or global formulation, and underperform in terms of SWKL, thus

[12] top-k, seq-cover, and DSSD are available in the implementation of the DSSD algorithm `http://www.patternsthatmatter.org/software.php#dssd/`

[13] Available in the Orange data mining toolkit `https://orangedatamining.com/`

Table 3: Algorithms included in the comparison and their functionalities. *Quality* represents the quality measure used to evaluate one single subgroup, *search* is the type of search algorithm supported, *swkl* shows if it supports SWKL to measure the quality of a subgroup set, *output* tells if the subgroups discovered form a list or a set, and '✓' and '−' represent if that type of target variable(s) is supported. MCTS stands for Monte Carlo Tree Search. * The algorithms only support WKL_μ for numeric targets (Eq. (7)), i.e., a Weighted Kullback-Leibler divergency that only takes into account the mean, contrary to the one used by RSD that also uses the variance (Eq. (8)). For the nominal target case there is only one WKL (the different WKL measures are explained in Section 3.5).

					nominal			numeric	
Algorithm	quality	search	output	swkl	bin.	nom.	multi	single	multi
RSD	WKL	beam	list	✓	✓	✓	✓	✓	✓
top-k	WKL^*_μ	beam	set	✓	✓	✓	✓	✓	✓
seq-cover	WKL^*_μ	beam	list	✓	✓	✓	✓	✓	✓
CN2-SD	entropy	beam	list	✓	✓	✓	-	-	-
DSSD	WKL^*_μ	beam	set	-	✓	✓	✓	✓	✓
MCTS4DM	WKL^*_μ	MCTS	set	-	✓	-	-	-	-
FSSD	$WRAcc$	DFS	list	✓	✓	-	-	-	-

those comparisons are relegated to Appendix G. As example, DSSD can indeed be applied to all types of target variables, but the fact that it uses weighted sequential covering makes it unsuitable to use the SWKL, making it unfairly underperform and unsuitable for a fair comparison (as shown in the Appendix). Also, note that we do not compare with machine learning algorithms that generate rules for classification or regression, such as RIPPER or CART, as the rules generated aim at making the best prediction possible, and not the highest difference from the dataset distribution, as shown theoretically in Appendix E.

Quality measures. As the quality of a set is measured using the SWKL, the most appropriate measure to use is the Weighted Kullback-Leibler (WKL) for the algorithms that support it. CN2-SD supports entropy which is related to WKL. FSSD only supports WRAcc at the moment. Note that for the case of numeric targets, except RSD, all use a WKL that only takes into account the mean, given by $WKL_\mu(s) = n_s/\hat{\sigma}_d(\hat{\mu_d} - \hat{\mu_s})^2$, in contrast to the deviation-aware measure of RSD in Eq. 34.

Hyperparameters. Most algorithms use beam search, thus only have three main hyperparameters: the maximum depth of search d_{max}; the width of the beam w_b; and the number of cut points to discretize numeric explanatory variables n_{cut}. The larger the values the better the performance but the slower the algorithms become, as time complexity is linear to each of them. To be fair and not over-search the hyperparameters, we selected the default values of the DSSD and seq-cover implementation for all beam-search algorithms: $d_{max} = 5$, $w_b = 100$, $n_{cut} = 5$. For the case of MCTS4DM, which requires a larger set of hyperparameters, only the number of iterations is set, $n_{iter} = 50\,000$, to

ensure good convergence, and the rest were set as default. FSSD only requires the maximum depth, which was set at 5.

2) Measures. In order to ascertain the quality of the subgroup sets we use three different measures. The first is our proposal to measure the overall quality of an ordered set of subgroups, the Sum of Weighted Kullback-Leibler (SWKL), as defined in Eq. (9). The other two are the number of subgroups $|S|$ and the average number of conditions per subgroup $|a|$, two commonly used measures for the interpretability/complexity of a set of rules. These two measures follow the law of parsimony and assume that fewer subgroups with fewer conditions are easier to understand by humans, which can be an invalid assumption in some situations. Nonetheless, it is widely used and its simple understanding typically make for a good proxy (Doshi-Velez and Kim, 2018). In machine learning, algorithms are tested on their generalization to unseen data, which is achieved by multiple runs using different test sets (e.g., cross-validation). Even though this could be of interest, subgroup discovery is always evaluated on the same dataset, as the goal is to describe the current dataset well. For this reason, and for the fact that existing implementations are not prepared to use a test set, we follow the standard approach in subgroup discovery of only testing on the current dataset.
3) Datasets. For a thorough analysis we use a total of 54 datasets—10-univariate binary; 10 univariate nominal; 9 multivariate nominal; 15 univariate numeric; and 9 multivariate numeric—that are listed in Tables 7 and 8 of Appendix F. The datasets are commonly used benchmarks of machine learning and subgroup discovery, which are publicly available from the UCI[14], Keel[15] and MULAN[16] repositories. The datasets were selected to be the most varied possible. In the case of the nominal target datasets in Table 7, the number of targets ranges from 1 to 374, the classes from 2 to 28, the samples from 150 to 45 222, and the variables from 3 to 1 186. In the case of the numeric target datasets in Table 8, the number of targets ranges from 1 to 16, the samples from 154 to 22 784. Note that we used multi-label datasets instead of multi-nominal as the latter are not widely available.

8.3 Nominal target results

The results obtained on binary, nominal and multi-label datasets with sequential subgroup set miners can be seen in Table 4, while the results for algorithms that ouput sets can be found in Table 9 in Appendix G. We can see that overall our algorithm gets 15 out of 29 best results, compared with seq-cover in second place with 13 best results. In terms of SWKL and per type of data, RSD achieves the smallest ranking for binary, seq-cover for nominal, and both are tied for multi-nominal. This small difference in the results between RSD and

[14] `https://archive.ics.uci.edu/ml/`
[15] `http://www.keel.es/`
[16] `http://mulan.sourceforge.net/datasets.html`

seq-cover is important for two reasons. First, it validates SWKL, as it shows that seq-cover is already implicitly maximizing it without knowing it. Second, it shows that RSD can obtain on par or slightly better results than other established approaches. Our non-diverse baseline, top-k, shows that covering different regions of the dataset is clearly important to maximize SWKL.
Regarding the number of found subgroups we can see that in most cases, all algorithms are in the same order of magnitude, with some clear exceptions where RSD obtains many more subgroups (for *adult*, *nursery*, *kr-vs-k*, and *mediamill*). These results can be explained by the use of normalized gain ($\beta = 1$) by RSD, together with the fact that these datasets have a large number of samples, few variables, and/or a large number of categories. First, let us recall that the normalized compression gain of Eq. (35) is composed of a data covering part and a model penalization part, and that both are normalized by the number of instances covered, which gives an advantage to subgroups that cover less data but are well-covered (only one category, or few categories). When the datasets are larger and the number of variables is reasonably small, like *adult* with 45 222 examples and 14 variables, there is a larger chance of finding more statistically "significant" subgroups, as there can be more regions where subgroups only (or almost only) cover one class, and the penalization of the model encoding is small as there are not many variables. On the other hand, subgroups that cover more data can more easily have a larger entropy in the class label distribution. For example, *kr-vs-k*, which is a reasonably large dataset with 28 056 and with 18 class labels, a subgroup that only covers one class label, as opposed to covering many class labels, will have a higher chance of being chosen. The number of subgroups found can be large, but it was shown in a classification setting that they generalize well (Proença and van Leeuwen, 2020). It is interesting to note that in the case of *corel-5k*, RSD does not find any "significant" subgroup to add.
Regarding the number of conditions per subgroup, the two best performing algorithms in terms of SWKL, RSD and seq-cover, tend to have similar and lower number of conditions than the other algorithms. Top-k, only covering the same region, has a tendency to be close to the maximum depth of 5.

8.4 Numeric target results

The results for the single-target and multi-target numeric datasets can be seen in Table 5. In general it can be seen that RSD obtains the best results for 23 out of 25 datasets. This is to be expected as SWKL and RSD take into account the dispersion/deviation of the subgroup target while top-k and seq-cover do not. This is clearly supported by the normalized standard deviation of the first subgroup found, where RSD tends to find subgroups with smaller deviation for 10 out of 15 cases. Comparing SWKL results for top-k with seq-cover and RSD shows that irrespective of dispersion-aware (RSD) or not (seq-cover), covering different regions of the data increases the quality of the list in terms of SWKL, validating the use of our measure. It should be noted that both top-

Table 4: Nominal target results. This includes single-binary, single-nominal, and multi-label, separated by horizontal lines in the table (top to bottom). The properties of the datasets can be seen in Table 7, and are ordered in ascending number of: 1) target variables; 2) number of classes; and 3) number of samples. The evaluation measures are {quality of the subgroup set swkl; number of subgroups $|S|$; and average number of conditions $|a|$}. 'avg. rank' stands for the average ranking for the respective target variable type, where 1 represents the best rank. Note that CN2-SD does not work for multi-label case and thus the empty values −. *as RSD produced no subgroups for corel-5k, seq-cover number of subgroups was used as a reference.

	top-k			seq-cover			CN2-SD			RSD		
datasets	swkl	$\|S\|$	$\|a\|$	swkl	$\|S\|$	$\|a\|$	swkl	$\|S\|$	$\|a\|$	swkl	$\|S\|$	$\|a\|$
sonar	0.24	2	4	**0.96**	9	2	0.67	11	2	0.43	2	3
haberman	0.08	1	5	**0.39**	20	4	0.18	12	4	0.04	1	1
breastCancer	0.37	6	2	0.80	13	2	0.80	11	2	**0.82**	6	2
australian	0.26	5	3	**0.69**	13	3	0.54	24	3	0.55	5	2
tictactoe	0.50	16	3	0.73	18	3	0.21	21	3	**0.87**	16	2
german	0.08	4	5	0.30	22	4	**0.42**	48	4	0.14	4	3
chess	0.25	17	3	0.87	13	2	0.68	51	3	**0.97**	17	2
mushrooms	0.49	12	4	0.92	11	1	**1.00**	36	1	**1.00**	12	1
magic	0.16	69	5	0.38	35	4	0.42	616	3	**0.47**	69	4
adult	0.11	103	5	0.27	79	4	0.43	1230	4	**0.31**	103	4
avg. rank	3.8	1.9	3.8	2.1	2.4	2.2	2.2	3.8	2.5	**1.9**	1.9	1.5
iris	0.53	4	2	**1.45**	5	2	0.96	4	2	1.44	4	1
balance	0.21	9	3	**0.80**	19	3	0.18	3	3	0.69	9	3
CMC	0.07	7	3	**0.30**	38	4	0.27	42	3	0.25	7	2
page-blocks	0.19	21	5	0.45	26	2	0.44	12	4	**0.49**	21	3
nursery	0.92	81	2	1.36	22	3	0.87	8	4	**1.63**	81	3
automobile	0.38	5	4	**1.61**	11	3	**1.54**	7	4	1.25	5	2
glass	1.01	5	2	1.55	5	2	**2.14**	6	2	1.92	5	1
dermatology	0.54	9	2	**2.28**	9	2	2.12	7	3	2.11	9	2
kr-vs-k	0.45	351	5	0.75	43	4	0.20	61	5	**1.83**	351	3
abalone	0.26	16	5	0.62	29	4	0.60	49	3	**0.74**	16	2
avg. rank	3.7	2.4	3.0	**1.6**	3.0	2.2	2.8	2.3	3.4	1.9	2.4	1.4
emotions	0.71	17	5	1.93	22	4	–	–	–	**2.68**	17	3
scene	0.39	49	5	1.85	33	4	–	–	–	**3.05**	49	4
birds	0.49	8	5	**2.02**	20	4	–	–	–	1.57	8	3
flags	0.44	5	4	**2.40**	17	4	–	–	–	1.21	5	2
yeast	0.49	35	5	1.83	55	5	–	–	–	**2.20**	35	5
genbase	0.88	15	2	5.51	12	1	–	–	–	**5.82**	15	1
mediamill	0.43	131	5	1.44	60	5	–	–	–	**2.96**	131	5
CAL500	1.46	1	5	**16.91**	36	4	–	–	–	1.24	1	5
corel5k*	5.81	144	3	**5.39**	144	4	–	–	–	0.00	0	0
avg. rank	2.7	1.9	2.7	**1.7**	2.3	1.9	–			**1.7**	1.8	1.4

k and seq-cover could in practice support taking into account the deviation but that would require several non-trivial modifications in their source code.

Table 5: Numeric target results. This includes single-numeric and multi-numeric, separated by a horizontal line in the table (top to bottom). The properties of the datasets can be seen in Table 8, and are ordered in ascending number of: 1) target variables; 2) number of classes; and 3) number of samples. The evaluation measures are { quality of the subgroup set swkl; number of subgroups $|S|$; normalized standard deviation of the first subgroup $\tilde{\sigma}_{t1}$; and average number of conditions $|a|$}. 'avg. rank' stands for the average ranking for the respective target variable type, where 1 represents the best ranking. Note that $\tilde{\sigma}_{t1}$ is not shown for the multi-numeric case as it is not easy to understand.

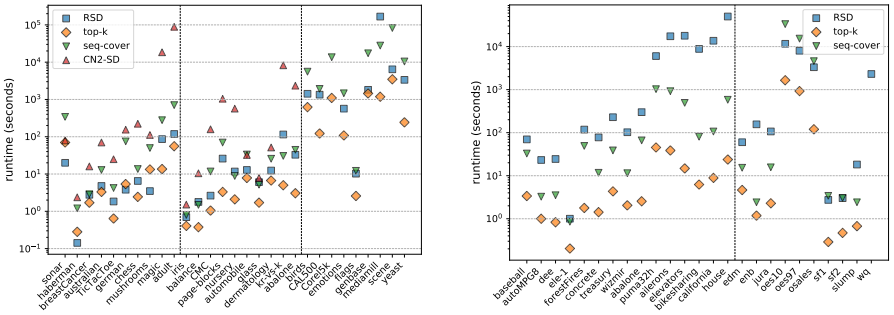
	top-k				seq-cover				RSD			
datasets	swkl	$\tilde{\sigma}_{t1}$	$\|S\|$	$\|a\|$	swkl	$\tilde{\sigma}_{t1}$	$\|S\|$	$\|a\|$	swkl	$\tilde{\sigma}_{t1}$	$\|S\|$	$\|a\|$
baseball	0.26	0.82	7	4	1.40	1.22	26	4	**1.86**	0.01	7	2
autoMPG8	0.43	0.54	8	4	1.45	1.85	22	4	**1.57**	0.18	8	2
dee	0.46	0.50	9	4	1.29	2.01	20	4	**1.35**	0.32	9	2
ele-1	0.29	1.06	8	4	1.14	0.94	22	4	**1.22**	1.24	8	2
forestFires	0.61	6.84	22	4	2.73	0.15	57	4	**3.91**	7.57	22	3
concrete	0.28	0.65	18	4	1.27	1.53	35	4	**1.31**	0.21	18	3
treasury	0.43	0.68	31	4	2.74	1.46	21	4	**3.85**	0.01	31	2
wizmir	0.70	0.31	22	4	2.15	3.22	26	4	**2.72**	0.15	22	2
abalone	0.23	0.59	26	4	0.47	1.68	126	5	**0.71**	1.32	26	3
puma32h	0.55	0.59	48	4	1.39	1.68	70	5	**1.44**	0.29	48	3
ailerons	0.24	1.23	98	4	1.04	0.82	105	4	**1.44**	0.98	98	4
elevators	0.23	1.44	158	4	0.83	0.69	150	5	**1.31**	1.40	158	4
bikesharing	0.26	1.09	136	4	1.24	0.92	91	4	**1.70**	0.02	136	4
california	0.19	0.90	174	4	0.69	1.11	116	5	**1.14**	0.00	174	4
house	0.19	1.59	269	4	0.91	0.63	143	5	**2.02**	2.83	269	5
avg. rank	3.0	2.1	1.8	2.0	2.0	2.3	2.3	2.7	**1.0**	1.6	1.8	1.3
edm	0.47	–	5	5	0.81	–	9	2	**1.88**	–	5	2
enb	2.73	–	41	2	3.54	–	19	2	**8.71**	–	41	2
slump	1.38	–	4	5	**2.74**	–	17	4	2.57	–	4	3
sf1	0.16	–	3	5	**2.06**	–	47	4	1.24	–	3	3
sf2	0.86	–	2	5	2.29	–	18	4	**0.91**	–	2	4
jura	0.47	–	15	5	2.38	–	28	4	**3.52**	–	15	3
osales	2.17	–	45	4	18.09	–	48	3	**26.44**	–	45	3
oes97	6.55	–	16	3	30.79	–	19	4	**34.36**	–	16	4
oes10	6.56	–	23	3	29.11	–	27	4	**40.65**	–	23	3
wq	0.87	–	62	5	2.06	–	47	4	**11.14**	–	62	4
avg. rank	3.0	–	1.7	2.4	1.7	–	2.6	1.8	**1.3**	–	1.7	1.8

Regarding the number of subgroups, seq-cover tends to have more rules than RSD for datasets with less than 5000 examples, while RSD tends to have more for higher number of examples. This makes sense as there is more evidence to identify possible significant subgroups.

Regarding the number of antecedents, RSD tends to have, on average, one condition fewer than seq-cover for single-target and a similar number for the multi-target case.

8.5 Runtime comparison

Runtimes of all algorithms compared, i.e., top-k, seq-cover, CN2-SD, and RSD, are shown in Figures 6a and 6b. In general, it can be seen that the runtime increases with the number of samples in the dataset for a fixed data type. For the nominal datasets it seems that there is an increase in runtime with the number of target variables, which does not seem to happen for numeric targets. This is due to the fact that for multivariate numeric targets the number of subgroups found was, in general, smaller.
Comparing the algorithms against each other, as expected, top-k was the fastest algorithm, as it only needs to search for the subgroups once, while the others need multiple iterations.
For nominal targets, CN2-SD was the slowest algorithm, which stems from the use of entropy as quality measure—experiments with WRAcc proved to be much faster. RSD seems to perform on par with seq-cover and is often even slightly faster.
For numeric targets RSD was one order of magnitude slower than seq-cover. One possible reason is the extra time to compute the variance, although this does not totally explain the difference between both algorithms. It seems that a further study of the numeric implementation could make for an interesting research direction.



(a) Nominal targets. (b) Numeric targets.

Fig. 6: Runtime in seconds for all algorithms for each dataset. The black vertical line divides the type of datasets, i.e., from left to right: univariate binary, nominal, and multi-label for nominal targets, and univariate and multivariate for numeric.

9 Case study: associations between socioeconomic background and university grades of Colombia Engineering students

In this section we apply RSD to a real use case to assess its usefulness and limitations. To this end, we aim at understanding how socioeconomic factors affect

the grades of engineering university students in Colombia on their national exams. The dataset used to study this is fully described by Delahoz-Dominguez et al. (2020). It contains socioeconomic variables and grades in national exams done at high-school and university level for engineering students in Colombia. For our specific case study we have selected two of their exam grades at the university for two reasons. First, the relationship between socioeconomic variables and university grades is weaker (than for high school grades), thus more interesting to see if we can find relations, and second, only having two exams grades improves the visualization of the results.

Dataset. The dataset used is composed of 12 412 samples, 22 explanatory variables, and 2 numeric target variables. The explanatory variables refer to the socioeconomic background of the students at the time of high school, and they are made of variables such as parents level of education, the household income, which type of high school they attended, the utilities available at home (e.g., internet and television), and their neighborhood stratum[17]. The numeric targets represent their grades, from 0% to 100%, in two national university-level exams, namely quantitative reasoning and English.
An additional reason for selecting this dataset is that it violates two of our model assumptions: 1) the target variables values are truncated between 0 and 100, thus violating the use of a continuous normal distribution to describe them; and 2) the target variables are not independent, as suggested by a correlation of 53%. If our approach is shown to work despite these violations, we may consider this is a good result.

9.1 Analysis of the subgroups obtained with RSD

The first four subgroups with absolute ($\beta = 0$) and normalized ($\beta = 1$) gain can be seen in Figures 7a and 7b, respectively. The distributions of the first two subgroups for both gains can be seen in Figures 8a, 8b, 8c and 8d. The two extreme gains were used to show that from an user perspective it can be interesting to use different gains depending on the goal of the data exploration, i.e., coarse versus fine-grained perspective.

Comparison of absolute and normalized gain. Overall, with absolute and normalized gain our method finds 7 and 34 subgroups that cover a total of 84% and 92% of the data, respectively. Looking at Figures 8a, 8b, 8c and 8d, it can be seen that normalized gain favors smaller and compact subgroups that deviate more from the dataset distribution, while absolute gain favors larger subgroups that deviate less from the dataset distribution. These conclusions can be verified by noting that normalized gain subgroups tend to have a smaller

[17] Stratum is a classification system unique to Colombia, where districts are ranked based on their affluence level from 1 to 6, where 1 is the lowest level `https://www.dane.gov.co/index.php/servicios-al-ciudadano/servicios-informacion/estratificacion-socioeconomica` (Accessed on 16 Feb. 2021).

standard deviation, between 5% and 9%, while absolute gain has values in the same order of magnitude of the dataset distribution, i.e., around 23%.

Interpretation of the results. Both normalized and absolute gain results point to the fact that having a 'better' socioeconomic background is associated with higher grades on average in both types of exams, and the contrary is associated with lower grades. This is clearer in the absolute gain case, as each subgroup covers more data. It is noticeable in Figure 8b that a subgroup with standard deviation similar to the dataset leads to subgroups that are spread throughout the whole range of values. Nonetheless, that subgroup covers more regions with lower grades than the dataset, making it a relevant result to understand the dataset better.
In general, it can be seen that some conditions appear often in the subgroups, such as *household_income* above and below 5 minimum wages and education of one of parents equal or above high school. It seems that presence or absence of these variables is highly associated with above or below average performance, respectively.
Looking at specific subgroups, it is interesting to see that in the 4^{th} subgroup of the absolute gain, the Quantitative reasoning grade is equal to the average behavior of the dataset (77%), while the English grade is 8% above average. Looking at the subgroups with normalized gain, we see that there are only slight variations of their descriptions and that they clearly belong to a similar socioeconomic macro group but with slight differences in their descriptions, which corresponds to small differences on their grades distribution.

Violation of the model assumptions. Here we can observe how our method behaves when some modeling assumptions are violated. Regarding the truncated values, it seems that the normalized gain is affected by grades around 100 (as seen in Figures 8c and 8d) as most of its subgroups capture these students, which increases the average and lowers the standard deviation, making them rank higher. Clearly our method was not developed for target values that are highly stratified, but the results seem to show that it is does not seem prohibitive to the use RSD in these cases as long as the stratification is mild and the user takes into account this fact.
Regarding the independence assumption, it seems that the subgroups found are still relevant although both grades are almost always taken into account together, i.e., as the values are positively correlated it is more likely to find subgroups with mean values that are high or low for both exams, but not high for one and low for the other. This is expected as the encoding of independent normal distributions does not take into account the covariance between target variables, and thus that case is not deemed a deviation by the current model formulation.

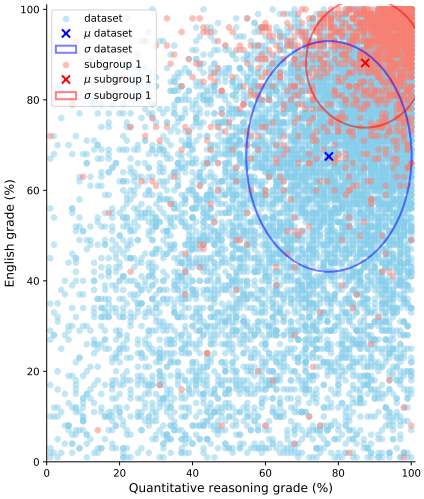
s	**description** of a student socioeconomic background	n_s	Quant.	English
1	household_income $\geq$ 5 min. wage & public_school = no & edu_mother > high_school & Microwave = yes	1676	87 ± 16	88 ± 14
2	household_income < 5 min. wage & stratum < 5 & public_school = yes	4031	72 ± 25	54 ± 26
3	gender = M & edu_father $\geq$ high_school & social_support = None & stratum > 3 & public_school = no	1478	85 ± 17	78 ± 20
4	social_support = None & edu_father > high_school & public_school = no & internet = yes & mobile = yes	997	77 ± 22	76 ± 19
	$\vdots$			
dataset distribution		1945*	77 ± 23	68 ± 26

(a) Subgroup list with absolute gain ($\beta = 0$). First 4 subgroups of a total of 7 and swkl = 0.41

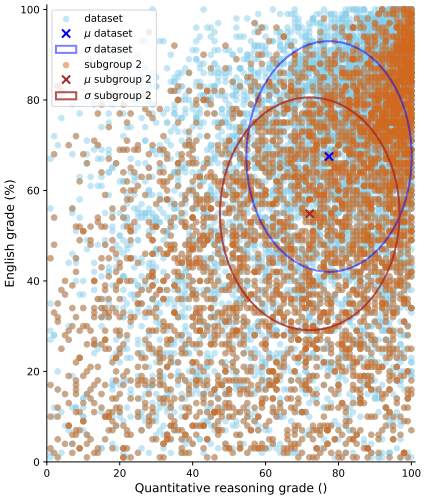
s	**description** of a student socioeconomic background	n_s	Quant.	English
1	household_income $\geq$ 5 min. wage & gender = M & household_size < 3 & edu_father > high-school & mobile = yes	39	96 ± 5	92 ± 6
2	household_income $\geq$ 5 min. wage & school_type = academic & occ._mother = retired & edu_father $\geq$ Undergrad	23	96 ± 5	95 ± 4
3	household_income $\geq$ 5 min. wage & job_mother = independent & stratum $\geq$ 4 & gender = M & job_father = independent	30	96 ± 5	93 ± 6
4	job_mother = executive & stratum $\geq$ 4 & mobile = yes & job_father = independent & public_school = no	32	93 ± 9	94 ± 6
	$\vdots$			
dataset distribution		942*	77 ± 23	68 ± 26

(b) Subgroup list with normalized gain ($\beta = 1$). First 4 subgroups of a total of 34 and swkl = 0.52

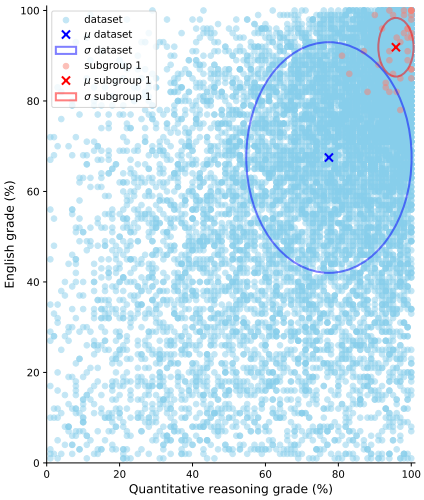
Fig. 7: *Colombia engineering students* performance in Quantitative Reasoning and English exams. The results of Fig. 7a and 7b were obtained by RSD with *absolute gain* ($\beta = 0$) and *normalized gain* ($\beta = 1$). The dataset contains two numeric target variable *Quantitative Reasoning* and *English* exams in a 0-100% scale. The dataset represents 12 412 engineering students in Colombia, their grades in university national exams and their social-economic background. *Description* contains information regarding students socio-enconomic background, n_s the number of instances covered, Quant. and English the average grade and standard deviation in the respective exams. * The n of the dataset is the total number of instances in the dataset.



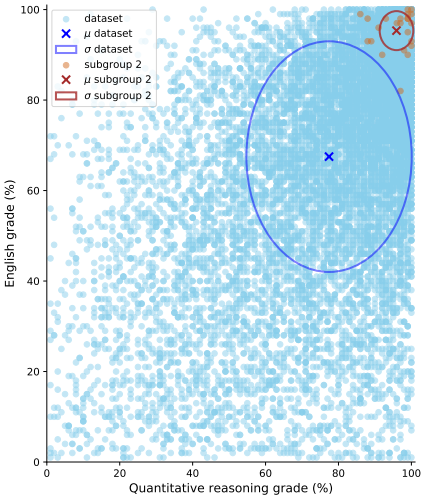
(a) 1^{st} subgroup with *absolute* gain.



(b) 2^{nd} subgroup with *absolute* gain.



(c) 1^{st} subgroup with *normalized* gain.



(d) 2^{nd} subgroup with *normalized* gain.

Fig. 8: Scatter plot of the grades of students for Quantitative Reasoning and English exam, together with the grades associated with the descriptions of the 1^{st} and 2^{nd} with *absolute* and *normalized* gain.

10 Conclusions

We showed that finding good subgroup lists (ordered sets) that are both non-redundant and statistically robust, i.e., *robust subgroup discovery*, is computationally feasible. To achieve this, we first defined what a subgroup list is and then proposed an optimal formulation of subgroup lists based on the MDL principle. We proposed a heuristic algorithm dubbed RSD that approximates this objective by means of a greedy search that adds the subgroup that locally minimizes the MDL criteria to the list in each consecutive iteration. This approximation was shown to be equivalent to a Bayesian test (factor) between subgroup and dataset marginal target distributions plus a penalty for multiple hypothesis testing, which guarantees that each subgroup added to the list is statistically sound.
These assertions are supported by empirical evidence obtained on a varied set of 54 datasets. In case of nominal targets our method performed on par in terms of subgroup list quality, while obtaining smaller lists with fewer conditions. In case of numeric targets and through the use of a deviation-aware measure, our method dominated in 92% of the cases.
Through a case study relating the socioeconomic background and national exams grades for Colombia engineering university students, we showed that RSD can be flexibly adapted to different goals of the user. In particular, it can change from a *fine grained* perspective of the data that finds many subgroups that cover small parts of the data well, to a *coarse* perspective that finds few subgroups that cover large parts of the data. Also, it was shown that our method is robust to mild violations of our model assumptions.

Limitations. Even though the RSD algorithm has some appealing local statistical properties, we do now know how far the found models are from the optimal subgroup lists as defined by the global MDL criteria we proposed. Also, it does not scale very well for numeric targets, which was to be expected from the time complexity analysis. At the moment, multiple target variables are assumed to be independent, which can produce erroneous results when this assumption is violated. Preliminary experiments show that for moderately correlated variables (e.g., with a correlation of 0.5) this does not seem to be an issue, but there is no quantification of its implications. Similarly, for numeric targets we use a normal distribution, and several datasets violate this assumption, either by behaving like a multi-modal or truncated distribution.

Future work. The main lines of research for future work can be divided in three categories: 1) extending subgroup lists to other target variables and/or distributions; 2) algorithmic developments; and 3) generalize this framework to other model classes. In the first category, an obvious extension would be to distributions that take into account multiple dependent target variables, such as multivariate-normal distributions for numeric targets and over itemsets for the nominal case. Another interesting and straightforward development would be the extension our work to mixed targets, combining both nominal and

numeric variables. In the second category, algorithmic developments could go from mere upper-and-lower bounds to improvements in search methods and to study the feasibility of global search such as Markov Chain Monte Carlo methods. In the third category, our approach could be formalized for subgroup sets, allowing for overlap between the subgroups.

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Appendices

A Normalized Maximum Likelihood independence for non-overlapping multinomials

For the purposes of this section, let us assume that we have a dataset $D = \{\mathbf{X}, Y\}$ and model M that forms a partition over the whole data. The model M divides the data D in ω parts, of the form $\{(\mathbf{X}^1, Y^1), \cdots, (\mathbf{X}^\omega, Y^\omega)\}$. Each part has an associated categorical distribution with estimated parameters $\hat{\Theta}^i$ over the target part Y^i (as defined in Section 3). Our goal in this section is to show that the NML encoding of a partition equals to the sum of the NML encoding of its parts:

$$L_{NML}(Y \mid \mathbf{X}, M) = \sum_{i=1}^{\omega} L_{NML}(Y^i). \tag{36}$$

Note that in the case of a subgroup list as the default rule does not require NML encoding, the M used in this section just represents the subgroups S, and D just represents the data covered by these. In the case of a tree or rule list, M represents the model that partitions the data at the level of leaves and rules (including default rule), respectively, and D the whole dataset. This is done without any loss of generality as the separation property allows us to separate the encoding of the default rule for a subgroup list.
First, lets recall the definition of the NML probability distribution (Shtar'kov, 1987):

$$L_{NML}(Y \mid \mathbf{X}, M) = -\log\left(\frac{\Pr(Y \mid \mathbf{X}; \hat{M}(Y \mid \mathbf{X}))}{\sum_{Z \in \mathcal{Y}^n} \Pr(Z \mid \mathbf{X}; \hat{M}(Z \mid \mathbf{X}))}\right),$$

where $\mathcal{Y}^n$ is the set of all possible sequences of n points with $k = |\mathcal{Y}|$ categories, $\hat{M}(Y \mid \mathbf{X})$ and $\hat{M}(Z \mid \mathbf{X})$ are the models with parameters estimated according to the maximum likelihood over the data Y and Z, respectively. Taking into account that our data is independent and identically distributed (*i.i.d.*), and that our model M partitions the data into ω parts, we can further develop the previous formula to:

$$\begin{aligned}
L_{NML}(Y \mid \mathbf{X}, M) &\overset{\text{i.i.d.}}{=} -\log\left(\frac{\prod_{i=1}^{n} \Pr(y^i \mid \mathbf{x}^i; \hat{M}(Y \mid \mathbf{X}))}{\sum_{Z \in \mathcal{Y}^n} \prod_{i=1}^{n} \Pr(z^i \mid \mathbf{x}^i; \hat{M}(Z \mid X))}\right) \\
&= -\log\left(\frac{\prod_{i'=1}^{\omega} \Pr(Y^{i'}; \hat{\Theta}(Y^{i'}))}{\sum_{Z \in \mathcal{Y}^n} \prod_{i'=1}^{\omega} \Pr(Z^{i'}; \hat{\Theta}(Z^{i'}))}\right) \\
&= -\log\left(\frac{\prod_{i'=1}^{\omega} l(\hat{\Theta}^{i'} \mid Y^{i'})}{g(Y, X, M)}\right) \\
&= -\log\left(\sum_{i'=1}^{\omega} l(\hat{\Theta}^{i'} \mid Y^{i'})\right) + \log g(Y, X, M),
\end{aligned} \tag{37}$$

where $l(\hat{\Theta}^{i'} \mid Y^{i'})$ is the likelihood function for each of the ω parts and $g(Y, X, M)$ is a complexity function that depends on these 3 variables.
The first term is already independent for each part, however the second is not.
Let us now look at $g(Y, X, M)$ in the case where we only have one part in the dataset, i.e., D^1. We will call this term the NML complexity of a multinomial distribution and denote it by $\mathcal{C}(n_1, k)$ of one part $D^1 = \{Y^1, X^1\}$, with $n_1 = |D^1|$ and $k = \mathcal{Y}$

$$\begin{aligned}\mathcal{C}(n_1, k) &= \log\left(\sum_{Z \in \mathcal{Y}^{n_1}} \Pr(Z^1; \hat{\Theta}(Z^1))\right) \\ &= \log\left(\sum_{Z \in \mathcal{Y}^{n_1}} \prod_{i=1}^{n_1} \Pr(z^i; \hat{\Theta}(Z^1))\right) \\ &= \log\left(\sum_{n_{11}+n_{12}+\ldots+n_{1k}=n_1} \frac{n_1!}{n_{11}!n_{12}!\ldots n_{1k}!} \prod_{c \in \mathcal{Y}} \left(\frac{n_{1c}}{n_1}\right)^{n_{1c}}\right)\end{aligned} \tag{38}$$

where n_{1c} is the number of points of category c in Y^1, and the passage from the second equality to the last is a property of multinomial distributions commonly used to make the computation of $\mathcal{C}(n_a, k)$ simpler (Grünwald, 2007). It is interesting to note that $\mathcal{C}(n_a, k)$ only depends on the number of points in Y^1 and its cardinality, not on the actual values. This term, i.e., the complexity of a multinomial distribution over n_1 points with k possible values, measures the likelihood of each possible sequence.

Table 6: All possible sequences of a partition of fixed length of the data in three parts. Fixed length means that all possible parts always have the same amount of points, as e.g. $|A_1| = |A_2| = \cdots = |A_a| = n_A$.

Part 1	Part 2	Part 3
A_1	B_1	C_1
A_1	B_1	C_2
$\vdots$	$\vdots$	$\vdots$
A_1	B_2	C_1
$\vdots$	$\vdots$	$\vdots$
A_a	B_b	C_c

Now we must generalize from a part to the whole partition of the dataset. To illustrate how to do this, let us first look at Table 6, which shows an example of all the possible sequences in a fixed-length three part partition of the data. Taking into account those three parts, let us look at how the probabilities of all those sequences could be computed:

$$\begin{aligned}\sum_{\forall a,b,c} \Pr(A_a)\Pr(B_b)\Pr(C_c) &= \left(\sum_{\forall a} \Pr(A_a)\right) \cdot \left(\sum_{\forall b,c} \Pr(B_b)\Pr(C_c)\right) \\ &= \left(\sum_{\forall a} \Pr(A_a)\right) \cdot \left(\sum_{\forall b} \Pr(B_b)\right) \cdot \left(\sum_{\forall c} \Pr(C_c)\right),\end{aligned}$$

where this follows naturally from the distributive property of the multiplication. It is easy to see that this generalizes to partitions of any number of parts. Thus, going back to the complexity term $g(Y, X, M)$, we can see that

$$\begin{aligned}\log g(Y,X,M) &= \log \sum_{Z\in\mathcal{Y}^n} \prod_{i'=1}^{\omega} \Pr(Z^{i'};\hat{\Theta}(Z^{i'})) \\ &= \log \prod_{i'=1}^{\omega} \sum_{Z^{i'}\in\mathcal{Y}^{n_{i'}}} \Pr(Z^{i'};\hat{\Theta}(Z^{i'})) \\ &= \sum_{i'=1}^{\omega} \log \sum_{Z^{i'}\in\mathcal{Y}^{n_{i'}}} \Pr(Z^{i'};\hat{\Theta}(Z^{i'})) \\ &= \sum_{i'=1}^{\omega} \log \mathcal{C}(n_{i'},k)\end{aligned} \tag{39}$$

Substituting this back into Eq. (37), we obtain what we wanted:

$$\begin{aligned}L_{NML}(Y \mid \mathbf{X}, M) &= -\log\left(\sum_{i=1}^{\omega} l(\hat{\Theta}^i \mid Y^i)\right) + \sum_{i=1}^{\omega} \log \mathcal{C}(n_i,k) \\ &= \sum_{i=1}^{\omega} l(\hat{\Theta}^i \mid Y^i) + \mathcal{C}(n_i,k) \\ &= \sum_{i=1}^{\omega} L_{NML}(Y^i)\end{aligned} \tag{40}$$

B Bayesian encoding of a normal distribution with mean and standard deviation unknown

Initially this derivation appeared in Proença et al. (2020) but for completeness we will repeat it here. For encoding a sequence of numeric valued i.i.d. observations such as $Y = (y_1, ..., y_n)$, the Bayesian encoding takes the following form:

$$P_{Bayes}(Y) = \int_{\Theta} f(Y \mid \Theta) w(\Theta)\, \mathrm{d}\Theta, \tag{41}$$

where f is the probability density function (pdf), Θ is the set of parameters of the distribution, and $w(\Theta)$ the prior over the parameters. In the case of a normal distribution $\Theta = \{\mu, \sigma\}$, with μ and σ being its mean and standard deviation, respectively, the pdf $f(Y \mid \Theta)$ over a sequence Y is the multiplication of the individual pdfs, thus:

$$f(Y \mid \mu, \sigma) = \frac{1}{(2\pi)^{n/2}\sigma^n} \exp\left[-\frac{1}{2\sigma^2}\sum_{i}^{n}(y^i-\mu)^2\right], \tag{42}$$

In order not to bias the encoding for specific values of the parameters, we choose to use a normal prior on the effect size $\rho = \mu/\sigma$ and the constant Jeffrey's prior of $1/\sigma^2$ for the unknown parameters μ and σ. Thus, our prior is given by:

$$w(\mu,\sigma) = \frac{1}{\sqrt{2\pi}\tau\sigma^2} \exp\left[-\frac{1}{2\sigma^2}\frac{\mu^2}{\tau^2}\right]. \tag{43}$$

Putting everything together, one obtains:

$$\begin{aligned}&P_{Bayes}(Y) = \\ &= (2\pi)^{-\frac{n+1}{2}}\tau^{-1}\int_{-\infty}^{+\infty}\int_{0}^{+\infty} \frac{1}{\sigma^{n+2}} \exp\left[-\frac{1}{2\sigma^2}\left(\sum_{i}^{n}(y^i-\mu)^2 + \frac{\mu^2}{\tau^2}\right)\right] \mathrm{d}\sigma\, \mathrm{d}\mu.\end{aligned} \tag{44}$$

The integrals over the whole space of the parameters μ and σ allow to penalize the fact that we do not know the statistics *a priori*, thus penalizing the fact that a distribution over n points could, by chance, have the same statistics as the one found in the data. Note that this prior choice is equal to the one of Gönen et al. (2005) for the Bayesian two-sample t-test, which was shown to converge to the Bayes Information Criteria (BIC) for large n (Rouder et al., 2009).

Note that using an improper prior requires that we somehow make it proper, i.e., we need to find a way to make the integration over the prior finite $\int\int w(\mu,\sigma) = K$, where K is a constant value. The usual way to make an improper prior finite is to condition on the k minimum number observations $Y^{|k} \in Y$ needed to make the integral proper (Grünwald, 2007), which in the case of two unknowns (μ and σ) is $k = 2$. Thus, instead of using $w(\mu,\sigma)$ we will in practice be using $w(\mu,\sigma \mid Y^{|2})$, and using the the chain rule and the Bayesian formula returns a total encoding of Y equal to

$$P(Y) = P_{Bayes}(Y \mid Y^{|2})P(Y^{|2}) = \frac{P_{Bayes}(Y)}{P_{Bayes}(Y^{|2})}P(Y^{|2}) \tag{45}$$

where $P(Y^{|2})$ is a non-optimal probability used to define $Y^{|2} = \{y^1, y^2\}$ that we will define later and y^1, y^2 chosen in a way that maximizes $P(Y)$. Now that we have all the ingredients to define $P(Y)$ we will start by defining $P_{Bayes}(Y)$ and then choose the appropriate probability for $P(Y^{|2})$.

To solve the first integral of $P_{Bayes}(Y)$ in Eq. (44), we integrate in σ and note that the formula is an instance of the gamma function,

$$\Gamma(k) = \int_0^{+\infty} z^{k-1}e^{-z}\,\mathrm{d}z, \tag{46}$$

with the corresponding variable transformation:

$$z = \frac{A}{2\sigma^2};\ \frac{1}{\sigma} = \frac{2^{1/2}z^{1/2}}{A^{1/2}};\ \mathrm{d}\sigma = -\frac{\sigma}{2z}\,\mathrm{d}z;\ A = \left[\sum_i^n (y^i-\mu)^2 + \frac{\mu^2}{\tau_\rho^2}\right], \tag{47}$$

Performing the variable transformation and noting that the minus sign of $\mathrm{d}z$ cancels with the reversing of the integral limits, we get:

$$\begin{aligned} &P_{Bayes}(Y) = \\ &= \tau^{-1}\Gamma(n/2)2^{\frac{n+1}{2}-1}(2\pi)^{-\frac{n+1}{2}}\int_{-\infty}^{+\infty}\left[\sum_i^n (y^i-\mu)^2 + \frac{1}{\tau^2}(0-\mu)^2\right]^{-\frac{n+1}{2}}\mathrm{d}\mu, \end{aligned} \tag{48}$$

which reveals that the prior on the effect size ρ, and specifically its standard deviation parameter τ, is equivalent to adding $1/\tau^2$ virtual points to the original data.

To solve the integral in μ we need to introduce the statistics $\hat{\mu}$ and $\hat{\sigma}$ as the values estimated from the data. We define these quantities as:

$$\hat{\mu} = \frac{1}{n}\sum_i^n y^i;\ \hat{\mu}' = \frac{n}{n+1/\tau^2}\hat{\mu};\ \hat{\sigma}^2 = \frac{1}{n}\sum_i^n (y^i-\hat{\mu})^2, \tag{49}$$

where $\hat{\mu}$ is the mean estimator over n data points, $\hat{\mu}'$ is an extension of the mean adding $1/\tau^2$ virtual points, and $\hat{\sigma}^2$ is the estimator of the variance. Note that for the variance the biased version with n was used instead of with $n-1$ as it allows to compute the Residual Sum of Squares (RSS) directly by $RSS = n\hat{\sigma}$.

Focusing now on the interior part of the integral of Eq. 48 and rewriting it in order to resemble the t-student distribution, we obtain:

$$\begin{aligned}
&\left[\sum_i^n (y^i-\mu)^2 + \frac{1}{\tau^2}(0-\mu^2)\right]^{-(n+1)/2} = \\
&\left[\sum_i^n (y^i)^2 - (n+1)\hat{\mu}'^2 + (n+1)\hat{\mu}'^2 - 2(n+1/\tau^2)\hat{\mu}'\mu^2 + (n+1/\tau^2)\mu^2\right]^{-(n+1)/2} = \\
&\left[\sum_i^n (y^i)^2 - n\hat{\mu}^2 + (n+1/\tau^2)(\hat{\mu}'-\mu)^2\right]^{-(n+1)/2} = \\
&\left[n\hat{\sigma}^2 + (n+1/\tau^2)(\hat{\mu}'-\mu)^2\right]^{-(n+1)/2} = \\
&\left[n\hat{\sigma}^2\right]^{-(n+1)/2}\left[1+\frac{(n+1/\tau^2)(\hat{\mu}'-\mu)^2}{n\hat{\sigma}^2}\right]^{-(n+1)/2} \\
&\left[n\hat{\sigma}^2\right]^{-(n+1)/2}\left[1+\frac{1}{n}\left(\frac{\hat{\mu}'-\mu}{s_s^2}\right)^2\right]^{-(n+1)/2},
\end{aligned} \tag{50}$$

where $s_s^2 = \hat{\sigma}/(n+1/\tau^2)$ is the "sampling" variance. Now, taking into account the fact that the integral of the t-student distribution over the whole space is equal to one, and reshuffling around its terms we get

$$\int_{-\infty}^{+\infty}\left[1+\frac{1}{n}\left(\frac{\hat{\mu}'-\mu}{s_s}\right)^2\right]^{-\frac{n+1}{2}} \mathrm{d}\mu = \frac{\Gamma\left(\frac{n}{2}\right)\sqrt{\pi n}s_s}{\Gamma\left(\frac{n+1}{2}\right)}. \tag{51}$$

Inserting this back in Eq. 44 we obtain:

$$\begin{aligned}
&P_{Bayes}(Y) = \\
&= \tau^{-1}\Gamma\left(\frac{n+1}{2}\right)2^{\frac{n+1}{2}-1}(2\pi)^{-\frac{n+1}{2}}\frac{\Gamma(\frac{n}{2})\sqrt{\pi n}s_s}{\Gamma(\frac{n+1}{2})}\left[n\hat{\sigma}^2\right]^{-(n+1)/2} \\
&= \tau^{-1}2^{-1}\pi^{-\frac{(n+1)}{2}}\Gamma\left(\frac{n}{2}\right)\frac{1}{\sqrt{n+1/\tau^2}}\left[n\hat{\sigma}^2\right]^{-\frac{n}{2}},
\end{aligned} \tag{52}$$

Returning to the the conditional probability of Eq. (45), we see that we still need to define $P(Y^{|2})$, the non-optimal probability of the first two-points. As in the case of our model class we assume that the dataset overall statistics are known, i.e., $\Theta = \{\hat{\mu}_d, \hat{\sigma}_d\}$, we will use this distribution to find the probability of the points $Y^{|2} = \{y^1, y^2\}$ as :

$$P(Y^{|2}) = \log 2\pi + \log\hat{\sigma}_d + \left[\frac{1}{2\hat{\sigma}_d^2}\sum_i^2 (y^i-\hat{\mu}_d)^2\right]\log e. \tag{53}$$

Finally, applying the minus logarithm base 2 to all the terms in Eq (45) to obtain the total code length in bits,

$$\begin{aligned}
&L_{Bayes2.0}(Y) = -\log P_{Bayes}(Y) + \log P_{Bayes}(Y^{|2}) - \log P(Y^{|2}) \\
&= 1 + \frac{n}{2}\log\pi - \log\Gamma\left(\frac{n}{2}\right) + \frac{1}{2}\log(n + 1/\tau^2) + \frac{n}{2}\log\left(n\hat{\sigma}_n^2\right) \\
&- 1 - \frac{2}{2}\log\pi + 0 - \frac{1}{2}\log(2 + 1/\tau^2) - \log\left(\sum_i^2 (y^i - \hat{\mu}_2)^2\right) \\
&+ \frac{2}{2}\log\pi + \log\hat{\sigma}_d + \left[\frac{1}{2\hat{\sigma}_d^2}\sum_i^2 (y^i - \hat{\mu}_d)^2\right]\log e \\
&= \frac{n}{2}\log\pi - \log\Gamma\left(\frac{n}{2}\right) + \frac{1}{2}\log(n + 1/\tau^2) + \frac{n}{2}\log\left(n\hat{\sigma}_n^2\right) + L_{cost}(Y^{|2}),
\end{aligned} \tag{54}$$

where $\hat{\mu}_2$ is the estimated mean of y^1, y^2 and $L_{cost}(Y^{|2})$ is the extra cost incurred of not being able to use a refined encoding for $Y^{|2}$. Now that the length of the encoding is defined we just need to choose the two points. i.e., y^1, y^2. Because we want to minimize this length, we notice that there are only two terms that contribute to it in $L_{cost}(Y^{|2})$, and thus by choosing the two observations close to $\hat{\mu}_d$ we can both minimize the encoding of $P(Y^{|2})$ and maximize $P_{Bayes}(Y^{|2})$ for most cases. There are exceptions to this, depending on the respective values of μ_d and y^1, y^2 but this are not significant to change the values too much and also requires less computational search to find the points.

C Bayesian encoding convergence to BIC for large n

In this section it is shown that for large number of instances n the Bayesian encoding of a normal distribution with unknown mean and standard deviation (Eq. (54)) converges to the encoding of a normal distribution with mean and standard deviation known plus $\log n$, i.e., proportional to the definition of the Bayes Information Criterion (BIC). First the encoding of a normal distribution with mean and standard deviation known over n *i.i.d.* points is equal to the sum of the individual encodings:

$$L(Y \mid \hat{\Theta}) = \frac{n}{2}\log 2\pi + \frac{n}{2}\log\hat{\sigma}^2 + \left[\frac{1}{2\hat{\sigma}^2}\sum_i^n (y^i - \hat{\mu})^2\right]\log e. \tag{55}$$

Second, we need to use the Stirling's approximation of the Gamma function for large n:

$$\begin{aligned}
&-\log\Gamma\left(\frac{n}{2}\right) \\
&\sim -\frac{1}{2}\log\pi - \frac{1}{2}\log(n-2) - \left(\frac{n}{2} - 1\right)\log\left(\frac{n}{2} - 1\right) + \left(\frac{n}{2} - 1\right)\log e,
\end{aligned} \tag{56}$$

and finally we insert it into Eq. (54) and assume $\tau = 1$ to obtain:

$$
\begin{aligned}
& L(Y) \sim \\
& \sim 1 + \frac{n-1}{2}\log\pi + \frac{1}{2}\log\left(\frac{n+1}{n-2}\right) + \frac{n}{2}\log\left(\frac{n\hat{\sigma}^2}{n/2-1}\right) + \left(\frac{n}{2}-1\right)\log e \\
& + \log\left(\frac{n}{2}-1\right) + L_{cost}(Y^{|2}) \\
& \sim \frac{n}{2}\log\pi + \frac{n}{2}\log 2\hat{\sigma}^2 + \left[\frac{1}{2\hat{\sigma}^2}\sum_i^n (y^i-\mu)^2\right]\log e + \log n - \log e + L_{cost}(Y^{|2}) \\
& = L(Y \mid \hat{\Theta}) + \log\frac{n}{e} + L_{cost}(Y^{|2}) \\
& \sim \frac{1}{2}\left(2L(Y \mid \hat{\Theta}) + 2\log n - 2\log e\right) \\
& = \frac{1}{2}BIC,
\end{aligned}
\tag{57}
$$

where from the second to the third line we assumed large n, making some of the terms disappear, while the definition $n\hat{\sigma}^2 = \sum_i^n (y^i-\mu)^2$ is used for making the third term of the third expression appear. From the fourth to the fifth expressions it was assumed that $L_{cost}(Y^{|2})$ is negligible, as it is the cost of not being able to encode the first two points optimally. For the Bayes information criterion we used its standard definition,

$$BIC = -2\ln\ell(\Theta \mid Y) + k\ln n, \tag{58}$$

where $\ell(\Theta \mid Y)$ is the likelihood as estimated from the data, and k is the number of parameters, which in our case is 2.

D Kullback-Leibler divergence between two normal distributions

Let us assume two normal probability distributions, $p(x) \sim \mathcal{N}(\mu_p, \sigma_p)$ and $q(x) \sim \mathcal{N}(\mu_q, \sigma_q)$. The Kullback-Leibler divergence of q from p is:

$$
\begin{aligned}
KL_{\mu,\sigma}(p;q) &= \int_{-\infty}^{+\infty} p(x)\log p(x)\,\mathrm{d}x - \int_{-\infty}^{+\infty} p(x)\log q(x)\,\mathrm{d}x \\
&= \mathbb{E}_p\left[\log p(x)\right] - \mathbb{E}_p\left[\log q(x)\right] \\
&= -\frac{1}{2}\left(\log e + \log 2\pi\sigma_p^2\right) + \frac{1}{2}\log 2\pi\sigma_q^2 + \mathbb{E}_p\left[\frac{(x-\mu_q)^2}{2\sigma_q^2}\log e\right] \\
&= -\frac{\log e}{2} + \log\frac{\sigma_p}{\sigma_q} + \mathbb{E}_p\left[\frac{x^2 - 2x\mu_q + \mu_q^2}{2\sigma_q^2}\log e\right] \\
&= -\frac{\log e}{2} + \log\frac{\sigma_q}{\sigma_p} + \frac{\sigma_p^2 + \mu_p^2 - 2\mu_p\mu_q + \mu_q^2}{2\sigma_q^2}\log e \\
&= -\frac{\log e}{2} + \log\frac{\sigma_q}{\sigma_p} + \frac{\sigma_p^2 + (\mu_p-\mu_q)^2}{2\sigma_q^2}\log e.
\end{aligned}
\tag{59}
$$

Note that in the specific case where the Kullback-Leibler divergence only takes into account the means and assumes both standard deviations equal, i.e., $p(x) \sim \mathcal{N}(\mu_p, \sigma)$ and $q(x) \sim \mathcal{N}(\mu_q, \sigma)$ one obtains:

$$KL_{\mu}(p;q) = \frac{(\mu_p-\mu_q)^2}{2\sigma^2}\log e, \tag{60}$$

and the weighted version of this KL_μ, i.e., $WKL_\mu = nKL_\mu(p;q)$, is similar to the most common subgroup discovery quality functions used for numeric targets that do not take into account the dispersion of the subgroup, such as the weighted relative accuracy or the mean-test (Van Leeuwen and Knobbe, 2012), which uses the square root of KL_μ. We will call this measure the Weighted Kullback-Leibler without dispersion.

E Difference between subgroup discovery and rule-based predictive models

In this section we show the difference between the objective being maximized for subgroup discovery and for predictive rules. We do this through the comparison of the equivalent maximization MDL scores for subgroup lists and classification rule lists (Proença and van Leeuwen, 2020) with only one rule/subgroup—without loss of generality for greater sizes or for regression tasks. To differentiate both model classes SL and RL will be used for subgroup lists and classification rule lists, respectively.
First, lets recall the form of a subgroup list SL as given in Figure 4:

$$\begin{aligned}\text{subgroup 1}: \textsc{if}\ a \sqsubseteq \mathbf{x}\ \textsc{then}\ y \sim Cat(\hat{\Theta}^a)\\ \text{dataset}: \textsc{else}\ y \sim Cat(\hat{\Theta}^d)\end{aligned}$$

where, $\hat{\Theta}^a$ are the estimated parameters of subgroup 1 and $\hat{\Theta}^d$ are the estimated parameters of the marginal distribution of the dataset and are thus constant for each dataset. On the other hand, the model form of a classification rule list RL takes the following form:

$$\begin{aligned}\text{rule 1}: \textsc{if}\ a \sqsubseteq \mathbf{x}\ \textsc{then}\ Cat(\hat{\Theta}^a)\\ \text{default}: \textsc{else}\ y \sim Cat(\hat{\Theta}^{\neg a})\end{aligned}$$

where $\hat{\Theta}^{\neg a}$ was used to emphasize that the default rule of a rule list is not fixed, and is equivalent to the 'not rule 1'. This is the key difference between between these two types of models, the default rule is fixed to the marginal distribution of the dataset for subgroup lists, and the default rule has the distribution of the negative set of the rules in the list for rule lists. It should be noted that there are many definitions of rule lists that use a fixed rule, however having a variable default rule that maximizes the prediction quality is the best representative of rule lists and of the objective of finding the best machine learning model, i.e., returning the best partition of the data with the smallest error possible. Note that a decision tree is also part of this family of models as any path starting at the root of the tree to one of its leaves also forms a rule, and thus, a decision tree is equivalent to a set of disjoint rules, i.e., none of the rules described in this way overlap on a dataset. For the type of classification rule lists defined above, the encoding of the first rule and default rule is given by Eq. 23 as for both rules the parameters are unknown.
Thus the MDL score of a rule list is given by:

$$L(D, RL) = L(Y^a \mid \mathbf{X}^a) + L(Y^{\neg a} \mid \mathbf{X}^{\neg a}) + L(RL), \tag{61}$$

and note that the model encoding $L(RL) = L(SL)$, has both lists can be described in the same manner.
Following the same steps as in Section 5.4 by turning the MDL score objective from a minimization to maximization by multiplying by minus one and adding the constant $L(Y^d \mid \boldsymbol{\Theta}^d)$, we obtain the same objective as in Eq. 5.4:

$$r^* = \arg\max_{s \in \mathcal{M}} \Big[L(Y^d \mid \boldsymbol{\Theta}^d) - L(Y \mid \mathbf{X}, RL) - L(RL) \Big],$$

where r is the rule that maximizes the objective. Working out this equation, maximization objective of a *classification rule list* for a target variable of k class labels is given by:

$$\begin{aligned} & L(Y \mid \hat{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(RL) \\ & = L(Y^a \mid \hat{\Theta}^d) + L(Y^{\neg a} \mid \hat{\Theta}^d) - L(Y^a \mid X_a) - L(Y^{\neg a} \mid \mathbf{X}^{\neg a}) - L(RL) \\ & = n_a KL(\hat{\Theta}^a; \hat{\Theta}^d) - \mathcal{C}(n_a, k) + n_{\neg a} KL(\hat{\Theta}^{\neg a}; \hat{\Theta}^d) - \mathcal{C}(n_{\neg a}, k) - L(RL), \end{aligned} \tag{62}$$

This should be contrasted with the maximization objective of *subgroup list* of Eq. 25, which is given by:

$$\begin{aligned} & L(Y \mid \hat{\Theta}^d) - L(Y \mid \mathbf{X}, M) - L(SL) = \\ & n_a KL(\hat{\Theta}^a; \hat{\Theta}^d) - \mathcal{C}(n_a, k) - L(SL). \end{aligned}$$

Comparing both of the last equations we can notice the most important distinction between subgroup discovery and classification: the *local* nature of subgroup discovery and the *global* nature of the classification task. In other words, subgroup discovery aims at finding subgroups that locally maximize their quality, independently of the rest of the dataset, and even though rules for classification try to maximize their *local* quality also, they have to take into account the quality of their negative set, i.e., a rule for classification cannot be considered by its quality alone, it has to be considered in terms of its *global* impact in the dataset. On the other hand, this result also shows the similarity between both tasks and where the confusion sometimes arises, i.e., in some particular cases the best subgroup can be also the best rule. An example of this would be a dataset that is very large (relatively to the number of observations covered by the rule), and the best rule/subgroup would cover a small number of observations compared to the rule formed by the negative set of that rule, i.e., $D^{\neg a}$, as a similar distribution to $\hat{\Theta}^d$, making $\hat{\Theta}^{\neg a} \sim \hat{\Theta}^d$. Nonetheless, this similarity decreases in the case of larger lists, as the default rule will always represent what is left and in a subgroup list it remains constant and representing what we consider uninteresting. The same result can be obtained for regression rule lists.

F Datasets for empirical experiments

The datasets selected are commonly used in machine learning and were retrieved from UCI (Dua and Graff, 2017), Keel (Alcalá-Fdez et al., 2011), MULAN (Tsoumakas et al., 2011) repositories. The datasets used for nominal and numeric targets experiments can be seen in Table 7 and 8, respectively.

Table 7: Nominal targets datasets: single-binary, single-nominal and multi-label. Dataset properties: number of {target variables T; target labels $|\mathcal{Y}|$; samples $|D|$; type of variables (nominal/numeric)}.

Dataset	T	$\lvert\mathcal{Y}\rvert$	$\lvert D\rvert$	$V(nom./num.)$
sonar	1	2	208	(0/60)
haberman	1	2	306	(0/3)
breastCancer	1	2	683	(0/9)
australian	1	2	690	(0/14)
TicTacToe	1	2	958	(9/0)
german	1	2	1 000	(13/7)
chess	1	2	3 196	(36/0)
mushrooms	1	2	8 124	(22/0)
magic	1	2	19 020	(0/10)
adult	1	2	45 222	(8/6)
iris	1	3	150	(0/4)
balance	1	3	625	(0/4)
CMC	1	3	1 473	(0/9)
page-blocks	1	5	5 472	(0/10)
nursery	1	5	12 960	(7/1)
automobile	1	6	159	(10/15)
glass	1	6	214	(0/10)
dermatology	1	6	358	(0/34)
kr-vs-k	1	18	28 056	(6/0)
abalone	1	28	4 174	(1/7)
emotions	6	2	593	(0/72)
scene	6	2	2407	(0/294)
flags	7	2	194	(9/10)
yeast	14	2	2417	(0/103)
birds	19	2	645	(/258)
genbase	27	2	662	(1186/0)
mediamill	101	2	43 907	(0/120)
CAL500	174	2	502	(0/68)
Corel5k	374	2	5000	(499/0)

Table 8: Numeric targets datasets: single-numeric and multi-numeric. Dataset properties: {number of target variables T; minimum and maximum target values $[min., max.]$; number of samples $|D|$; number of type of variables (nominal/numeric)}.

Dataset	T	$[min.; max.]$	$\lvert D\rvert$	$V(nom./num.)$
baseball	1	$[109; 6100]$	337	(4/12)
autoMPG8	1	$[9; 46.6]$	392	(0/6)
dee	1	$[0.8; 5.1]$	365	(0/6)
ele-1	1	$[80; 7675]$	495	(0/2)
forestFires	1	$[0; 1091]$	517	(0/12)
concrete	1	$[3; 21]$	1030	(0/8)
treasury	1	$[29; 90]$	1049	(0/15)
wizmir	1	$[29; 90]$	1461	(0/9)
abalone	1	$[1; 29]$	4177	(0/8)
puma32h	1	$[-0.0867; 0.0898]$	8192	(0/32)
ailerons	1	$[-0.0036; 0]$	13750	(0/40)
elevators	1	$[0.012; 0.078]$	16599	(0/18)
bikesharing	1	$[1; 977]$	17379	(2/10)
california	1	$[14999; 500001]$	20640	(0/8)
house	1	$[0; 500001]$	22784	(0/16)
edm	2	$[-1; 1]$	154	(0/16)
enb	2	$[6.01; 48.03]$	768	(0/8)
slump	3	$[0; 78]$	103	(0/7)
sf1	3	$[0; 4]$	323	(0/10)
sf2	3	$[0; 8]$	1066	(0/10)
jura	3	$[0.135; 166.4]$	359	(0/15)
osales	12	$[500; 795000]$	639	(0/413)
wq	14	$[0; 5]$	1060	(0/16)
oes97	16	$[30; 48890]$	334	(0/263)
oes10	16	$[30; 64560]$	403	(0/298)

G Empirical results of non-sequential subgroup discovery algorithms

The comparison of RSD with subgroup set discovery algorithms that return sets (and not lists) can be seen in Table 9.

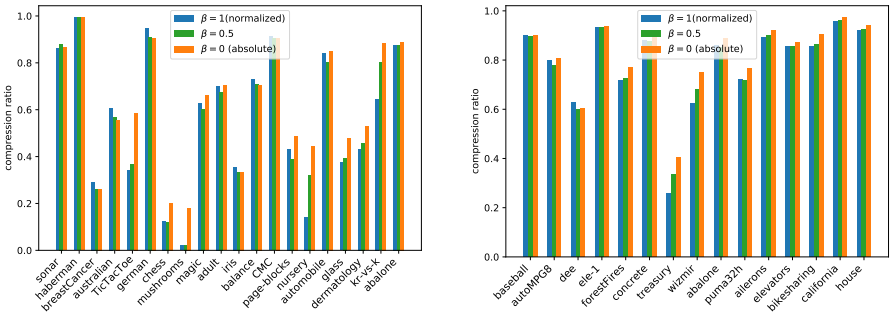
Table 9: Single nominal target results for non-sequential methods plus RSD. This includes single-binary, single-nominal, respectively separated by an horizontal line in the table. The properties of the datasets can be seen in Table 7, and are ordered by number target variables, number of classes, and number of samples, in this order. The evaluation measures are {quality of the subgroup set swkl; number of subgroups $|S|$; and average number of conditions $|a|$}. Note that FSSD does not work for single-nominal case and MCTS4DM only works for datasets with the same type of explanatory variables and thus the empty values −. *as DSSD does have a stopping criteria the maximum number of subgroups was selected as the number of subgroups found by RSD, and total overlapping subgroups were posteriorly removed.

	DSSD			MCTS4DM			FSSD			RSD		
datasets	swkl	$\|S\|*$	$\|a\|$	swkl	$\|S\|$	$\|a\|$	swkl	$\|S\|$	$\|a\|$	swkl	$\|S\|$	$\|a\|$
sonar	0.33	2	5	–	–	–	0.05	1	43	**0.43**	2	3
haberman	**0.08**	1	4	**0.08**	1	3	0.04	11	3	0.04	1	1
breastCancer	0.79	6	3	0.81	6	4	0.35	6	9	**0.82**	6	2
australian	0.50	3	3	0.54	7	6	0.33	15	12	**0.55**	5	2
tictactoe	0.50	4	3	–	–	–	0.20	5	3	**0.87**	16	2
german	**0.15**	4	5	–	–	–	0.10	6	11	0.14	4	3
chess	0.76	11	4	–	–	–	0.34	4	15	**0.97**	17	2
mushrooms	0.97	3	4	–	–	–	0.40	5	20	**1.00**	12	1
magic	0.30	40	3	–	–	–	0.06	3	10	**0.47**	69	4
adult	0.24	31	5	–	–	–	0.00	1	10	**0.31**	103	4
avg. rank	1.8	1.7	2.0	–	–	–	3.0	1.9	2.9	**1.2**	2.5	1.1
iris	1.44	3	2	**1.45**	4	3	–	–	–	1.44	4	1
balance	0.63	9	3	–	–	–	–	–	–	**0.69**	9	3
CMC	0.18	7	3	0.16	20	4	–	–	–	**0.25**	7	2
page-blocks	0.36	19	3	–	–	–	–	–	–	**0.49**	21	3
nursery	0.92	2	3	–	–	–	–	–	–	**1.63**	81	3
automobile	0.85	5	5	–	–	–	–	–	–	**1.25**	5	2
glass	1.55	3	1	1.12	5	6	–	–	–	**1.92**	5	1
dermatology	1.85	6	3	1.02	9	6	–	–	–	**2.11**	9	2
kr-vs-k	0.62	13	3	–	–	–	–	–	–	**1.83**	351	3
abalone	0.53	14	3	–	–	–	–	–	–	**0.74**	16	2
avg. rank	1.9	1.2	1.7		–	–	–	–	–	**1.1**	1.9	1.3

H Empirical analysis of compression gain

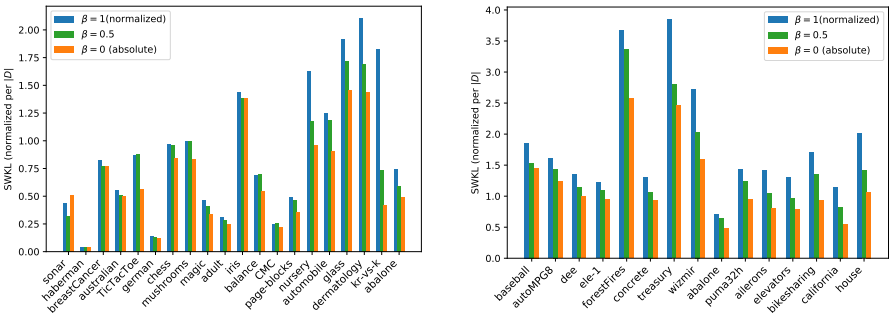
In this section we present a thorough comparison of the normalization terms β of RSD, where $\beta = 1$ is the *normalized* gain and $\beta = 0$ the *absolute* gain. RSD is executed with the same parameters (beam width, number of cut points for numerical variables, and maximum depth of search) as in the experiments section, i.e., $w_b = 100$, $n_{cut} = 5$, $d_{max} = 5$. The different types of gain are compared for all the benchmark datasets described in the paper in terms of their compression ratio (defined later) in Figure 9, Sum of Weighted Kullback-Leibler divergency (SWKL) in Figure 10, and number of rules in Figure 11. The compression ratio is the length of the found model $L(D, M)$ divided by the length of encoding the data with the dataset distribution (a model without subroups) $L(D \mid \hat{\Theta}^d)$, and formally it has the following form:

$$L\% = \frac{L(D, M)}{L(D \mid \hat{\Theta}^d)} \tag{63}$$



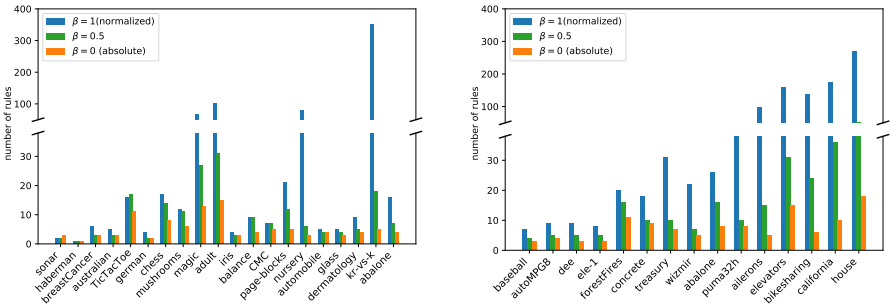
(a) Univariate nominal target. (b) Univariate numeric target.

Fig. 9: Compression ratio obtained with $\beta = 0$ (absolute gain), $\beta = 0.5$, and $\beta = 1$ (normalized gain).



(a) Univariate nominal target. (b) Univariate numeric target.

Fig. 10: Normalized SWKL obtained with $\beta = 0$ (absolute gain), $\beta = 0.5$, and $\beta = 1$ (normalized gain).



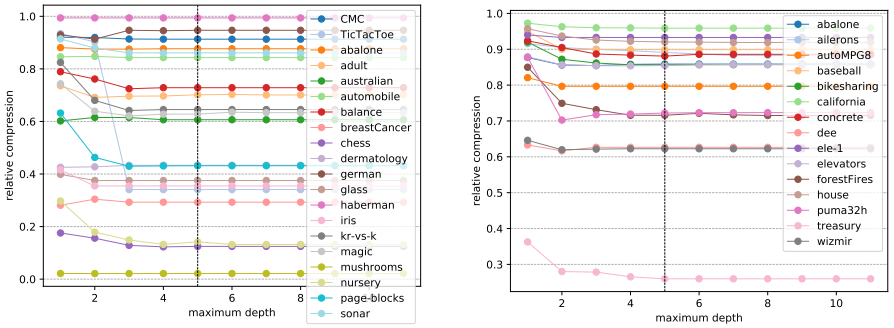
(a) Univariate nominal target. (b) Univariate numeric target.

Fig. 11: Number subgroups obtained with $\beta = 0$ (absolute gain), $\beta = 0.5$, and $\beta = 1$ (normalized gain).

I Empirical analysis of the influence of the beam search hyperparameters

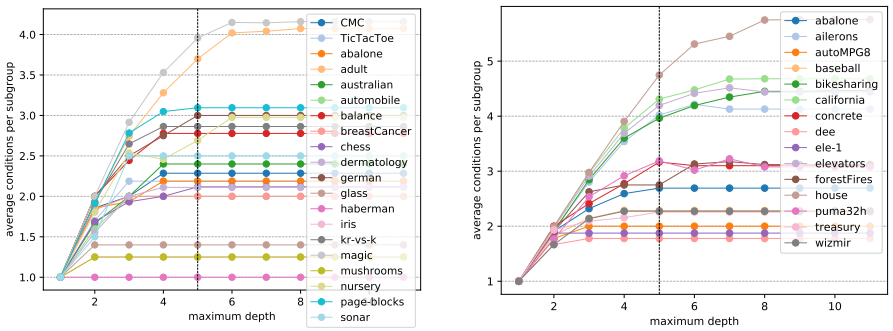
In this section we present a thorough comparison of the influence of the hyperparameters of the beam search of RSD on its results. As a complete search over the whole combination of parameters is unfeasible we present here a exploration over the parameters used for the experimental comparison in the paper ($w_b = 100$, $n_{cut} = 5$, $d_{max} = 5$), i.e., we fix two of the parameters on the aforementioned values and then proceed to change the selected parameter of interest, and we do this for all the 3 parameters. The line between the dots of the same color does not represent an interpolation and is merely used to aid visualization and suggest trends.

Note on relative compression. It may seem that the values of the relative compression remain constant but that is an illusion due to the scale of the y axis. As the compression ratio is given by the division of large values (usually above the thousands) its value with two decimal digits can be misleading. Nonetheless, in general, when zooming over the figures one can discern a slight improvement (smaller values) for larger values of the hyperparameters.



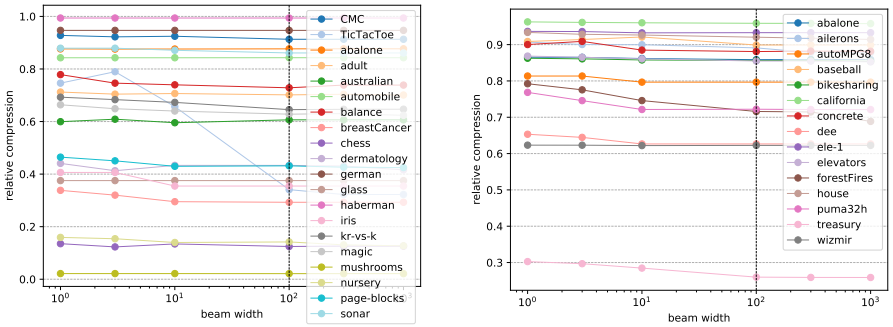
(a) Univariate nominal target. (b) Univariate numeric target.

Fig. 12: Compression ratio obtained by varying the maximum search depth fixing $w_b = 100$, $n_{cut} = 5$ and $\beta = 1$ (normalized gain). The black vertical line represents the value used in Experiments section of the paper.



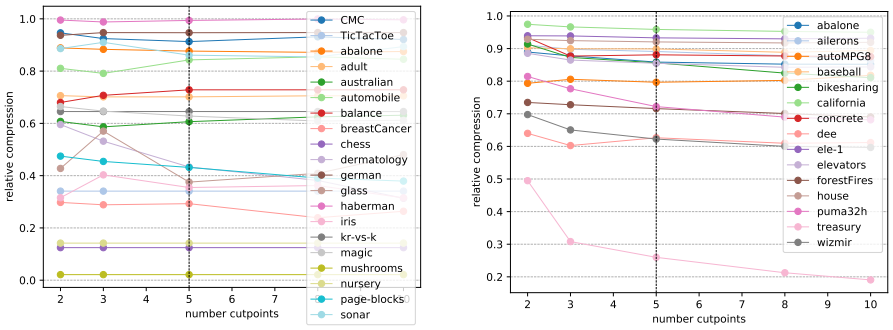
(a) Univariate nominal target. (b) Univariate numeric target.

Fig. 13: Average number of conditions per subgroup obtained by varying the maximum search depth fixing $w_b = 100$, $n_{cut} = 5$ and $\beta = 1$ (normalized gain). The black vertical line represents the value used in Experiments section of the paper.



(a) Univariate nominal target. (b) Univariate numeric target.

Fig. 14: Compression ratio obtained by varying the beam width and fixing $d_{max} = 5$, $n_{cut} = 5$ and $\beta = 1$ (normalized gain). The black vertical line represents the value used in Experiments section of the paper.



(a) Univariate nominal target. (b) Univariate numeric target.

Fig. 15: Compression ratio obtained by varying the number of cut points and fixing $w_b = 100$, $d_{max} = 5$ and $\beta = 1$ (normalized gain). The black vertical line represents the value used in Experiments section of the paper

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