MiSoSouP: Mining Interesting Subgroups with Sampling and Pseudodimension

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"Miso makes a soup loaded with flavour that saves you the hassle of making stock." – Y. Ottolenghi

ABSTRACT

We present MiSoSouP, a suite of algorithms for extracting high-quality approximations of the most interesting subgroups, according to different interestingness measures, from a random sample of a transactional dataset. We describe a new formulation of these measures that makes it possible to approximate them using sampling. We then discuss how pseudodimension, a key concept from statistical learning theory, relates to the sample size needed to obtain an high-quality approximation of the most interesting subgroups. We prove an upper bound on the pseudodimension of the problem at hand, which results in small sample sizes. Our evaluation on real datasets shows that MiSoSouP outperforms state-of-the-art algorithms offering the same guarantees, and it vastly speeds up the discovery of subgroups w.r.t. analyzing the whole dataset.

CCS CONCEPTS

• **Mathematics of computing → Probabilistic algorithms**; • **Information systems → Data mining**; • **Theory of computation → Sketching and sampling**; **Sample complexity and generalization bounds**;

KEYWORDS

Pattern Mining, Statistical Learning Theory

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1 INTRODUCTION

A fundamental task within data mining is *subgroup discovery* [8, 10, 32], which requires to identify *interesting subsets* (the subgroups) of a dataset, for which the distribution of a specific feature (the *target*) within the subgroup largely differs from the distribution of that feature in the entire dataset. The notion of *interestingness* is captured by a formally-defined measure of *quality* that combines the frequency of the subgroup in the dataset and the difference between the mean of the target within the subgroup and the mean of the target in the entire dataset. Subgroup discovery is a broadly applicable task and is relevant in many domains: in market basket analysis, it uncovers groups of customers with a particular interest in buying a product; in social networks, it identifies members attracted to a given topic; in biomedicine, it discovers groups of patients associated with a clinical phenotype (e.g., response to therapy).

Many exact algorithms for subgroup discovery have been proposed [10, 32] (see also the comprehensive reviews by Herrera et al. [5] and Atzmueller [2]). They naturally require to process the entire dataset, but the sheer amount of data may render such (full) computation infeasible. A general approach to deal with very large datasets is to only analyze a *small random sample* of the data. Random sampling has been successful in many areas of knowledge discovery, such as frequent itemsets mining [21, 22] and graph analysis [23]. The main challenge in using sampling for subgroup discovery is understanding how close the qualities of the subgroups observed in the sample are to their exact values, which are unknown as they can only be obtained by processing the entire dataset. Solving this challenge requires the derivation of a sample size S such that, with high probability, on a sample of size S, all the sample qualities are within ε from the exact ones, where ε is an user-specified parameter (to be fixed with domain knowledge) controlling the maximum allowed error.

The derivation of such sample size for subgroup discovery is more complex than in other scenarios (e.g., than in frequent itemsets mining [21, 22]), since estimating the quality of a subgroup requires to approximate both the frequency of the subgroup in the dataset and the mean of the target *within the subgroup*. The latter is an especially challenging inferential task since the target mean is a *conditional* expectation. This increased complexity is reflected in the lack of rigorous sampling algorithms for subgroup discovery, with even popular approaches [25] not providing rigorous quality guarantees on their output, as we discuss in the supplementary materials [24].

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1.1 Contributions

The main focus of this work is the extraction of a high-quality approximation of the top-k most interesting subgroups from a random sample of the dataset. Our contributions are the following.

- We precisely define the concept of *ε-approximation* of the set of top-k subgroups according to various interestingness measures, extending and strengthening an existing definition by Scheffer and Wrobel [25, Def. 2]. The user-defined parameter ε controls the quality of the approximation.
- We give a *new formulation of the 1-quality*, one of the key measures of subgroup interestingness, and as a consequence also of other fundamental measures. This novel formulation is crucial to enable the estimation of the interestingness of subgroups from a sample.
- We present MiSoSouP, a suite of algorithms that use *random sampling* to extract, with probability at least $1 - \delta$, ε-approximations of the set of top-k interesting subgroups from a small random sample of the dataset. MiSoSouP is the first algorithm to obtain such approximations, while previous work [25] does not actually provide rigorous guarantees (see the supplementary materials [24]). The only parameters of MiSoSouP are ε, k, and the confidence parameter δ, which are all easily interpretable, therefore making our algorithms very practical.
- We derive the sample size employed by MiSoSouP using *pseudodimension* [19], a key concepts from statistical learning theory [30]. We show an upper bound to the pseudodimension of the task of subgroup discovery, which is independent from the size of the dataset and only depends on properties of the set of possible subgroups (i.e., the language) and on the number of columns of the dataset. The computation of the upper bound is essentially cost-free. To the best of our knowledge, ours is the first application of pseudodimension to the field of subgroup discovery, and in general to pattern mining.
- We perform an extensive experimental evaluation showing that MiSoSouP identifies rigorous approximations to the most interesting subgroups using a small fraction of the dataset, and it provides a significant speed-up w.r.t. other sampling approaches with the same guarantees.

2 RELATED WORK

Many measures for evaluating the quality (i.e., interestingness) of subgroups have been proposed in the literature, and many subgroup discovery algorithms are available. We discuss some of the measures in Sect. 3, and refer the reader to the surveys by Herrera et al. [5] and Atzmueller [2] for details about the algorithms. In this work we treat these algorithms as black-boxes: we run them on a small random sample of the dataset and we are interested in how well the so-obtained collection of interesting subgroups approximates the one we would obtain by mining the whole dataset.

Scheffer and Wrobel [25] first studied the use of sampling for subgroups: they present GSS, a progressive sampling algorithm to compute an approximation of the most interesting subgroups. Unfortunately, the analysis of GSS has some issues. The first concern is that the quantities of interest (e.g., the number of subgroups at iteration i) are random variables, while the analysis assumes that they are fixed values. Another major issue is that the analysis uses a Chernoff bound for the probability of deviation for the *unusualness* of a subgroup, but such bound cannot be employed since the unusualness is a *conditional* probability, hence it cannot be obtained as the average of a binary function over *all* transactions in the sample. Other issues and possible partial solutions are discussed more in depth in the supplementary materials [24]. Even when (partially) corrected, the analysis of GSS relies on the availability of probabilistic confidence intervals on the estimated quality of each subgroup under consideration, and then on a union bound over all possible subgroups, in order to obtain simultaneous guarantees on the confidence intervals of all subgroups. The union bound is, by design, loose in many practical situations, effectively assuming that the considered events are independent. As a results, the stopping condition used by GSS cannot be satisfied at small sample sizes. MiSoSouP instead relies on pseudodimension [19], which allows us to use very small sample sizes.

Some works focused on the issue of the statistical significance of subgroups. Duivesteijn et al. [3] designed a permutation-based approach to estimate the distribution of false discoveries, which is used to assess the ability of various quality measures to distinguish between statistically significant patterns and false discoveries. Van Leeuwen and Ukkonen [29] showed that several real datasets contain large numbers of high-quality subgroups, many more than are expected from randomly drawn subgroups. Terada et al. [27] introduced LAMP, a method to identify a minimum generality threshold to find subgroups while bounding the family-wise error rate (FWER), where the significance of a subgroup is given by its association with a binary target variable as assessed by Fisher exact test. Minato et al. [15] subsequently improved LAMP by employing a more efficient mining strategy. We do not investigate the issue of statistical significance of subgroups, but one of the quality measures we study (i.e., the 1/2-quality measure, see Sect. 3) is a proxy for the z-score, a well-defined measure of statistical significance.

Our approach is orthogonal to heuristic approaches that sample *subgroups* to speed-up the discovery of interesting subgroups [17]. In contrast, MiSoSouP samples *transactions* while providing rigorous guarantees on the relation between the qualities of the subgroups obtained from the sample and their exact qualities (i.e., obtained from the entire dataset). In fact, any exact or heuristic algorithm can be used to mine the sample from MiSoSouP while maintaining the aforementioned guarantees for the resulting subgroups. The use of sampling is also orthogonal to techniques that aim at reducing the redundancy in the output collection of subgroups [28]. Indeed these approaches could be applied to the collection of subgroups obtained by MiSoSouP.

Pseudodimension [19] is a key concept from statistical learning theory [30]. Like many other measures of sample complexity, such as Rademacher averages, it has long been considered only of theoretical interest, but recent applications [4, 7, 20, 22, 23] of these quantities have shown that they can be extremely useful in practice, especially on very large datasets. Pseudodimension is closely related to the concept of Vapnik-Chervonenkis dimension that has been used in the context of frequent itemsets mining by Riondato and Upfal [21]. Despite the relative similarity between subgroup discovery and frequent itemset mining, using pseudodimension

for the former presents significant challenges, such as lack of anti-monotonicity in the quality measures, that do not allow to use the same approach by Riondato and Upfal [21]. To the best of our knowledge, ours is the first application of concepts from statistical learning theory to the task of subgroup discovery.

3 PRELIMINARIES

In this section we formally introduce the core definitions and theorems that we use throughout the article.

3.1 Subgroup discovery

We now define the fundamental concepts of subgroup mining [9] and the quality measures used to rank the subgroups.

Let $\mathcal{D}$ be a *dataset*, i.e., a bag of $(z+1)$-dimensional tuples, known as *transactions*, over the attributes $\{A_1, \ldots, A_z, T\}$. The attributes A_i, $1 \leq i \leq z$ are known as *description* attributes, while T is the *target* attribute. Transactions take value in $\mathcal{Y}_1 \times \cdots \times \mathcal{Y}_z \times \mathcal{Y}_T$, where each $\mathcal{Y}_i$ is the (categorical or numerical) domain of attribute A_i, while $\mathcal{Y}_T$ is Boolean (i.e., $\mathcal{Y}_T = \{0, 1\}$).

A *subgroup* is a *conjunction* of disjunctions of conditions on the description attributes. An example of subgroup is: $(A_1 =$ "blue" $\vee$ $A_1 =$ "red") $\wedge$ $(A_2 > 4)$. A transaction $t \in \mathcal{D}$ *supports* a subgroup A if the values of t's attributes satisfy A. The *cover* $C_{\mathcal{D}}(A)$ *of* A *on* $\mathcal{D}$ is the bag of transactions in $\mathcal{D}$ that support A. The *generality* $\mathrm{g}_{\mathcal{D}}(A)$ *of a subgroup* A *on* $\mathcal{D}$ is the ratio between the size of the cover of A on $\mathcal{D}$ and the size of $\mathcal{D}$:

$$\mathrm{g}_{\mathcal{D}}(A) = \frac{|C_{\mathcal{D}}(A)|}{|\mathcal{D}|} \ .^{1}$$

Given a bag $\mathcal{B}$ of transactions, let

$$\mu(\mathcal{B}) = \frac{1}{|\mathcal{B}|} \sum_{t \in \mathcal{B}} t.T$$

be the *target mean* of $\mathcal{B}$, where $t.T$ denotes the value in the target attribute of the tuple t. If $\mathcal{B} = \emptyset$, $\mu(\mathcal{B}) = 0$. The *target mean of a subgroup* A *on* $\mathcal{D}$ is

$$\mu_{\mathcal{D}}(A) = \mu(C_{\mathcal{D}}(A)) \ .$$

The *unusualness*[2] $\mathrm{u}_{\mathcal{D}}(A)$ *of* A *on* $\mathcal{D}$ is the difference between the target mean of A and the target mean of $\mathcal{D}$:

$$\mathrm{u}_{\mathcal{D}}(A) = \mu_{\mathcal{D}}(A) - \mu(\mathcal{D}) \ .$$

The generality and the unusualness are used to define quality measures for the subgroups (see Sect. 3.1.1).

A *description language* $\mathcal{L}$ is a set of subgroups that are of potential interest, and is *fixed in advance* by the user before analyzing the dataset. It could be a superset or a subset of the subgroups that actually appear in the dataset, and it expresses the constraint that only subgroups in the description language should be considered in the mining process. For example, given some integer m, one may consider the description language of all and only the subgroups composed of up to m conjunctions of equality conditions on the attributes.

[1] We use $|B|$ to denote the size of a bag B, i.e., the number of elements in B, counting repeated elements multiple times.

[2] Scheffer and Wrobel [25] use the term *statistical unusualness*. We choose to drop the adjective to avoid confusion with *statistical significance*.

3.1.1 Quality measures.

A *quality measure* for the subgroups in $\mathcal{L}$ on a dataset $\mathcal{D}$ is a function $\phi_{\mathcal{D}} : \mathcal{L} \to \mathbb{R}$ which assigns a numerical score to each subgroup $A \in \mathcal{L}$ based on its generality and unusualness. In this work we consider the most popular subgroup quality measures [10], which differ from each other for the relative weight given to generality and unusualness.

Definition 3.1 ([8, 18, 32]). Let $p \in \{1/2, 1, 2\}$. The *p-quality of a subgroup* A *on a dataset* $\mathcal{D}$ is

$$\mathrm{q}^{(p)}_{\mathcal{D}}(A) = (\mathrm{g}_{\mathcal{D}}(A))^p \, \mathrm{u}_{\mathcal{D}}(A) \ .$$

The 1-quality is also known as *Weighted Relative Accuracy* (WRAcc).[3] The 1/2-quality is proportional to the z-score[4] for the statistic $|C_{\mathcal{D}}(A)|\mathrm{u}_{\mathcal{D}}(A)$, which can be used to test whether a subgroup shows statistical association with the target variable. Thus, the 1/2-quality can be used as a proxy for the statistical significance of the subgroup A [8, 25, 29]. The domain $\mathcal{Y}_T$ of the target attribute is Boolean, thus $\mathrm{q}^{(p)}_{\mathcal{D}}(A) \in [-1, 1]$ for any subgroup A. There exist variants of the p-qualities that consider the *absolute value* of the unusualness [25]. MiSoSouP can be easily adapted to work with such measures.

3.1.2 Subgroup discovery task.

Fix $p \in \{1/2, 1, 2\}$. Let $\mathcal{L}_{\mathcal{D}}$ be the subset of $\mathcal{L}$ containing only the subgroups of $\mathcal{L}$ that actually appear in $\mathcal{D}$ (i.e., those with generality strictly greater than zero). We do not assume to know $\mathcal{L}_{\mathcal{D}}$: it is only needed for the following definition. Assume to sort the subgroup in $\mathcal{L}_{\mathcal{D}}$ in decreasing order according to their p-quality in $\mathcal{D}$, ties broken arbitrarily. Let $k > 0$ be an integer and let $\mathrm{r}^{(p)}_{\mathcal{D}}(k)$ be the p-quality of the k-th subgroup in the sorted order.

Definition 3.2. The *subgroup discovery* task consists in extracting the set $\mathrm{TOP}_p(k, \mathcal{D})$ of the *top-k subgroups in* $\mathcal{L}_{\mathcal{D}}$ *w.r.t. the p-quality in* $\mathcal{D}$, i.e., the set of subgroups with p-quality at least $\mathrm{r}^{(p)}_{\mathcal{D}}(k)$:

$$\mathrm{TOP}_p(k, \mathcal{D}) = \left\{ A \in \mathcal{L}_{\mathcal{D}} \ : \ \mathrm{q}^{(p)}_{\mathcal{D}}(A) \geq \mathrm{r}^{(p)}_{\mathcal{D}}(k) \right\} \ .$$

$\mathrm{TOP}_p(k, \mathcal{D})$ may contain more than k elements when many subgroups have p-quality equal to $\mathrm{r}^{(p)}_{\mathcal{D}}(k)$.[5]

A variant of the task allows the user to specify a constraint on the minimum generality of returned subgroups. MiSoSouP can handle this case with minor modifications.

3.1.3 Approximations.

We want to obtain an *ε-approximation to the set* $\mathrm{TOP}_p(k, \mathcal{D})$ from a small *random sample* of the dataset, where $\varepsilon \in (0, 1)$ is an user-defined parameter that controls the maximum acceptable error. Formally this concept is defined as follows.

Definition 3.3. Let $\varepsilon \in (0, 1)$. An ε-approximation to $\mathrm{TOP}_p(k, \mathcal{D})$ is a set $\mathcal{B}$ of pairs (A, q_A) where A is a subgroup and q_A is a value in $[-1, 1]$, and $\mathcal{B}$ is such that:

[3] Van Leeuwen and Ukkonen [29] denote the 1/2-quality as "WRAcc", but all other references we found (e.g., [5, 12]) use this name to denote the 1-quality.

[4] The z-score for a test statistic X is $(X - \mathbb{E}[X])/\sigma_X$, where $\mathbb{E}[X]$ is the expectation and σ_X is the standard deviation of X (under the null hypothesis). For subgroups, under the null hypothesis of no association of a subgroup with the target variable, the z-score is $(|C_{\mathcal{D}}(A)|\mu_{\mathcal{D}}(A) - |C_{\mathcal{D}}(A)|\mu(\mathcal{D}))/\sqrt{C_{\mathcal{D}}(A)\mu(\mathcal{D})(1-\mu(\mathcal{D}))}$.

[5] This definition of the task is therefore slightly different from the one given in [25, Definition 1], where the size of $\mathrm{TOP}_p(k, \mathcal{D})$ is limited to exactly k elements.

(1) for any $A \in \mathsf{TOP}_p(k, \mathcal{D})$, there is a pair $(A, q_A) \in \mathcal{B}$; and
(2) there is no pair $(A, q_A) \in \mathcal{B}$ such that $\mathsf{q}^{(p)}_{\mathcal{D}}(A) < \mathsf{r}^{(p)}_{\mathcal{D}}(k) - \varepsilon$; and
(3) for each pair $(A, q_A) \in \mathcal{B}$, $|\mathsf{q}^{(p)}_{\mathcal{D}}(A) - q_A| \leq \varepsilon/4$.

MiSoSouP computes (with high probability) an ε-approximation from a random sample of the dataset.

An ε-approximation can act as a set of candidates for $\mathsf{TOP}_p(k, \mathcal{D})$, as it contains a pair (A, q_A) for each subgroup A in this set. Scheffer and Wrobel [25, Definition 2] present a slightly different definition of approximation. Such an approximation is *not* a set of candidates for $\mathsf{TOP}_p(k, \mathcal{D})$, and in particular its intersection with this set may be empty. On the other hand, if we sort the pairs in an ε-approximation by decreasing order of their second component, ties broken arbitrarily, the set of the subgroups in the first k pairs according to this order is an approximation in the sense defined by Scheffer and Wrobel [25]. The choice of ε, similar to the choice of k in Def. 3.2 must be informed, at least in part, by domain knowledge. The quantity $1 - \mu(\mathcal{D})$ can act, in some sense, as an upper bound to the possible choice of ε, as no subgroup can have 1-quality greater than this quantity. Approximations guaranteeing a multiplicative bound on the error are also possible and we will discuss them in an extended version of this work.

3.2 Pseudodimension

We now introduce the main concepts and results on *VC-dimension* [31] and *pseudodimension* [19], specializing some of them to our settings. [6]

3.2.1 VC-dimension. Let $\mathcal{W}$ be a finite domain and let $\mathcal{R} \subseteq 2^{\mathcal{W}}$ be a collection of subsets of $\mathcal{W}$, where $2^{\mathcal{W}}$ is the set of all subsets of $\mathcal{W}$. We call $\mathcal{R}$ a *rangeset on* $\mathcal{W}$, and call its members *ranges*. The set $A \subseteq \mathcal{W}$ is *shattered* by $\mathcal{R}$ if $\{R \cap A \ : \ R \in \mathcal{R}\} = 2^A$. The *VC-dimension* $\mathsf{VC}(\mathcal{W}, \mathcal{R})$ of $(\mathcal{W}, \mathcal{R})$ is the size of the largest subset of $\mathcal{W}$ that can be shattered by $\mathcal{R}$.

3.2.2 Pseudodimension. Pseudodimension [19] is an extension of VC-dimension [31] to *real-valued* functions, defined as follows.

Let $\mathcal{F}$ be a family of functions from a finite domain $\mathcal{H}$ onto $[a, b] \subset \mathbb{R}$. In this work $\mathcal{H}$ will be the dataset $\mathcal{D}$, and $\mathcal{F}$ will contain one function f_A for each subgroup $A \in \mathcal{L}$ (see Sect. 4.1.1). Consider, for each $f \in \mathcal{F}$, the subset R_f of $\mathcal{H} \times [a, b]$ defined as

$$R_f = \{(x, t) \ : \ t \leq f(x)\} \ .$$

Let

$$\mathcal{F}^+ = \{R_f, f \in \mathcal{F}\},$$

be a rangeset on $\mathcal{H} \times [a, b]$. The *pseudodimension* $\mathsf{PD}(\mathcal{F})$ *of* $\mathcal{F}$ is the VC-dimension of $(\mathcal{H} \times [a, b], \mathcal{F}^+)$ [1, Sect. 11.2]:

$$\mathsf{PD}(\mathcal{F}) = \mathsf{VC}(\mathcal{H} \times [a, b], \mathcal{F}^+) \ .$$

3.2.3 Uniform convergence. Let $\mathcal{S} = \{x_1, \ldots, x_\ell\}$ be a *bag* of elements of $\mathcal{H}$, sampled independently and uniformly at random, with replacement. For each $f \in \mathcal{F}$, define

$$\mathsf{m}_{\mathcal{H}}(f) = \frac{1}{|\mathcal{H}|} \sum_{x \in \mathcal{H}} f(x) \quad \text{and} \quad \mathsf{m}_{\mathcal{S}}(f) = \frac{1}{\ell} \sum_{i=1}^{\ell} f(x_i) \ .$$

[6] For an in-depth discussion of these topics see, e.g., the books by Shalev-Shwartz and Ben-David [26] and by Anthony and Bartlett [1].

We call $\mathsf{m}_{\mathcal{S}}(f)$ the *empirical average of* f *on* $\mathcal{S}$. It holds $\mathbb{E}[\mathsf{m}_{\mathcal{S}}(f)] = \mathsf{m}_{\mathcal{H}}(f)$. The following result connects an upper bound to the pseudodimension of $\mathcal{F}$ to the number of samples needed to simultaneously approximate all the expectations of all the functions in $\mathcal{F}$ using their sample averages.

Theorem 3.4 ([13]). *Let* $\mathsf{PD}(\mathcal{F}) \leq d$. *Fix* $\xi, \eta \in (0, 1)$. *When* $\mathcal{S}$ *is a collection of*

$$|\mathcal{S}| = \frac{(b-a)^2}{\xi^2} \left(d + \log \frac{1}{\eta} \right) \tag{1}$$

elements sampled independently and uniformly at random with replacement from $\mathcal{H}$, *then, with probability at least* $1 - \eta$ *over the choice of* $\mathcal{S}$, *it holds*

$$|\mathsf{m}_{\mathcal{H}}(f) - \mathsf{m}_{\mathcal{S}}(f)| < \xi, \ \textit{for every } f \in \mathcal{F} \ .$$

The following two lemmas by Riondato and Upfal [23, Lemmas 3.7 and 3.8] are useful when proving upper bounds to the pseudodimension of a family of functions.

Lemma 3.5. *If* $B \subseteq \mathcal{H} \times [a, b]$ *is shattered by* $\mathcal{F}^+$, *it may contain* at most one *element* $(d, x) \in \mathcal{H} \times [a, b]$ *for each* $d \in \mathcal{H}$.

Lemma 3.6. *If* $B \subseteq \mathcal{H} \times [a, b]$ *is shattered by* $\mathcal{F}^+$, *it cannot contain* any *element in the form* (d, a), *for any* $d \in \mathcal{H}$.

4 ALGORITHMS

In this section we present MiSoSouP, our suite of algorithms to compute ε-approximations of $\mathsf{TOP}_p(k, \mathcal{D})$. We present only the case for $p = 1$, and discuss the variants for the other p-qualities in the supplementary materials [24].

4.1 MiSoSouP for 1-quality

We start by introducing a family $\mathcal{P}$ of functions which we use to give a novel expression for the 1-quality of a subgroup. We then present a sufficient condition for extracting an ε-approximation from a sample, and derive bounds to the sample size sufficient to ensure that the condition holds with high probability. Finally ,we describe the algorithm.

4.1.1 A novel formulation of the 1-quality. The family $\mathcal{P}$ contains one function ρ_A from $\mathcal{D}$ to $\{-\mu(\mathcal{D}), 0, 1 - \mu(\mathcal{D})\}$ for each subgroup $A \in \mathcal{L}$, defined, for $t \in \mathcal{D}$, as:

$$\rho_A(t) = \begin{cases} 1 - \mu(\mathcal{D}) & \text{if } t \in C_{\mathcal{D}}(A) \text{ and } t.T = 1 \\ -\mu(\mathcal{D}) & \text{if } t \in C_{\mathcal{D}}(A) \text{ and } t.T = 0 \\ 0 & \text{otherwise} \end{cases} \ .$$

We assume to know the exact value of $\mu(\mathcal{D})$, which is a standard and reasonable assumption (made also by Scheffer and Wrobel [25]), since $\mu(\mathcal{D})$ can be computed with a very quick scan of the target attribute on $\mathcal{D}$, or kept up-to-date while collecting the data.

The 1-quality of a subgroup A can be expressed as the average over the transactions in the dataset of the function ρ_A:

$$\begin{aligned} \mathsf{m}_{\mathcal{D}}(\rho_A) &= \frac{1}{|\mathcal{D}|} \sum_{t \in \mathcal{D}} \rho_A(t) \\ &= \frac{1}{|\mathcal{D}|} \left((1 - \mu(\mathcal{D})) \mu_{\mathcal{D}}(A) |C_{\mathcal{D}}(A)| - \mu(\mathcal{D}) |C_{\mathcal{D}}(A)| (1 - \mu_{\mathcal{D}}(A)) \right) \\ &= \frac{|C_{\mathcal{D}}(A)|}{|\mathcal{D}|} \left(\mu_{\mathcal{D}}(A) - \mu(\mathcal{D}) \right) = \mathsf{g}_{\mathcal{D}}(A) \mathsf{u}_{\mathcal{D}}(A) = \mathsf{q}^{(1)}_{\mathcal{D}}(A) \ . \end{aligned} \tag{2}$$

This equivalence is a novel insight of *crucial importance* to enable the efficient estimation of the 1-quality from a sample of the dataset.

Let now $\mathcal{S} = \{t_1, \ldots, t_\ell\}$ be a collection of transactions sampled uniformly and independently at random with replacement from $\mathcal{D}$. It holds, following the same steps as in (2), that

$$\mathrm{m}_{\mathcal{S}}(\rho_A) = \frac{1}{\ell}\sum_{i=1}^{\ell}\rho_A(t_i) = \mathrm{g}_{\mathcal{S}}(A)\,(\mu_{\mathcal{S}}(A) - \mu(\mathcal{D})) \quad .$$

Note that this quantity is different from $\mathrm{q}^{(1)}_{\mathcal{S}}(A)$, as it uses $\mu(\mathcal{D})$ rather than $\mu(\mathcal{S})$. As mentioned earlier, it is reasonable to assume knowledge of $\mu(\mathcal{D})$. We define the *approximate 1-quality of A on $\mathcal{S}$* as

$$\tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A) = \mathrm{m}_{\mathcal{S}}(\rho_A) \quad .$$

4.1.2 Sufficient condition for an ε-approximation. We now show a condition on the sample $\mathcal{S}$ that is sufficient to allow the computation of an ε-approximation of $\mathsf{TOP}_1(k, \mathcal{D})$ from $\mathcal{S}$. Assume to sort the subgroups in $\mathcal{L}$ in decreasing order by their approximate 1-quality on $\mathcal{S}$, ties broken arbitrarily. Let $\tilde{\mathrm{r}}^{(1)}_{\mathcal{S}}(k)$ be the *approximate* 1-quality on $\mathcal{S}$ of the k-th subgroup in this order.

Theorem 4.1. *If $\mathcal{S}$ is such that*

$$|\tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A) - \mathrm{q}^{(1)}_{\mathcal{D}}(A)| \le \frac{\varepsilon}{4} \text{ for every } A \in \mathcal{L}, \tag{3}$$

then the set

$$\mathcal{B} = \left\{\left(A, \tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A)\right) \;:\; \tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A) \ge \tilde{\mathrm{r}}^{(1)}_{\mathcal{S}}(k) - \frac{\varepsilon}{2}\right\} \tag{4}$$

is an ε-approximation to $\mathsf{TOP}_1(k, \mathcal{D})$.

Proof. Equation (3) holds in particular for subgroups appearing in the pairs in $\mathcal{B}$. Thus, $\mathcal{B}$ satisfies Property 3 from Definition 3.3.

It holds

$$\tilde{\mathrm{r}}^{(1)}_{\mathcal{S}}(k) \ge \mathrm{r}^{(1)}_{\mathcal{D}}(k) - \frac{\varepsilon}{4} \tag{5}$$

because all the subgroups in $\mathsf{TOP}_1(k, \mathcal{D})$, which are at least k, have, from (3), approximate 1-quality in $\mathcal{S}$ at least $\mathrm{r}^{(1)}_{\mathcal{D}}(k) - \varepsilon/4$.

Another consequence of (3) is that

$$\tilde{\mathrm{r}}^{(1)}_{\mathcal{S}}(k) \le \mathrm{r}^{(1)}_{\mathcal{D}}(k) + \frac{\varepsilon}{4} \tag{6}$$

because only subgroups with exact 1-quality in $\mathcal{D}$ strictly greater than $\mathrm{r}^{(1)}_{\mathcal{D}}(k)$ can have an approximate 1-quality in $\mathcal{S}$ strictly greater than $\mathrm{r}^{(1)}_{\mathcal{D}}(k) + \varepsilon/4$, and there are only at most $k-1$ such subgroups.

It then holds from (6) and (3) that

$$\tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(Z) \ge \tilde{\mathrm{r}}^{(1)}_{\mathcal{S}}(k) - \frac{\varepsilon}{2} \text{ for all } Z \in \mathsf{TOP}_1(k, \mathcal{D}) \quad .$$

Thus $\mathcal{B}$ satisfies Property 1 of Definition 3.3.

Let now A be any subgroup with $\mathrm{q}^{(1)}_{\mathcal{D}}(A) < \mathrm{r}^{(1)}_{\mathcal{D}}(k) - \varepsilon$. It follows from (3) that

$$\tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A) \le \mathrm{r}^{(1)}_{\mathcal{D}}(k) - 3\varepsilon/4,$$

and using (5) we get

$$\tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A) < \tilde{\mathrm{r}}^{(1)}_{\mathcal{S}}(k) - \varepsilon/2,$$

hence $\left(A, \tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A)\right) \notin \mathcal{B}$, as required by Property 2 of Definition 3.3. □

4.1.3 Loose bounds to the sufficient sample size. Intuition correctly suggests that if the sample $\mathcal{S}$ is large enough, then with high probability over the choice of $\mathcal{S}$, $\mathcal{S}$ satisfies the condition in (3), thus allowing the computation of an ε-approximation of $\mathsf{TOP}_1(k, \mathcal{D})$ from $\mathcal{S}$. To warm up, and as a baseline, we first present a loose bound on how large $\mathcal{S}$ should be for the above to happen.

Theorem 4.2. *Let $\delta \in (0,1)$, $\varepsilon \in (0,1)$, and $k \ge 1$. Let $\mathcal{S}$ be a collection of*

$$|\mathcal{S}| \ge \frac{16}{\varepsilon^2}\left(\ln|\mathcal{L}_{\mathcal{D}}| + \ln\frac{2}{\delta}\right) \tag{7}$$

transactions sampled uniformly at random with replacement from $\mathcal{D}$. With probability at least $1-\delta$ (over the choice of $\mathcal{S}$), the set

$$\mathcal{B} = \left\{\left(A, \tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A)\right) \;:\; \tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A) + \frac{\varepsilon}{2} \ge \tilde{\mathrm{r}}^{(1)}_{\mathcal{S}}(k)\right\}$$

is an ε-approximation to $\mathsf{TOP}_1(k, \mathcal{D})$.

The proof is in the supplementary material [24]. It uses Hoeffding's inequality [6] and the union bound [16, Lemma 1.2].

The quantity in (7) is a loose upper bound to the sample size sufficient to probabilistically obtain an ε-approximation, due to the use of the union bound. It is also somewhat intuitive that the sample size should not depend on just the size of $\mathcal{L}_{\mathcal{D}}$, but on a quantity that better describes the relationship between the language and the dataset, as will be the case for the sample size used by MiSoSouP. Another drawback is that the sample size in (7) can only be computed when the *size* of $\mathcal{L}_{\mathcal{D}}$ is known, which is almost never the case. A loose upper bound to $|\mathcal{L}_{\mathcal{D}}|$ can be computed with a full scan of the dataset, which is potentially expensive (see details in Sect. 5). The sample size used by MiSoSouP, presented next, does not suffer from these downsides.

4.1.4 Bounds to the pseudodimension and to the sample size. In this section we present a novel upper bound to the number of samples needed to satisfy the condition in (3), and therefore compute an high-quality approximation of $\mathsf{TOP}_1(k, \mathcal{D})$. It relies on the following bound to the *pseudodimension* [19] (see Sect. 3.2) of the family $\mathcal{P}$ introduced in Sect. 4.1.1.

Theorem 4.3. *Let d be the maximum number of subgroups from $\mathcal{L}$ that may appear in a transaction of $\mathcal{D}$. Then, the pseudodimension $\mathsf{PD}(\mathcal{P})$ of $\mathcal{P}$ satisfies:*

$$\mathsf{PD}(\mathcal{P}) \le \lfloor \log_2 d \rfloor + 1 \quad .$$

We need some intermediate results before proving this theorem. Define, for every subgroup $A \in \mathcal{L}$, the range

$$R_A = \{(t, x) \;:\; t \in \mathcal{D} \text{ and } x \le r_A(t)\},$$

and let $\mathcal{R} = \{R_A, A \in \mathcal{L}\}$ be a rangeset on $\mathcal{D} \times [-\mu(\mathcal{D}), 1-\mu(\mathcal{D})]$.

Lemma 3.6 tells us that only subsets of $\mathcal{D} \times (-\mu(\mathcal{D}), 1-\mu(\mathcal{D})]$ may be shattered by $\mathcal{R}$. The following lemmas further restrict the collection of sets that may be shattered.

For any $x \in (-\mu(\mathcal{D}), 1-\mu(\mathcal{D})]$ let

$$\mathrm{c}(x) = \begin{cases} 1-\mu(\mathcal{D}) & \text{if } 0 < x \le 1-\mu(\mathcal{D}) \\ 0 & \text{if } -\mu(\mathcal{D}) < x \le 0 \end{cases} \quad .$$

Lemma 4.4. *A set $B \subseteq \mathcal{D} \times (-\mu(\mathcal{D}), 1-\mu(\mathcal{D})]$ is shattered by $\mathcal{R}$ if and only if the set*

$$B' = \{(t, \mathrm{c}(x)) \;:\; (t, x) \in B\}$$

is also shattered by $\mathcal{R}$. Note that $|B| = |B'|$.

Proof. It follows from the definition of R_A, $A \in \mathcal{L}$, that (t, x) belongs to all and only the R_A's that $(t, \mathrm{c}(x))$ belongs to. Hence if B is shattered then the same ranges that shatter it also shatter B', and vice versa.

The equality $|B| = |B'|$ follows from 1) the fact that clearly it is impossible that $|B'| > |B|$; and 2) Lemma 3.5 as it ensures that if B is shattered then it cannot contain more than a single element (t, y) for a fixed $t \in \mathcal{D}$ and some $y \in (-\mu(\mathcal{D}), 1 - \mu(\mathcal{D})]$, hence it is impossible that two or more elements of B are mapped by $\mathrm{c}(\cdot)$ to the same element of B'. □

Lemma 4.5. *Let $t \in \mathcal{D}$ be any transaction such that $t.T = 0$. No $B \subseteq \mathcal{D} \times \{0, 1 - \mu(\mathcal{D})\}$ such that $(t, 1 - \mu(\mathcal{D})) \in B$ can be shattered by $\mathcal{R}$.*

Proof. There is no subgroup $A \in \mathcal{L}$ such that $(t, 1-\mu(\mathcal{D})) \in R_A$, thus, for any B containing $(t, 1 - \mu(\mathcal{D}))$, it is impossible to find an $A \in \mathcal{L}$ such that $R_A \cap B = \{(t, 1 - \mu(\mathcal{D}))\}$, hence B cannot be shattered. □

Lemma 4.6. *Let $t \in \mathcal{D}$ be any transaction such that $t.T = 1$. No $B \subseteq \mathcal{D} \times \{0, 1 - \mu(\mathcal{D})\}$ such that $(t, 0) \in B$ can be shattered by $\mathcal{R}$.*

Proof. The element $(t, 0)$ belongs to R_A for any $A \in \mathcal{L}$, so for any B containing $(t, 0)$, it is impossible to find an $A \in \mathcal{L}$ such that $R_A \cap B = \emptyset$, hence B cannot be shattered. □

It follows from Lemmas 3.6, 4.4, 4.5, and 4.6 that, to prove Theorem 4.3, we can focus our attention only on trying to shatter subsets of $\mathcal{D} \times [-\mu(\mathcal{D}), 1 - \mu(Ds)]$ containing elements that are either in the form $(t, 1 - \mu(\mathcal{D}))$ with $t.T = 1$, or in the form $(t, 0)$ with $t.T = 0$. The two following lemmas show upper bounds to the sizes of such subsets that can be shattered by $\mathcal{R}$. Theorem 4.3 is then an immediate consequence.

Lemma 4.7. *Let $B \subseteq \mathcal{D} \times \{0, 1 - \mu(\mathcal{D})\}$ be a set that is shattered by $\mathcal{R}$ and such that B contains an element $(t, 1 - \mu(\mathcal{D}))$, for some $t \in \mathcal{D}$. Then it must be*

$$|B| \leq \lfloor \log_2 d \rfloor + 1,$$

for d as in Theorem 4.3.

Proof. The proof is in part inspired by the one for [21, Theorem 4.5]. Consider one of the elements in the form $(t, 1 - \mu(\mathcal{D}))$ belonging to B. By hypothesis there is at least one such element. Let us denote it as $a = (t, 1 - \mu(\mathcal{D}))$.

Denote the $2^{|B|-1}$ non-empty subsets of B containing a as C_i, $1 \leq i \leq 2^{|B|-1}$, labelling them in an arbitrary order. Since B is shattered, for each of the C_i's there must be an A_i such that $R_{A_i} \cap B = C_i$. Since $C_i \neq C_j$ for each $i \neq j$, $1 \leq i, j \leq 2^{|B|-1}$, it must hold $R_{A_i} \neq R_{A_j}$. The element a belongs to each R_{A_i}, $1 \leq i \leq 2^{|B|-1}$. From Lemma 4.5 it follows that, since B is shattered, then it must be $t.T = 1$. Thus the element a belongs to all and only the ranges R_Z for $Z \in \mathcal{L}$ such that $t \in C_{\mathcal{D}}(Z)$. There are at most d such Z's, hence it must be $2^{|B|-1} \leq d$. □

Lemma 4.8. *Let $B \subseteq \mathcal{D} \times \{0, 1 - \mu(\mathcal{D})\}$ be a set that is shattered by $\mathcal{R}$ and such that B contains an element $(t, 0)$, for some $t \in \mathcal{D}$. Then it must be*

$$|B| \leq \lfloor \log_2 d \rfloor + 1,$$

for d as in Theorem 4.3.

Proof. Consider one of the elements in the form $(t, 0)$ that belong to B. By hypothesis there is at least one such element. Let us denote it as $a = (t, 0)$. The proof is similar to the one for Lemma 4.7, but with one profound difference, i.e., we essentially consider the subsets of B that *do not* contain a.

Denote the $2^{|B|-1}$ subsets of B *not* containing a as C_i, $1 \leq i \leq 2^{|B|-1}$, labelling them in an arbitrary order. Note that there must be an i such that $C_i = \emptyset$. Since B is shattered, for each of the C_i's there must be a subgroup A_i such that $R_{A_i} \cap B = C_i$. Since $C_i \neq C_j$ for each $i \neq j$, $1 \leq i, j \leq 2^{|B|-1}$, it must hold $R_{A_i} \neq R_{A_j}$. The element a does not belong to any R_{A_i}, $1 \leq i \leq 2^{|B|-1}$. From Lemma 4.4 it follows that, since B is shattered, then it must be $t.T = 0$. Thus the element a does not belong only to the ranges R_Z for $Z \in \mathcal{L}$ such that $t \in C_{\mathcal{D}}(Z)$. There are at most d such Z's, hence it must be $2^{|B|-1} \leq d$. □

It is common to choose $\mathcal{L}$ to be the set of subgroups involving up to c conjunctions of simple *equality* conditions on the attributes, for some $c \geq 1$. The following corollary is a reformulation of Theorem 4.3 using the maximum number of subgroups from $\mathcal{L}$ that may appear in a transaction of $\mathcal{D}$ for such cases.

Corollary 4.9. *Let C be the number of description attributes in $\mathcal{D}$ (i.e.,* not *counting the target attribute). Let $\mathcal{L}$ be the set of subgroups of conjuctions of equality conditions on up to c attributes, for some $1 \leq c \leq C$. Then*

$$\mathrm{PD}(\mathcal{P}) \leq \left\lfloor \log_2 \sum_{i=1}^{c} \binom{C}{i} \right\rfloor + 1 \ . \tag{8}$$

We conjecture that these bounds to the pseudodimension are strict, in the sense that there are datasets attaining the bounds. We will investigate this conjecture in the extended version of this work.

By combining Theorem 4.3 with Theorem 3.4 we obtain the following result.

Theorem 4.10. *Let $\delta \in (0, 1)$, $\varepsilon \in (0, 1)$, and $k \geq 1$. Let d as in Theorem 4.3. Let*

$$S = \frac{16}{\varepsilon^2} \left(\lfloor \log_2 d \rfloor + 1 + \ln \frac{1}{\delta} \right). \tag{9}$$

The probability that a collection $\mathcal{S}$ of S transactions sampled independently and uniformly at random with replacement from $\mathcal{D}$ satisfies (3) is at least $1 - \delta$.

The improvement of (9) over (7) is evident: $\lfloor \log_2 d \rfloor + 1$ is usually much much smaller, potentially orders of magnitude so, than $\ln |\mathcal{L}_{\mathcal{D}}|$.

4.1.5 The algorithm. We now have all the ingredients to describe and analyze MiSoSouP-1, our algorithm for extracting, with probability at least $1 - \delta$ (over the runs of the algorithm), an ε-approximation to $\mathrm{TOP}_1(k, \mathcal{D})$. The input of the algorithm is the tuple $(\mathcal{D}, k, \varepsilon, \delta)$.

MiSoSouP-1 starts by creating the sample $\mathcal{S}$ by drawing S transactions independently and uniformly at random with replacement from $\mathcal{D}$, for S as in (9). An exact algorithm for subgroup discovery is used to extract from $\mathcal{S}$ the set $\mathcal{B}$ defined in (4). Any exact algorithm can be used for the discovery step, but it needs to be slightly modified to use $\tilde{\mathrm{q}}^{(1)}_{\mathcal{S}}(A)$ as measure for the interestingness of a subgroup A, instead of $\mathrm{q}^{(1)}_{\mathcal{S}}(A)$. This modification is straightforward. The set $\mathcal{B}$ is then returned in output. By combining Theorem 4.1 with Theorem 4.10 we obtain the following result on the quality guarantees of MiSoSouP-1.

Theorem 4.11. *With probability at least $1-\delta$ (over its runs),* MiSoSouP-1 *outputs an ε-approximation to $\mathrm{TOP}_1(k, \mathcal{D})$.*

5 EXPERIMENTAL EVALUATION

We now discuss our experimental evaluation to assess the performances of MiSoSouP. We report here a subset of the results for $p = 1$. Additional and qualitatively similar results for the other measures are available in the supplementary materials [24].

5.1 Goals

Our experiments have two goals: *1)* evaluate the speed-up of MiSoSouP w.r.t. sampling-based approximation algorithms offering the same quality guarantees; and *2)* evaluate the quality of the approximations returned by MiSoSouP, in terms of the accuracy of the estimates of the quality of the returned subgroups, and of the number of returned subgroups.

5.2 Baselines

We compare the performances of MiSoSouP against a baseline algorithm UB.[7] Like MiSoSouP, UB computes, with probability at least $1-\delta$, an ε-approximation to $\mathrm{TOP}_p(k, \mathcal{D})$ by analyzing a sample of the dataset. The *only difference* between MiSoSouP and UB is that UB uses, as sample size, the r.h.s. of (7) (or similar equations for $p \neq 1$). We use UB-1 to denote the variant of UB for 1-quality. As is evident from (7), UB requires, to compute its sample size, the number of subgroups in $\mathcal{L}$ that actually appear in $\mathcal{D}$ or an upper bound to such number. An *upper bound* can be computed by considering the size of the (effective) domains of the columns in the dataset, and taking the sum, over all r-subsets C of columns, for r from 1 to some *maxlen*, of the products of the sizes of the column domains in C. Computing the sizes of the column domains requires a linear scan of the dataset. Despite the fact that this step can be relatively expensive and its cost grows with the size of the dataset, we do not include the time for such computation in the runtime of UB we report, therefore favoring UB in our comparisons. Note that MiSoSouP relies on (8) to compute the upper bound d to the pseudodimension used in (9) to obtain its sample size, and the cost of evaluating the r.h.s. of (8) is essentially nil, as all values are known by MiSoSouP, since $\mathcal{L}$ and thus c are fixed in advance, and the number of columns of $\mathcal{D}$ is an immediately available quantity.

We do not compare MiSoSouP with algorithms that mine the whole dataset and output the exact collection $\mathrm{TOP}_p(k, \mathcal{D})$ because MiSoSouP (and also UB) have sample sizes that are independent on the size of the dataset, while an exact algorithm would take time proportional to this quantity. As a result, on modern-sized datasets, an exact algorithm is always much slower than a sampling-based algorithm. We also do not to compare against GSS [25] because the algorithm does not actually offer the claimed guarantees (see the supplementary materials [24]). Additionally, an implementation is not available.

[7] UB was not presented before in the literature. We introduce it only for comparison with MiSoSouP, which, as we will see, offers several practical advantages.

Dataset	Size	Attributes	Max. Length
Car	6912×10^4	6	4
Mushroom	32496×10^4	22	4
Tic-Tac-Toe	3832×10^4	9	5

Table 1: Characteristics of the datasets

5.3 Datasets and languages

We use datasets from the UCI repository [14]. Since these datasets are quite small for today's standards, we replicate them 20,000 times (i.e., each transaction is copied 20,000 times) and then shuffle the order of the transactions in the replicated copy. This way, we obtain significantly larger datasets while *preserving the distribution* of the p-qualities of the subgroups appearing in the original datasets. This approach does not change the search space of any algorithm and does not give any advantage to MiSoSouP over UB. Table 1 shows the descriptive statistics of the datasets we used. We consider the description language $\mathcal{L}$ of subgroups of up to "Max. Length" conjunctions of *equality* conditions.

5.4 Implementation and environment

We implemented MiSoSouP and UB in C++17. The implementation uses a simple exhaustive search algorithm for extracting the subgroups from the sample (any algorithm can be used for this step, we just found it more practical to write our own implementation than to modify an existing implementation of a more efficient algorithm). We run our experiments on a cluster of GNU/Linux machines, except for the timing experiments, which were performed on a machine with an AMD Phenom™ II X4 955 processor and 16GB of RAM, running FreeBSD 12. The code is included in the supplementary materials [24].

5.5 Parameters

We report results for $k \in \{10, 50, 100, 200, 500, 1000, 2000\}$, $\varepsilon \in \{0.05, 0.02, 0.01, 0.0075\}$, and for $\delta = 0.1$. We tested different values for δ, but given that both MiSoSouP and UB have (the same) logarithmic dependence on δ, varying δ has limited quantitative effect and no qualitative effect. We run MiSoSouP and UB five times for each combination of parameters: the results were extremely stable and we report them for a randomly chosen run among the five.

5.6 Results

We first show the results on runtime and sample sizes (Sect. 5.6.1), then discuss the accuracy of the estimates of the 1-qualities obtained by MiSoSouP-1 (Sect. 5.6.2), and finally analyze the number of false positives it reports (Sect. 5.6.3).

Dataset	ε	$\lvert\mathcal{S}\rvert$	Reduction w.r.t. UB-1	Runtime (s)	Reduction w.r.t. UB-1	Absolute error ($\times 10^4$) (for $k = 1000$) Min.	1st Q.	Median	3rd Q.	Max.	$\varepsilon/4$
Car	0.05	53137	-25.07%	1.50	-1.5%	< 0.01	0.32	0.76	1.88	25.50	125
	0.02	332104		2.13	-10.55%	< 0.01	0.14	0.32	0.73	8.20	50
	0.01	1328414		4.42	-17.68%	< 0.01	0.07	0.15	0.36	10.78	25
	0.0075	2361625		6.67	-20.16%	< 0.01	0.05	0.11	0.26	4.98	18.75
Mushroom	0.05	104337	-11.98%	88.66	-8.64%	0.17	8.22	13.35	21.09	45.75	125
	0.02	652104		467.97	-13.86%	0.40	5.63	6.56	8.45	22.86	50
	0.01	2608414		1816.05	-11.45%	0.05	2.53	4.27	4.63	7.45	25
	0.0075	4637180		3274.01	-10.70%	0.05	3.41	3.77	4.43	8.85	18.75
Tic-Tac-Toe	0.05	72337	-17.35%	2.34	-12.96%	< 0.01	0.87	2.04	4.11	48.88	125
	0.02	452104		9.72	-16.66%	< 0.01	0.34	0.77	1.53	28.58	50
	0.01	1808414		35.36	-17.47%	< 0.01	0.32	0.68	1.21	7.86	25
	0.0075	3214958		59.31	-19.72%	< 0.01	0.29	0.64	1.11	5.14	18.75

Table 2: Sample size, runtime, and accuracy (absolute error) evaluation for MiSoSouP-1

5.6.1 Sample size reduction and speed-up. We compare the number of samples used by MiSoSouP-1 and by UB-1 as ε varies. In both cases, the sample size is independent from k: k enters into play only when computing the final output, so it can be chosen after the "sampling phases" of the algorithms have run. The results are presented in the 3rd and 4th column from the left of Table 2. W.r.t. the whole dataset (whose size is reported in Table 1), MiSoSouP-1 looks at a small fraction of the transactions, and *this quantity does not grow as the dataset grows*, which is one of the main advantages of sampling-based approaches.[8] MiSoSouP-1 achieves a very large reduction in the sample size w.r.t. UB-1 (only a single number is reported for each dataset because the two sample sizes have the same dependency on ε and δ, and do not depend on k). The reduction is extremely significant because, especially when ε is small, UB-1 would require to analyze a sample *larger* than the original dataset, defeating the whole purpose of sampling, while MiSoSouP-1 would still shine.[9] Hence, MiSoSouP-1 can be used with success in situations where UB-1 would be useless. There are other scenarios where UB-1 would not work but MiSoSouP-1 would: if given just a sample and no information on the *size* of the language, UB-1 would not be able to compute the sample size, while MiSoSouP-1 would have no issues. Thus, MiSoSouP-1 requires fewer transactions than UB-1, while being more flexible.

The runtime of MiSoSouP-1 and the reduction over UB-1 are reported in the 5th and 6th columns of Table 2. We remark once again that the runtime of UB-1 did not include the time to compute an upper bound to the size of language, which on large datasets is significant. Thus the improvement of MiSoSouP-1 over UB-1 is actually even larger than reported. At small sample sizes (i.e., large values of ε), both algorithms have fixed costs that dominate over the part of the running time that depends on the size of the sample, thus the reduction in MiSoSouP-1's runtime w.r.t. UB-1's is not proportional to the reduction in the sample size. The sample-size-dependent costs dominate when ε is small (larger sample sizes) and in these cases the speed-up becomes essentially equal to the reduction in the sample size.

5.6.2 Accuracy. We evaluate the accuracy of the output of MiSoSouP-1 by measuring, for each subgroup A in the output, the *absolute error* on the sample $\mathcal{S}$: $\mathrm{err}_{\mathcal{S}}^{(p)}(A) = \left|\tilde{\mathrm{q}}_{\mathcal{S}}^{(p)}(A) - \mathrm{q}_{\mathcal{D}}^{(p)}(A)\right|$. The quality guarantees of MiSoSouP-1 ensure that, with probability at least $1-\delta$, the absolute error is bounded by $\varepsilon/4$ for all subgroups. A first important result is that the above was true in *all* the thousands of runs of MiSoSouP-1 we performed, i.e., not just with probability $1-\delta$. Hence MiSoSouP-1 has, in practice, even higher confidence than it guarantees theoretically. We will further comment later on this aspect. In the six rightmost columns of Table 2 we report the minimum, first quartile, median, third quartile, and maximum absolute error, and the value of $\varepsilon/4$ for comparison. We report results for $k = 1000$ (the full table for all values of k is available in the supplementary materials [24], with qualitatively similar results). We can see that not only the maximum absolute error was approximately between two to seven times smaller than the maximum allowed ($\varepsilon/4$), but the majority of the distribution of the error (over the subgroups) is highly concentrated around values that are often orders of magnitude smaller, with the median being at times even more than 100 times smaller than $\varepsilon/4$. Additionally we see how, as ε decreases, the distribution of the error becomes more concentrated, with the maximum values decreasing faster than the third quartiles and the medians.

A possible explanation for the fact that the estimation of the 1-qualities is much better than what is guaranteed by the theory is that the analysis uses an *upper bound* to the pseudodimension, which itself is a *worst-case* measure of complexity. This looseness is

[8] This property of sampling-based approached is also the reason why we did not perform evaluate the scalability of MiSoSouP as the dataset size grows.

[9] For extremely small values of ε and only moderately large datasets, MiSoSouP-1 would also require a sample size larger than the datasets. This weakness is implicit in all sampling-based approaches, but for MiSoSouP-1, it appears at much smaller values of ε than for UB-1.

ε	k	$\lvert\text{TOP}_1(k,\mathcal{D})\rvert$	FP	% of all Acceptable FP
	10	10	29	19.72
	50	50	120	22.64
0.05	100	100	232	25.86
	200	200	399	32.83
	500	546	764	34.80
	1000	1013	850	17.63
	2000	2004	4030	15.26
	10	10	14	56.00
	50	50	48	57.83
0.02	100	100	57	40.42
	200	200	141	51.64
	500	546	361	59.66
	1000	1013	284	42.83
	2000	2004	949	31.96
	10	10	2	14.28
	50	50	17	36.95
0.01	100	100	26	45.61
	200	200	46	34.07
	500	546	67	18.55
	1000	1013	129	41.88
	2000	2004	455	48.50
	10	10	2	100.00
	50	50	8	34.78
0.0075	100	100	26	78.78
	200	200	35	35.00
	500	546	47	16.60
	1000	1013	92	46.23
	2000	2004	246	36.71

Table 3: Output evaluation for MiSoSouP-1 on Mushroom

somewhat inevitable, but it suggests that there is room for improvement in the analysis. We plan to investigate the use of Rademacher averages [11] to obtain tighter sample-dependent bounds to the deviations of the sample qualities from their exact values.

5.6.3 Output properties. The set of subgroups returned by MiSoSouP-1 is a superset of $\text{TOP}_p(k,\mathcal{D})$. This was always the case in all the runs, so the *recall* of MiSoSouP-1 is, in practice, 100%. MiSoSouP-1 therefore effectively exceeds the theoretical guarantees it offers. As for the precision, we must remark that a sampling-based algorithm can obviously not guarantee 100% precision, especially if it gives 100% recall like MiSoSouP-1 does.

Nevertheless, MiSoSouP-1 guarantees that *False Positives (FP)*, i.e., subgroups not in $\text{TOP}_p(k,\mathcal{D})$) that may be included in the output, can only be among those subgroups with 1-quality in $\mathcal{D}$ at least $\text{r}^{(1)}_{\mathcal{D}}(k)-\varepsilon$, i.e., at most ε less than the 1-quality of the top-k-th subgroup in $\mathcal{D}$. The number of these "acceptable" FP depends on the distribution of the 1-qualities in the dataset, and cannot be controlled by the algorithm. Thus, the precision may be very low if there are many (potentially $\gg k$) subgroups that would be acceptable FP, and these FP are the price to pay for the speed-up in analyzing the dataset. It is arguable that in these cases the exact choice of k becomes somewhat arbitrary, because there are many subgroups with p-qualities very close to each other. In any case, the output of MiSoSouP-1 is a superset of $\text{TOP}_1(k,\mathcal{D})$ and can be refined to obtain this set with a fast linear scan of the dataset.

We report in Table 3, for the Mushroom dataset, the number of FP in the output and to what percentage of the acceptable FP that number corresponds to. The tables for other datasets are available in the supplementary materials [24]. As expected, for a fixed value of k, the number of FP included in the output decreases as ε becomes smaller, but notice that the percentage may not decrease because the set of acceptable FP changes with ε. The absolute number of FP tends to grow with k, because the number of acceptable FP also tends to grow with k, which is a consequence of the power-law distribution of the qualities of the subgroups.

In the end, the amount of FP is either a small number (either in absolute terms or relatively to k) or a relatively small fraction of the total number of acceptable FP. This fact can be explained by the "excessive" accuracy of MiSoSouP-1 in estimating the 1-quality of the subgroups, as discussed in Sect. 5.6.2. As mentioned, MiSoSouP-1 gives no guarantees that only a small subset of the acceptable FP would be included in the output, so the fact that in most cases less than half of them are actually present is a witness to the good performances of the algorithm.

6 CONCLUSIONS

We introduced MiSoSouP, the first family of algorithms based on random sampling that compute probabilistically-guaranteed high-quality approximations of the collection of the top-k most interesting subgroups in a dataset. Our analysis relies on pseudodimension, a fundamental concept from statistical learning theory. This connection is novel for subgroup discovery.

Our experimental evaluation shows that MiSoSouP requires much smaller sample sizes than state-of-the-art solutions to obtain approximations with the same guarantees, therefore providing the first viable tool to efficiently identify the most interesting subgroups for ever-more-massive datasets.

Our algorithms hinge on defining quality measures as averages of specific functions. This approach can be used in concert with Rademacher averages to design progressive-sampling methods for subgroups discovery, as done for other mining tasks [22]. We will investigate this direction in the near future.

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