MiSoSouP: Mining Interesting Subgroups with Sampling and Pseudodimension

Full Version with Supplementary Materials

Matteo Riondato Labs Two Sigma Investments, LP New York, NY, USA matteo@twosigma.com Fabio Vandin
Department of Information Engineering
Università di Padova
Padova, Italy
fabio.vandin@unipd.it

ABSTRACT

"Miso makes a soup loaded with flavour that saves you the hassle of making stock." – Y. Ottolenghi [19]

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

ACM Reference Format:

1 INTRODUCTION

A fundamental task within data mining is *subgroup discovery* [10, 12, 36], which requires to identify *interesting subsets* (the subgroups) of a dataset, for which the distribution of a specific feature (the

Permission to make digital or hard copies of part or all of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for third-party components of this work must be honored. For all other uses, contact the owner/author(s).

KDD'18, August 19–23, 2018, London, UK

© 2018 Copyright held by the owner/author(s).

ACM ISBN 978-x-xxxx-xxxx-x/YY/MM.

https://doi.org/10.1145/nnnnnn.nnnnnn

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 [12, 36] (see also the comprehensive reviews by Herrera et al. [7] and Azmuller [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 [23, 24] and graph analysis [25]. 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 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 [23, 24]), 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 [29] not providing rigorous quality guarantees on their output, as we discuss in Appendix C.

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 [29, 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 [29] does not actually provide rigorous guarantees (see Appendix C). 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* [21], a key concepts from statistical learning theory [34]. 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. [7] and Azmueller [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 [29] 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 Appendix C). 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 [21], which allows us to use very small sample sizes.

Some works [5, 16, 31, 33] focused on the issue of the statistical significance of subgroups. Duivesteijn et al. [5] 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 [33] showed that several real datasets contain large numbers of high-quality subgroups, many more than are expected from randomly drawn subgroups. Terada et al. [31] 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. [16] subsequently improved LAMP by employing a more efficient mining strategy. We do not investigate this problem, 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.

The use of sampling is also orthogonal to techniques that aim at reducing the redundancy in the output collection of subgroups [32]. Indeed these approaches could be applied to the collection of subgroups obtained by MiSoSouP.

Pseudodimension [21] is a key concept from statistical learning theory [34]. Like many other measures of sample complexity, such as Rademacher averages, it has long been considered only of theoretical interest, but recent applications [6, 9, 22, 24, 25] 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 [23]. Despite the relative similarity between subgroup discovery and frequent itemset mining, using pseudodimension for the former presents significant challenges, such as lack of antimonotonicity in the quality measures, that do not allow to use the same approach by Riondato and Upfal [23]. 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 [11] 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 , $1 \le i \le z$ 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: $(A_1 = \text{``blue''} \lor A_1 = \text{``red''}) \land (A_2 > 4)$. 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 $g_{\mathcal{D}}(A)$ 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} :

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

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 $unusualness^2$ $u_{\mathcal{D}}(A)$ of A on \mathcal{D} is the difference between the target mean of A and the target mean of \mathcal{D} :

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

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.

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 [12], which differ from each other for the relative weight given to generality and unusualness.

Definition 3.1 ([10, 20, 36]). Let $p \in \{1/2, 1, 2\}$. The p-quality of a subgroup A on a dataset \mathcal{D} is

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

The 1-quality is also known as *Weighted Relative Accuracy* (WRAcc).³ The 1/2-quality is proportional to the *z*-score⁴ for the statistic $C_{\mathcal{D}}(A)$ 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 [10, 29, 33]. The domain \mathcal{Y}_T of the target attribute is Boolean, thus $q_{\mathcal{D}}^{(p)}(A) \in [-1, 1]$ for any subgroup A. There exist variants of the p-qualities that consider the *absolute value* of the unusualness [29]. 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 $r_{\mathcal{D}}^{(p)}(k)$ 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 $\mathsf{TOP}_p(k,\mathcal{D})$ 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 $\mathsf{r}_{\mathcal{D}}^{(p)}(k)$:

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

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

- (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 $q_{\mathcal{D}}^{(p)}(A) < r_{\mathcal{D}}^{(p)}(k) \varepsilon$; and
- (3) for each pair $(A, q_A) \in \mathcal{B}$, $|q_{\mathcal{D}}^{(p)}(A) q_A| \le \varepsilon/4$.

MiSoSouP computes (with high probability) an ε -approximation from a random sample of the dataset. For the 1/2-quality, we define slightly different conditions for an ε -approximation (presented in Section A.2).

 $^{^1\}mbox{We}$ use |B| to denote the size of a bag B, i.e., the number of elements in B, counting repeated elements multiple times.

²Scheffer and Wrobel [29] use the term *statistical unusualness*. We choose to drop the adjective to avoid confusion with *statistical significance*.

 $^{^3}$ Van Leeuwen and Ukkonen [33] denote the 1/2-quality as "WRAcc", but all other references we found (e.g., [7, 18]) use this name to denote the 1-quality.

⁴The *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 $(|C_{\mathcal{D}}(A)|\mu_{\mathcal{D}}(A) - |C_{\mathcal{D}}(A)|\mu(\mathcal{D}))/\sqrt{C_{\mathcal{D}}(A)\mu(\mathcal{D})(1 - \mu(\mathcal{D}))}$.

⁵This definition of the task is therefore slightly different from the one given in [29, Definition 1], where the size of $\mathsf{TOP}_p(k,\mathcal{D})$ is limited to exactly k elements.

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 [29, 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 [29]. 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 [35] and pseudodimension [21], specializing some of them to our settings. 6

3.2.1 VC-dimension. Let 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 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 [21] is an extension of VC-dimension [35] 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

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

Let

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

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

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

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

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

We call $m_{\mathcal{S}}(f)$ the *empirical average of f on S*. It holds $\mathbb{E}[m_{\mathcal{S}}(f)] = m_{\mathcal{H}}(f)$. 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 ([14]). Let $PD(\mathcal{F}) \leq d$. Fix $\xi, \eta \in (0,1)$. When \mathcal{S} is a collection of

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

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

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

The following two lemmas by Riondato and Upfal [26, Lemmas B.1 and B.2] 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 $TOP_p(k, \mathcal{D})$. We present only the case for p = 1, and discuss the variants for the other p-qualities in App. A.

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:

$$\rho_{A}(t) = \begin{cases} 1 - \mu(\mathcal{D}) & \text{if } t \in C_{\mathcal{D}}(A) \text{ and } t.T = 1\\ -\mu(\mathcal{D}) & \text{if } t \in C_{\mathcal{D}}(A) \text{ and } t.T = 0\\ 0 & \text{otherwise} \end{cases}$$
 (2)

We assume to know the exact value of $\mu(\mathcal{D})$, which is a standard and reasonable assumption (made also by Scheffer and Wrobel [29]), 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 :

$$m_{\mathcal{D}}(\rho_{A}) = \frac{1}{|\mathcal{D}|} \sum_{t \in \mathcal{D}} \rho_{A}(t)$$

$$= \frac{1}{|\mathcal{D}|} \left((1 - \mu(\mathcal{D})) \mu_{\mathcal{D}}(A) |C_{\mathcal{D}}(A)| - \mu(\mathcal{D}) |C_{\mathcal{D}}(A)| (1 - \mu_{\mathcal{D}}(A)) \right)$$

$$= \frac{|C_{\mathcal{D}}(A)|}{|\mathcal{D}|} \left(\mu_{\mathcal{D}}(A) - \mu(\mathcal{D}) \right) = g_{\mathcal{D}}(A) u_{\mathcal{D}}(A) = q_{\mathcal{D}}^{(1)}(A) . \tag{3}$$

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 $S = \{t_1, \dots, t_\ell\}$ be a collection of transactions sampled uniformly and independently at random with replacement from \mathcal{D} . It holds, following the same steps as in (3), that

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

 $^{^6{\}rm For}$ an in-depth discussion of these topics see, e.g., the books by Shalev-Shwartz and Ben-David [30] and by Anthony and Bartlett [1].

524

525

526

527

528

529

530

531

532

533

534

535

536

537

538

539

540

541

542

543

544

545

546

547

548

549

550

551

552

553

554

555

556

557

558

559

560

562

563

564

565

566

567

568

569

570

571

572

573

575

576

577 578

579

580

465

466

467

468

469

470

471

472

473

474

475

476

477

478

479

480

481

482

483

484

485

486

487

488

489

490

491

492

493

494

495

496

497

498

499

500

501

502

503

504

505

506

507

508

509

510

511

512

513

514

515

516

517

518

519

520

521

522

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

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

4.1.2 Sufficient condition for an ε -approximation. We now show a condition on the sample S that is sufficient to allow the computation of an ε -approximation of TOP₁(k, \mathcal{D}) from \mathcal{S} . Assume to sort the subgroups in $\mathcal L$ in decreasing order by their approximate 1-quality on S, ties broken arbitrarily. Let $\tilde{r}_{S}^{(1)}(k)$ be the *approximate* 1-quality on S of the k-th subgroup in this order.

Theorem 4.1. If S is such that

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

then the set

$$\mathcal{B} = \left\{ \left(A, \tilde{\mathsf{q}}_{\mathcal{S}}^{(1)}(A) \right) \ : \ \tilde{\mathsf{q}}_{\mathcal{S}}^{(1)}(A) \ge \tilde{\mathsf{r}}_{\mathcal{S}}^{(1)}(k) - \frac{\varepsilon}{2} \right\} \tag{5}$$

is an ε -approximation to $TOP_1(k, \mathcal{D})$.

PROOF. Equation (4) holds in particular for subgroups appearing in the pairs in \mathcal{B} . Thus, \mathcal{B} satisfies Property 3 from Definition 3.3. It holds

$$\tilde{\mathsf{r}}_{\mathcal{S}}^{(1)}(k) \ge \mathsf{r}_{\mathcal{D}}^{(1)}(k) - \frac{\varepsilon}{4} \tag{6}$$

because all the subgroups in $TOP_1(k, \mathcal{D})$, which are at least k, have, from (4), approximate 1-quality in S at least $r_{\mathcal{D}}^{(1)}(k) - \varepsilon/4$.

Another consequence of (4) is that

$$\tilde{\mathsf{r}}_{\mathcal{S}}^{(1)}(k) \le \mathsf{r}_{\mathcal{D}}^{(1)}(k) + \frac{\varepsilon}{4} \tag{7}$$

because only subgroups with exact 1-quality in $\mathcal D$ strictly greater than $r_{\mathcal{D}}^{(1)}(k)$ can have an approximate 1-quality in \mathcal{S} strictly greater than $r_{\mathcal{D}}^{(1)}(k) + \varepsilon/4$, and there are only at most k-1 such subgroups. It then holds from (7) and (4) that

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

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

Let now *A* be any subgroup with $q_{\mathcal{D}}^{(1)}(A) < r_{\mathcal{D}}^{(1)}(k) - \varepsilon$. It follows from (4) that $\tilde{q}_{S}^{(1)}(A) \le r_{D}^{(1)}(k) - 3\varepsilon/4$, and using (6) we get $\tilde{q}_{S}^{(1)}(A) < \varepsilon/4$ $\tilde{\mathbf{r}}_{S}^{(1)}(k) - \varepsilon/2$, hence $(A, \tilde{\mathbf{q}}_{S}^{(1)}(A)) \notin \mathcal{B}$, 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 S is large enough, then with high probability over the choice of S, S satisfies the condition in (4), 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 S should be for the above to happen.

Theorem 4.2. Let $\delta \in (0,1)$, $\varepsilon \in (0,1)$, and $k \geq 1$. Let S be a collection of

$$|S| \ge \frac{16}{\varepsilon^2} \left(\ln |\mathcal{L}_{\mathcal{D}}| + \ln \frac{2}{\delta} \right)$$
 (8)

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

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

is an ε -approximation to $TOP_1(k, \mathcal{D})$.

The proof is in App. B. It uses Hoeffding's inequality [8] and the union bound [17, Lemma 1.2].

The quantity in (8) 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 MiSo-SouP. Another drawback is that the sample size in (8) 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 (4), and therefore compute an high-quality approximation of $TOP_1(k, \mathcal{D})$. It relies on the following bound to the pseudodimension [21] (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 $PD(\mathcal{P})$ of \mathcal{P} satisfies:

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

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

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

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

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

is also shattered by 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, 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

640

641

642

646

647

648

649

650

651

652

653

654

655

656

657

658

659

660

661

665

666

667

668

669

670

671

672

673

674

675

676

678

679

680

681

682

683

684

685

686

687

688

689

691

692

693

694

695

696

589

595

596

597

603 604 605

607 608 609

618

636

impossible that two or more elements of *B* are mapped by $c(\cdot)$ 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

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

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

for d as in Theorem 4.3.

PROOF. The proof is in part inspired by the one for [23, 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 , $1 \le a$ $i \leq 2^{|B|-1}$, 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} , $1 \le i \le 2^{|B|-1}$. 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 $2^{|B|-1} < d$.

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

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

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 , $1 \le i \le$ $2^{|B|-1}$, 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} , $1 \le i \le 2^{|B|-1}$. 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 $2^{|B|-1} < d$.

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 $c \ge 1$. 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 $1 \le c \le C$. Then

$$PD(\mathcal{P}) \le \left| \log_2 \sum_{i=1}^c \binom{C}{i} \right| + 1 . \tag{9}$$

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

$$S = \frac{16}{\varepsilon^2} \left(\lfloor \log_2 d \rfloor + 1 + \ln \frac{1}{\delta} \right). \tag{10}$$

The probability that a collection S of S transactions sampled independently and uniformly at random with replacement from $\mathcal D$ satisfies (4) is at least $1 - \delta$.

The improvement of (10) over (8) is evident: $\lfloor \log_2 d \rfloor + 1$ is usually much much smaller, potentially orders of magnitude so, than $\ln |\mathcal{L}_{\mathcal{D}}|$. The quantity d depends on both the dataset and the language: it is intuitively more "natural" that the sample size should depend on the relationship between the two, rather than just on the language.

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 $\mathsf{TOP}_1(k,\mathcal{D})$. The input of the algorithm is the tuple $(\mathcal{D}, k, \varepsilon, \delta)$.

MiSoSouP-1 starts by creating the sample S by drawing S transactions independently and uniformly at random with replacement from \mathcal{D} , for S as in (10). An exact algorithm for subgroup discovery is used to extract from S the set B defined in (5). Any exact algorithm can be used for the discovery step, but it needs to be slightly modified to use $\tilde{q}_{S}^{(1)}(A)$ as measure for the interestingness of a subgroup A, instead of $q_{\mathcal{S}}^{(1)}(A)$. 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 TOP₁(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 App. D.

5.1 Goals

Our experiments have two goals: 1) evaluate the speed-up of Mi-SoSouP 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. Like MiSoSouP, UB computes, with probability at least $1 - \delta$, an ε -approximation to $TOP_p(k, \mathcal{D})$ 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 (8) (or similar equations for $p \neq 1$). We use UB-1 to denote the variant of UB for 1-quality. As is evident from (8), 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 (9) to compute the upper bound d to the pseudodimension used in (10) to obtain its sample size, and the cost of evaluating the r.h.s. of (9) 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 $\mathsf{TOP}_p(k,\mathcal{D})$ 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 [29] because the algorithm does not actually offer the claimed guarantees (see App. C). Additionally, an implementation is not available.

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 [15]. 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 PhenomTM II X4 955 processor and 16GB of RAM, running FreeBSD 12. The code is included in the same archive where you found this version of the work.

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).

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*

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

						A	bsolute	error (×10	⁴) (for <i>k</i>	= 1000)	
Dataset	ε	$ \mathcal{S} $	Reduction w.r.t. UB-1	Runtime (s)	Reduction w.r.t. UB-1	Min.	1 st Q.	Median	3 rd Q.	Max.	$\varepsilon/4$
	0.05	53137		1.50	-1.5%	< 0.01	0.32	0.76	1.88	25.50	125
Car	0.02	332104	-25.07%	2.13	-10.55%	< 0.01	0.14	0.32	0.73	8.20	50
Car	0.01	1328414	-25.07%	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
	0.05	104337		88.66	-8.64%	0.17	8.22	13.35	21.09	45.75	125
Mushroom	0.02	652104	-11.98%	467.97	-13.86%	0.40	5.63	6.56	8.45	22.86	50
Musiffooiii	0.01	2608414	-11.90%	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
	0.05	72337		2.34	-12.96%	< 0.01	0.87	2.04	4.11	48.88	125
Tic-Tac-Toe	0.02	452104	17.2507	9.72	-16.66%	< 0.01	0.34	0.77	1.53	28.58	50
11c-1ac-10e	0.01	1808414	-17.35%	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

quantity does not grow as the dataset grows, which is one of the main advantages of sampling-based approaches. 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. 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 S: $\operatorname{err}_{S}^{(p)}(A) = \left|\tilde{\mathsf{q}}_{S}^{(p)}(A) - \mathsf{q}_{D}^{(p)}(A)\right|$. 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 App. D. 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 somewhat inevitable, but it suggests that there is room for improvement in the analysis. We plan to investigate the use of Rademacher averages [13] 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 $TOP_p(k,\mathcal{D})$. 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.

 $^{^8\}mathrm{This}$ property of sampling-based approached is also the reason why we did not perform evaluate the scalability of MiSoSouP as the dataset size grows.

 $^{^{5}}$ 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	$ TOP_1(k,\mathcal{D}) $	FP	% of all Acceptable Fl
	10	10	29	19.73
	50	50	120	22.6
0.05	100	100	232	25.8
	200	200	399	32.83
	500	546	764	34.80
	1000	1013	850	17.63
	2000	2004	4030	15.20
	10	10	14	56.0
	50	50	48	57.83
0.02	100	100	57	40.42
	200	200	141	51.6
	500	546	361	59.6
	1000	1013	284	42.83
	2000	2004	949	31.9
	10	10	2	14.23
	50	50	17	36.9
0.01	100	100	26	45.6
	200	200	46	34.0
	500	546	67	18.5
	1000	1013	129	41.8
	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	36.7
	500 1000	546 1013	47 92	16.0 46.1

Nevertheless, MiSoSouP-1 guarantees that False Positives (FP),
i.e., subgroups not in $TOP_p(k, \mathcal{D})$) that may be included in the
output, can only be among those subgroups with 1-quality in ${\mathcal D}$ at
least $\mathbf{r}_{\mathcal{D}}^{(1)}(k) - \varepsilon$, 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 $TOP_1(k, \mathcal{D})$ 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 App. D. 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 1quality 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.

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 [24]. We will investigate this direction in the near future.

REFERENCES

- Martin Anthony and Peter L. Bartlett. 1999. Neural Network Learning Theoretical Foundations. Cambridge University Press.
- Martin Atzmueller. 2015. Subgroup discovery. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery 5, 1 (2015), 35-49.
- Michele Borassi and Emanuele Natale, 2016, KADABRA is an ADaptive Algorithm for Betweenness via Random Approximation. In 24th Annual European Symposium on Algorithms (ESA '16), 20:1-20:18.
- Victor De la Peña and Evarist Giné. 1999. Decoupling: from dependence to independence. Springer.
- Wouter Duivesteijn, Ad Feelders, and Arno Knobbe. 2012. Different slopes for different folks: mining for exceptional regression models with Cook's distance. In Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining (KDD '12). ACM, 868-876.
- Tapio Elomaa and Matti Kääriäinen. 2002. Progressive Rademacher Sampling. In AAAI/IAAI, Rina Dechter and Richard S. Sutton (Eds.). AAAI Press / The MIT Press, 140-145
- [7] Franciso Herrera, Cristóbal José Carmona, Pedro González, and María José Del Jesus. 2011. An overview on subgroup discovery: foundations and applications. Knowledge and information systems 29, 3 (2011), 495-525
- Wassily Hoeffding. 1963. Probability Inequalities for Sums of Bounded Random Variables. J. American Statistical Assoc. 58, 301 (1963), 13-30.
- Matti Kääriäinen, Tuomo Malinen, and Tapio Elomaa. 2004. Selective Rademacher Penalization and Reduced Error Pruning of Decision Trees. Journal of Machine Learning Research 5 (Dec. 2004), 1107-1126
- [10] Willi Klösgen. 1992. Problems for knowledge discovery in databases and their treatment in the Statistics Interpreter Explora. International Journal of Intelligent Systems 7 (1992), 649-673.
- Willi Klösgen. 1995. Assistant for knowledge discovery in data. In Assisting Computer: A New Generation of Support Systems, P. Hoschka (Ed.).
- Willi Klösgen. 1996. Explora: A multipattern and multistrategy discovery assistant. In Advances in knowledge discovery and data mining. American Association for Artificial Intelligence, 249-271.

1046

1047

1048

1049

1050

1051

1052

1053

1054

1055

1061

1062

1064

1065

1066

1067

1068

1071

1072

1073

1074

1075

1076

1077

1078

1079

1080

1081

1082

1085

1086

1087

1088

1089

1090

1091

1092

1093

1094

1095

1098

1099

1100

1101

1102

1103

1104

1105

1106

1107

1108

1109

1110

1111

1112

1113

1114

1115

1116

1117

1118

1119

1120

1121

1122

1123

1124

1125

1128

1129

1130

1131

1132

1133

1134

1135

1136

1137

1138

1139

1141

1142

1143

1144

1145

1146

1147

1148

1149

1150

1151

1152

1153

1155

1156

1157

1158

1159

1160

- [13] Vladimir Koltchinskii. 2001. Rademacher penalties and structural risk minimization. IEEE Transactions on Information Theory 47, 5 (July 2001), 1902–1914.
- [14] Yi Li, Philip M. Long, and Aravind Srinivasan. 2001. Improved Bounds on the Sample Complexity of Learning. J. Comput. System Sci. 62, 3 (2001), 516–527.
- [15] M. Lichman. 2013. UCI Machine Learning Repository. http://archive.ics.uci.edu/ml. (2013).
- [16] Shin-ichi Minato, Takeaki Uno, Koji Tsuda, Aika Terada, and Jun Sese. 2014. A fast method of statistical assessment for combinatorial hypotheses based on frequent itemset enumeration. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases. Springer, 422–436.
- [17] Michael Mitzenmacher and Eli Upfal. 2005. Probability and Computing: Randomized Algorithms and Probabilistic Analysis. Cambridge University Press.
- [18] Petra Kralj Novak, Nada Lavrač, and Geoffrey I Webb. 2009. Supervised descriptive rule discovery: A unifying survey of contrast set, emerging pattern and subgroup mining. Journal of Machine Learning Research 10, Feb (2009), 377–403.
- [19] Yotam Ottolenghi. 2012. Yotam Ottolenghi's recipes for char-grilled sprouting broccoli with sweet tahini, plus gingery fish balls in miso soup. https://www.theguardian.com/lifeandstyle/2012/feb/03/ grilled-broccoli-fishball-soup-recipes. (feb 2012).
- [20] Gregory Piatetsky-Shapiro. 1991. Discovery, analysis, and presentation of strong rules. Knowledge discovery in databases (1991), 229–248.
 - [21] David Pollard. 1984. Convergence of stochastic processes. Springer-Verlag.
 - [22] Theodoros Rekatsinas, Manas Joglekar, Hector Garcia-Molina, Aditya Parameswaran, and Christopher Ré. 2017. SLiMFast: Guaranteed Results for Data Fusion and Source Reliability. In Proceedings of the 2017 ACM International Conference on Management of Data (SIGMOD '17). ACM, New York, NY, USA, 1399–1414.
 - [23] Matteo Riondato and Eli Upfal. 2014. Efficient Discovery of Association Rules and Frequent Itemsets through Sampling with Tight Performance Guarantees. ACM Trans. Knowl. Disc. from Data 8, 4 (2014), 20. https://doi.org/10.1145/2629586
 - [24] Matteo Riondato and Eli Upfal. 2015. Mining Frequent Itemsets through Progressive Sampling with Rademacher Averages. In Proceedings of the 21st ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD '15). ACM, 1005–1014. Extended version available from http://matteo.rionda.to/papers/RiondatoUpfal-FrequentItemsetsSamplingRademacher-KDD.pdf.
 - [25] Matteo Riondato and Eli Upfal. 2016. Approximating Betweenness Centrality in Static and Dynamic Graphs with Rademacher Averages. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD '16). ACM, 1145–1154.
 - [26] Matteo Riondato and Eli Upfal. 2016. Approximating Betweenness Centrality in Static and Dynamic Graphs with Rademacher Averages. (2016). Extended Version available from http://matteo.rionda.to/papers/RiondatoUpfal-ABRA-ext.pdf.
 - [27] Matteo Riondato and Fabio Vandin. 2014. Finding the True Frequent Itemsets. In Proceedings of the 2014 SIAM International Conference on Data Mining, Philadelphia, Pennsylvania, USA, April 24-26, 2014, Mohammed Javeed Zaki, Zoran Obradovic, Pang-Ning Tan, Arindam Banerjee, Chandrika Kamath, and Srinivasan Parthasarathy (Eds.). SIAM, 497-505. https://doi.org/10.1137/1.9781611973440.57
 - [28] Matteo Riondato and Fabio Vandin. 2018. MiSoSouP: Mining Interesting Subgroups with Sampling and Pseudodimension – Extended version. (Feb 2018). Available at http://matteo.rionda.to/papers/misosoup-ext.tar.bz2.
 - [29] Tobias Scheffer and Stefan Wrobel. 2002. Finding the most interesting patterns in a database quickly by using sequential sampling. J. Mach. Learn. Res. 3 (Dec. 2002), 833–862.
 - [30] Shai Shalev-Shwartz and Shai Ben-David. 2014. Understanding Machine Learning: From Theory to Algorithms. Cambridge University Press.
 - [31] Aika Terada, Mariko Okada-Hatakeyama, Koji Tsuda, and Jun Sese. 2013. Statistical significance of combinatorial regulations. Proceedings of the National Academy of Sciences 110, 32 (2013), 12996–13001.
 - [32] Matthijs Van Leeuwen and Arno Knobbe. 2011. Non-redundant subgroup discovery in large and complex data. In Machine Learning and Knowledge Discovery in Databases (ECML PKDD '11). 459–474.
 - [33] Matthijs Van Leeuwen and Antti Ukkonen. 2016. Expect the Unexpected On the Significance of Subgroups. In Proceedings of Discovery Science (DS '16).
 - [34] Vladimir N. Vapnik. 1998. Statistical learning theory. Wiley.
 - [35] Vladimir N. Vapnik and Alexey J. Chervonenkis. 1971. On the Uniform Convergence of Relative Frequencies of Events to Their Probabilities. Theory of Probability and its Applications 16, 2 (1971), 264–280. https://doi.org/10.1137/1116025
 - [36] Stefan Wrobel. 1997. An algorithm for multi-relational discovery of subgroups. In European Symposium on Principles of Data Mining and Knowledge Discovery (PKDD '97). 78–87.
 - [37] Shengjia Zhao, Enze Zhou, Ashish Sabharwal, and Stefano Ermon. 2016. Adaptive Concentration Inequalities for Sequential Decision Problems. In Advances In Neural Information Processing Systems (NIPS '16). 1343–1351.

A MISOSOUP FOR OTHER QUALITY MEASURES

A.1 MiSoSouP for 2-quality

In this section we present MiSoSouP-2, the variant of MiSoSouP for computing an ε -approximation to TOP₂(k, \mathcal{D}). To obtain upper bounds on the number of samples needed by MiSoSouP-2, we will combine the result obtained in the previous section with variants of results by Riondato and Vandin [27] on the number of samples needed to compute a high-quality approximation of the frequent itemsets from a random sample of a transactional dataset.

We start by defining another family \mathcal{G} of functions, in addition to \mathcal{P} defined in Section 4.1.1. The domain of the functions in \mathcal{G} is \mathcal{D} . For each subgroup $A \in \mathcal{L}$ there is one function $g_A \in \mathcal{G}$, defined as follows, for $t \in \mathcal{D}$:

$$g_A(t) = \mathbb{1}_{C_{\mathcal{D}}(A)}(t) = \begin{cases} 1 & \text{if } t \in C_{\mathcal{D}}(A) \\ 0 & \text{otherwise} \end{cases}$$
 (11)

It holds

$$\mathsf{m}_{\mathcal{D}}(g_A) = \frac{1}{|\mathcal{D}|} \sum_{t \in \mathcal{D}} g_A(t) = \frac{|C_{\mathcal{D}}(A)|}{|\mathcal{D}|} = \mathsf{g}_{\mathcal{D}}(A) \ .$$

Let now $S = \{t_1, \dots, t_\ell\}$ be a collection of transactions sampled uniformly and independently at random with replacement from \mathcal{D} . It holds

$$\mathsf{m}_{\mathcal{S}}(g_A) = \frac{1}{\ell} \sum_{i=1}^{\ell} g_A(t_i) = \mathsf{g}_{\mathcal{S}}(A)$$

For any subgroup $A \in \mathcal{L}$, we define the *approximate 2-quality of A* on \mathcal{S} as

$$\tilde{\mathbf{q}}_{\mathcal{S}}^{(2)}(A) = \mathbf{m}_{\mathcal{S}}(g_A) \mathbf{m}_{\mathcal{S}}(\rho_A) = \mathbf{g}_{\mathcal{S}}(A) \tilde{\mathbf{q}}_{\mathcal{S}}^{(1)}(A) \ .$$

As was the case for p = 1, it holds $\tilde{q}_{\mathcal{S}}^{(2)}(A) \neq q_{\mathcal{S}}^{(2)}(A)$.

The following lemma shows how a bound on the deviations of the values taken by the functions in \mathcal{G} on \mathcal{S} from their values on \mathcal{D} , together with a bound on the deviations of the approximate 1-qualities on \mathcal{S} of all subgroups, give a bound to the approximate 2-qualities on \mathcal{S} of all subgroups.

Lemma A.1. Let $\varepsilon \in (0, 1)$. If

(1)
$$\sup_{A \in \mathcal{L}} \left| \tilde{q}_{S}^{(1)}(A) - q_{D}^{(1)}(A) \right| \le \sqrt{1 + \varepsilon/4} - 1$$
; and

(2)
$$\sup_{A \in \mathcal{L}} |g_{\mathcal{S}}(A) - g_{\mathcal{D}}(A)| \le \sqrt{1 + \varepsilon/4} - 1$$
,

then

$$\sup_{A\in\mathcal{L}} \left| \tilde{\mathsf{q}}_{\mathcal{S}}^{(2)}(A) - \mathsf{q}_{\mathcal{D}}^{(2)}(A) \right| \leq \frac{\varepsilon}{4} \ .$$

Proof. We show the proof for a more general case. For any $\eta_{\rm q}$ and $\eta_{\rm g}$, assume it holds

(1)
$$\sup_{A \in \mathcal{L}} \left| \tilde{\mathsf{q}}_{\mathcal{S}}^{(1)}(A) - \mathsf{q}_{\mathcal{D}}^{(1)}(A) \right| \leq \eta_{\mathsf{q}}; \text{ and }$$

(2)
$$\sup_{A \in \mathcal{L}} |g_{\mathcal{S}}(A) - g_{\mathcal{D}}(A)| \le \eta_{g}$$
.

From the above, it holds, for any $A \in \mathcal{L}$,

$$\begin{split} \tilde{q}_{S}^{(2)}(A) &= g_{S}(A)\tilde{q}_{S}^{(1)}(A) \leq (g_{D}(A) + \eta_{g}) \left(q_{D}^{(1)}(A) + \eta_{q} \right) \\ &\leq q_{D}^{(2)}(A) + q_{D}^{(1)}(A)\eta_{g} + g_{D}(A)\eta_{q} + \eta_{g}\eta_{q} \\ &\leq q_{D}^{(2)}(A) + \eta_{g} + \eta_{q} + \eta_{g}\eta_{q} \; . \end{split}$$
(12)

1220

1221

1222

1224

1225

1226

1227

1228

1229

1230

1231

1232

1233

1234

1235

1236

1237

1238

1239

1240

1241

1243

1244

1245

1246

1247

1248

1249

1250

1251

1252

1253

1254

1255

1256

1257

1258

1259

1260

1261

1262

1263

1264

1265

1266

1267

1268

1269

1270

1271

1272

1273

1274

1275

1276

Additionally, again from the hypothesis, for any $A \in \mathcal{L}$ it holds

$$\tilde{q}_{S}^{(2)}(A) = g_{S}(A)\tilde{q}_{S}^{(1)}(A) \ge (g_{D}(A) - \eta_{g}) \left(q_{D}^{(1)}(A) - \eta_{q}\right)
\ge q_{D}^{(2)}(A) - q_{D}^{(1)}(A)\eta_{g} - g_{D}(A)\eta_{q} + \eta_{g}\eta_{q}
\ge q_{D}^{(2)}(A) - \eta_{g} - \eta_{q} - \eta_{g}\eta_{q} .$$
(13)

Thus, by combining, we obtain

1161

1162

1163

1164

1165

1166

1167

1168

1169

1170

1171

1172

1173

1174

1175

1176

1178

1179

1180

1181

1182

1183

1184

1185

1187

1188

1189

1190

1191

1192

1193

1194

1195

1196

1197

1198

1199

1200

1201

1202

1203

1204

1205

1206

1207

1208

1209

1210

1211

1212

1213

1214

1215

1216

1217

1218

$$\sup_{A \in \mathcal{I}} \left| \tilde{\mathsf{q}}_{\mathcal{S}}^{(2)}(A) - \mathsf{q}_{\mathcal{D}}^{(2)}(A) \right| \leq \eta_{\mathsf{g}} + \eta_{\mathsf{q}} + \eta_{\mathsf{g}} \eta_{\mathsf{q}} \ .$$

The thesis follows by setting $\eta_q = \eta_g = \sqrt{1 + \varepsilon/4} - 1$.

This lemma sheds light on how to obtain ε -approximations of $\mathsf{TOP}_2(k,\mathcal{D})$ from a sample \mathcal{S} : the sample must offer *simultaneous* guarantees on two family of functions, \mathcal{P} and \mathcal{G} . We discussed the case for family \mathcal{P} when presenting MiSoSouP-1, so we now focus on \mathcal{G} . An application of the union bound will ensure the simultaneous guarantees.

Consider a rangeset \mathcal{R}_g containing a range

$$R_A = \{t \in \mathcal{D} : A \in t\}$$

for each $A \in \mathcal{L}$ appearing in at least one transaction of \mathcal{D} .

As shown by Riondato and Vandin [27, Sect. 4], the VCdimension of this rangeset is also upper bounded by $\lfloor \log_2 d \rfloor + 1$, for d as in Theorem 4.3. An equivalent of Theorem 3.4 also holds for families of binary functions with bounded VC-dimension, with the same sample size as in (1), and therefore relates the sample size of ${\mathcal S}$ with the maximum deviation from the second condition of Lemma A.1.

A.1.1 The algorithm. We are now ready to describe MiSo-SouP-2. The input is the same tuple $(\varepsilon, \delta, k, \mathcal{D})$ as in MiSoSouP-1. After creating a sample S of size

$$S = \frac{1}{\left(\sqrt{1+\varepsilon/4} - 1\right)^2} \left(\lfloor \log_2 d \rfloor + 1 + \ln \frac{2}{\delta} \right),\tag{14}$$

MiSoSouP-2 runs on S a modified variant of an exact algorithm for subgroup discovery that uses $\tilde{q}^{(2)}$ as the interestingness measure. Let $\tilde{r}_{S}^{(2)}(k)$ be the top-k highest approximate 2-quality on S, ties broken arbitrarily. The output set $\mathcal B$ is defined as

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

The following theorem states the guarantees of MiSoSouP-2.

THEOREM A.2. With probability at least $1 - \delta$ (over its runs), Mi-SoSouP-2 outputs an ε -approximation to TOP₂ (k, \mathcal{D}) .

SKETCH. An application of the union bound and of Theorem 3.4 and its corresponding version for VC-dimension gives that the probability that S satisfies the hypothesis of Lemma 4.5 is at least $1 - \delta$. When that is the case, then the thesis of that lemma holds, i.e.,

$$\sup_{A\in\mathcal{L}}\left|\tilde{\mathsf{q}}_{\mathcal{S}}^{(2)}(A)-\mathsf{q}_{\mathcal{D}}^{(2)}(A)\right|\leq\frac{\varepsilon}{4}\ .$$

From here, the proof continues essentially as the one for Theo-

A.2 MiSoSouP for 1/2-quality

We now present MiSoSouP-1/2, the variant of MiSoSouP for computing an approximation of the top-k subgroups in $\mathcal D$ w.r.t. 1/2quality and with generality $g_{\mathcal{D}}(A) \geq \sigma$, where σ is a user-defined threshold. Let \mathcal{L}_{σ} be the set of subgroups A in \mathcal{L} with $g_{\mathcal{D}}(A) \geq \sigma$. Assume to rank the subgroups in \mathcal{L}_{σ} in decreasing order according to their 1/2-quality in \mathcal{D} , ties broken arbitrarily. Let k > 0 be an integer and let ${\bf r}_{\mathcal{D}}^{(1/2)}(k)$ be the p-quality of the k-th subgroup in the ranking. We then define

$$\mathsf{TOP}_{1/2}(k,\sigma,\mathcal{D}) = \left\{ A \in \mathcal{L}_\sigma \ : \ \mathsf{q}_{\mathcal{D}}^{(1/2)}(A) \geq \mathsf{r}_{\mathcal{D}}^{(1/2)}(k) \right\} \ .$$

The additional constraint on the generality of the subgroups is needed for technical purposes of the analysis. Other algorithms based on sampling for computing approximations of the original set $\mathsf{TOP}_{1/2}(k,\mathcal{D})$ [29] do not require this additional constraint but they also do not actually offer the promised quality guarantees (see the supplementary materials [28]).

The guarantees offered by MiSoSouP-1/2 take into account the additional constraint as follows.

Definition A.3. Let $\varepsilon \in (0, 3/4\sigma)$. A ε -approximation to the set $\mathsf{TOP}_{1/2}(k, \sigma, \mathcal{D})$ is a set \mathcal{B} of pairs (A, q_A) where A is a subgroup

- (1) for any $A \in \mathsf{TOP}_{1/2}(k, \sigma, \mathcal{D})$, there is a $(A, q_A) \in \mathcal{B}$;
- (2) there is no pair $(A, q_A) \in \mathcal{B}$ such that $A \in \mathcal{L}_{\sigma}$ and q $_{\mathcal{D}}^{(1/2)}(A) < \frac{1}{4}r_{\mathcal{D}}^{(1/2)}(k) - \varepsilon;$ (3) there is no pair $(A, q_A) \in \mathcal{B}$ such that $g_{\mathcal{D}}(A) < \sigma - \varepsilon/2;$ (4) for each pair $(A, q_A) \in \mathcal{B}$ with $A \in \mathcal{L}_{\sigma}, \frac{1}{\sqrt{2}}q_A - \varepsilon/2 \le$
- $q_{\mathcal{O}}^{(1/2)}(A) \le 2q_A + \varepsilon/2.$

As for p = 1, 2, an ε -approximation can be used as a set of candidates for $TOP_{1/2}(k, \sigma, \mathcal{D})$, as it contains a pair (A, q_A) for each subgroup *A* in this set.

The following lemma shows that, similarly to the 2-quality, a bound to the approximate 1/2-qualities on S, for subgroups A in \mathcal{L}_{σ} , is obtained by combining a bound on the deviations of the values taken by the functions in ${\cal G}$ (defined in Section A.1) on ${\cal S}$ from their values on \mathcal{D} , together with a bound on the deviations of the approximate 1-qualities on ${\mathcal S}$ of all subgroups in ${\mathcal L}_\sigma$ and a minor requirement on the relationship between σ and ε .

LEMMA A.4. If

- (1) $\sup_{A \in \mathcal{L}_{\sigma}} |g_{\mathcal{S}}(A) g_{\mathcal{D}}(A)| \leq \frac{\varepsilon}{4}$; and
- (2) $\sup_{A \in \mathcal{L}_{\sigma}} \left| \tilde{\mathsf{q}}_{\mathcal{S}}^{(1)}(A) \mathsf{q}_{\mathcal{D}}^{(1)}(A) \right| \leq \frac{\varepsilon \sqrt{\sigma}}{4}$; and

- (1) $\sup_{A \in \mathcal{L}_{\sigma}} \left| \tilde{\mathsf{q}}_{\mathcal{S}}^{(1/2)}(A) 2\mathsf{q}_{\mathcal{D}}^{(1/2)}(A) \right| \leq \frac{\varepsilon}{2}; and$ (2) $\sup_{A \in \mathcal{L}_{\sigma}} \left| \mathsf{q}_{\mathcal{D}}^{(1/2)}(A) / \sqrt{2} \tilde{\mathsf{q}}_{\mathcal{S}}^{(1/2)}(A) \right| \leq \frac{\varepsilon}{2}.$

PROOF. We prove the general case for positive reals η_0 and η_g < 3/4. Assume $\sup_{A \in \mathcal{L}_{\sigma}} |g_{\mathcal{S}}(A) - g_{\mathcal{D}}(A)| \le \eta_g$, $\sup_{A\in\mathcal{L}_{\sigma}}\left|\tilde{\mathsf{q}}_{S}^{(1)}(A)-\mathsf{q}_{\mathcal{D}}^{(1)}(A)\right|\leq\eta_{\mathsf{q}}.$ From the hypothesis it holds,

for any $A \in \mathcal{L}_{\sigma}$,

$$\begin{split} \tilde{q}_{\mathcal{S}}^{(1/2)}(A) &= \tilde{q}_{\mathcal{S}}^{(1)}(A) / \sqrt{g_{\mathcal{S}}(A)} \leq \frac{q_{\mathcal{D}}^{(1)}(A) + \eta_{q}}{\sqrt{g_{\mathcal{D}}(A) - \eta_{g}}} \\ &\leq \frac{q_{\mathcal{D}}^{(1)}(A)}{\sqrt{g_{\mathcal{D}}(A) - \eta_{g}}} + \frac{\eta_{q}}{\sqrt{g_{\mathcal{D}}(A) - \eta_{g}}} \\ &\leq 2q_{\mathcal{D}}^{(1/2)}(A) + 2\frac{\eta_{q}}{\sqrt{g_{\mathcal{D}}(A)}} \\ &\leq 2q_{\mathcal{D}}^{(1/2)}(A) + 2\frac{\eta_{q}}{\sqrt{\sigma}}, \end{split}$$

where the second inequality follows from

$$\mathsf{g}_{\mathcal{D}}(A) - \eta_\mathsf{g} \geq \mathsf{g}_{\mathcal{D}}(A) - \frac{3}{4} \mathsf{g}_{\mathcal{D}}(A) = \frac{\mathsf{g}_{\mathcal{D}}(A)}{4} \ .$$

In addition, again from the hypothesis, for any $A \in \mathcal{L}_{\sigma}$ it holds

$$\begin{split} \tilde{q}_{\mathcal{S}}^{(1/2)}(A) &= \tilde{q}_{\mathcal{S}}^{(1)}(A)/\sqrt{g_{\mathcal{S}}(A)} \geq \frac{q_{\mathcal{D}}^{(1)}(A) - \eta_{q}}{\sqrt{g_{\mathcal{D}}(A) + \eta_{g}}} \\ &\geq \frac{q_{\mathcal{D}}^{(1)}(A)}{\sqrt{g_{\mathcal{D}}(A) + \eta_{g}}} - \frac{\eta_{q}}{\sqrt{g_{\mathcal{D}}(A) + \eta_{g}}} \\ &\geq \frac{q_{\mathcal{D}}^{(1)}(A)}{\sqrt{2}\sqrt{g_{\mathcal{D}}(A)}} - \frac{\eta_{q}}{\sqrt{g_{\mathcal{D}}(A)}} \\ &\geq \frac{1}{\sqrt{2}}q_{\mathcal{D}}^{(1/2)}(A) - \frac{\eta_{q}}{\sqrt{\sigma}}, \end{split}$$

where the third inequality follows from $\eta_g \leq \frac{3}{4} g_{\mathcal{D}}(A)$.

The thesis follows by setting $\eta_g = \frac{\varepsilon}{4}$ and $\eta_q = \frac{\varepsilon\sqrt{\sigma}}{4}$.

A.2.1 The algorithm. We now describe MiSoSouP-1/2. The input is a tuple $(\varepsilon, \delta, k, \mathcal{D}, \sigma)$, where ε, δ, k , and \mathcal{D} are the same as in MiSoSouP-1 and MiSoSouP-2, while σ is a minimum generality threshold for the subgroups of interest. In addition, MiSoSouP-1/2 requires that $\varepsilon \leq \frac{3}{4}\sigma$.

After creating a sample of ${\mathcal S}$ of size

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

MiSoSouP-1/2 runs on $\mathcal S$ a variant of an exact algorithm for subgroup discovery that uses $\tilde{\mathfrak q}^{(1/2)}$ as interesting measure. Let $\tilde{\mathfrak r}_{\mathcal S}^{(1/2)}(k)$ be the top-k highest approximate 1/2-quality on $\mathcal S$ for groups A with $g_{\mathcal S}(A) \geq \sigma - \frac{\varepsilon}{4}$, ties broken arbitrarily. The output set $\mathcal B$ is defined as

$$\mathcal{B} = \left\{ \left(A, \tilde{q}_{\mathcal{S}}^{(1/2)}(A) \right) : g_{\mathcal{S}}(A) \ge \sigma - \varepsilon/4, \\ \tilde{q}_{\mathcal{S}}^{(1/2)}(A) + (\varepsilon/2) \ge \tilde{r}_{\mathcal{S}}^{(1/2)}(k) \right\} .$$

The following establishes the theoretical guarantees of MiSo-SouP-1/2.

Theorem A.5. With probability at least 1 – δ (over its runs), Mi-SoSouP-1/2 outputs an ε-approximation to TOP_{1/2}(k, σ , \mathcal{D}).

Sketch. The proof follows the same lines as the proof for Theorem A.2, but leveraging on Lemma A.4 instead of Lemma 4.5. $\ \Box$

B ADDITIONAL THEORETICAL RESULTS

We show here the proof for Theorem 4.2. We first recall the two-tailed Hoeffding's inequality [8].

Theorem B.1. Let f be a function from a domain \mathcal{Y} to $[a,b] \subseteq \mathbb{R}$. Let $\mathcal{S} = (x_1,\ldots,x_\ell)$ be a collection of independent samples from \mathcal{Y} , and let $\xi \in (0,1)$. Then

$$\Pr\left(|\mathsf{m}_{\mathcal{S}}(f) - \mathbb{E}\left[\mathsf{m}_{\mathcal{S}}(f)\right]| \geq \xi\right) \leq 2\exp\left(-\frac{n\xi^2}{(b-a)^2}\right) \ .$$

Then Theorem 4.2 is a straightforward application of Theorem. B.1 (using $\varepsilon/4$ as ξ , and the fact that b-a=1 for the functions in \mathcal{P}) and the union bound [17, Lemma 1.2].

A similar quantity can be obtained for the 2-quality through an additional application of Hoeffding's inequality to bound the deviation of the estimation of the generality from its expectation, and an application of the union bound.

Theorem B.2. Let
$$\delta \in (0, 1)$$
, $\varepsilon \in (0, 1)$, and $k \ge 1$. Let

$$\xi = \sqrt{1 + \varepsilon/4} - 1 \ .$$

With probability at least $1 - \delta$, if S is a collection of

$$|S| \ge \frac{1}{\xi^2} \left(\ln |\mathcal{L}| + \ln \frac{4}{\delta} \right)$$
 (15)

transactions sampled uniformly at random with replacement from \mathcal{D} , then

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

is an ε -approximation top $TOP_2(k, \mathcal{D})$.

Proof (Sketch). With probability at least 1 – δ it holds simultaneously that

$$\sup_{A \in \mathcal{L}} |\tilde{\mathsf{q}}_{\mathcal{S}}^{(1)}(A) - \mathsf{q}_{\mathcal{D}}^{(1)}(A)| \le \xi$$

and

$$\sup_{A \in \mathcal{L}} |g_{\mathcal{S}}(A) - g_{\mathcal{D}}(A)| \le \xi .$$

An application of Lemma A.1 with $\eta_g = \eta_q = \xi$ concludes the proof.

Obtaining an upper bound for the 1/2-quality is not straightforward, but it would be interesting for completeness and to actually allow for a corrected version of GSS, as discussed in the previous section.

C ON THE CORRECTNESS OF THE **GSS** ALGORITHM

In this section we present our concerns on the correctness of the GSS algorithm by Scheffer and Wrobel [29]. We borrow the same notation used in that work.

C.1 Random stopping time and hypothesis sets

The proofs of [29, Lemmas 13 and 14] do not appear to be correct. Let's start with the proof for [29, Lemma 14] first, as it is easier to explain and it will clarify the situation for [29, Lemma 13]. The issue is that the value i_{max} is a random variable, and so is the set $H_{i_{max}}$, and thus its size. All these quantities are functions of the sequence of random variables $(t_i)_{i\geq 1}$, where t_i is the transaction

sampled by the algorithm at time i. In [29, Lemma 14], all these quantities are assumed to be fixed, i.e., the results are obtained conditioned on the realized values of i_{max} and $H_{i_{max}}$. One may wish to believe that it is therefore sufficient to apply the law of total probability over all possible values of i_{max} and $H_{i_{max}}$ [17, Thm. 1.6], and given that each conditional probability is bounded by $\delta/2$, then so is the unconditional probability. As observed by Borassi and Natale [3, Section 3], this approach is not justified a priori. The solution presented by Borassi and Natale [3, Section 2], although for a different problem, can only partially be imported to "save" GSS, as it does not solve the problem that the set H_i of hypotheses under consideration at iteration i is a random variable for every i > 1. One may be tempted to try to fix the correctness of the algorithm, at least as far as it concerns this issue, by removing the possibility for the algorithm to stop when $E(i, \delta/(2|H_i|))$ is less than or equal to $\varepsilon/2$ (third condition on line 3 of the pseudocode in [29, Table 1]), and replace it with a condition that is satisfied when the number of sampled transactions is equal to M (defined on line 2 of [29, Table 1]), but these changes would not be sufficient to guarantee the correctness of the algorithm, and additional changes must be made, as we discuss in Section C.2.

For more details on the topic of randomly stopped sequences of random variables, we refer the reader to the book by De La Peña and Giné [4, Ch. 2] and for recent developments to the paper by Zhao et al. [37].

The issue with [29, Lemma 13] is similar to the one described above: the event in the probability on the line above [29, Equation 131] is defined conditioned on the sets H_i , but this conditioning must be justified and handled appropriately. In order to try to fix this issue, one could consider the worst case when all the H_i equal H. Then the assumption A1 would be modified to have |H| instead of $|H_i|$ and the same modification would be made in the algorithm on lines 3.e.i and 3.e.ii in [29, Table 1], and to [29, Equations 85 and 104]. These changes are not sufficient and must be complemented with those we discuss in the following section.

C.2 Use of the Chernoff bounds

Scheffer and Wrobel [29, Section 4.1] discuss how to use Chernoff bounds [17, Chapter 4] to compute a probabilistic tail bound for the deviation of a relative frequency (i.e., a sample average of a 0–1 binary function) from its expectation. The function $E(m,\delta)$ in [29, Equation 4] gives a value such that the probability that a sample average computed from a sample of m transactions deviates from its expectation by more than $E(m,\delta)$ is at most δ , as shown in [29, Equations 5–7].

The correctness of the above statement, i.e., of the properties of $E(m,\delta)$ depends crucially on the fact that the sample average is the average of m values. This is definitively the case for the functions presented in [29, Section 4.1], but not for the functions presented in [29, Sections 4.2, 4.3, 4.4]. This fact is recognized by Scheffer and Wrobel [29], who develop sequences of insightful inequalities to show how to upper bound the probability that a sample estimate of the p-quality, $p \in \{1/2, 1, 2\}$, deviates from its expectations by more than some quantity with a sum of the probabilities that the sample

estimates of the generality and the usefulness deviate from their expectation by more than some other quantities. The derivations of these upper bound are presented in [29, Equation 16–22] for the 1-quality, [29, Equation 36–43] for the 2-quality, ¹¹ and [29, Equation 59–67] for the 1/2-quality.

The issue in these derivations is that Scheffer and Wrobel [29] consider the sample estimate for the unusualness (which they denote as \hat{p}) as the average of a 0-1 function over the m elements in the sample (the function is 0 if the target attribute is 0, 1 otherwise), but this is not correct. For a subgroup $A \in \mathcal{L}$, one could see \hat{p} of A as the average of such 0-1 function only over the cover of A on the sample, i.e., over at most m transactions, but potentially and often many fewer than m. The consequences are quite impactful. For example, the rightmost probability in [29, Equation 42] is (implicitly) upper bounded in [29, Equation 43] using an exponential quantity obtained from the Chernoff bound, but this quantity is valid only for averages of 0-1 functions over m elements, which \hat{p} , as discussed, is not. Essentially the same issue is observed in the passage between [29, Equation 63] and [29, Equation 64], and in the passage between [29, Equation 21] and [29, Equation 22]. Note that we solve these issue by defining the function ρ_A , $A \in \mathcal{L}$, as a non-binary function over all transactions, not just those in the cover of A.

Because of the issues mentioned in the previous paragraph, the "instantiation" of the GSS algorithm for the p-qualities are not correct. One can instead use the function $\rho_A(t)$ defined in (2): its average over all transactions in the sample is an estimate for the 1-quality (see Section 4.1), and this can be combined with the sample average of the generality g_A to obtain an estimate for the 2-quality, as we do in Section A.1. Fixing the result for the 1/2-quality seems more complicate, as it was also deriving MiSoSouP-1/2.

Additionally, instead of using the Chernoff bound to compute tail bounds for the sample estimation of unusualness, one must use Hoeffding's inequality, as we discuss in Section 4.1.3.

D ADDITIONAL EXPERIMENTAL RESULTS

In this section we present additional experimental results that did not fit in the main part of the paper.

D.1 Additional results for p=1

See tables 4 to 8.

D.2 Results for p=2

We now discuss the results for p=2. Most of the results are qualitatively similar to those for p=1, so we only give additional details where the results differ.

D.2.1 Sample size reduction and speed-up. The results for the sample size and the runtime are reported in Table 9. We compare the performances of MiSoSouP-2 with those of UB-2, which uses a sample size computed as $\frac{1}{\left(\sqrt{1+\epsilon/4}-1\right)^2}\left(\ln|\mathcal{L}|+\ln\frac{2}{\delta}\right)$. We can

see that the improvement of MiSoSouP-2 over UB-2 in terms of the used sample size is similar to the case for p = 1. In absolute,

 $^{^{10}}$ To be specific, i_{max} is a *stopping time* [17, Section 12.2] for the sequence of random variables $(t_i)_{i\geq 1}$.

 $^{^{11} \}mbox{There}$ is a typo in the second line of [29, Equation 41]: the ">" sign should be "<".

Table 4: Accuracy (absolute error) evaluation – Car – p = 1

			Absol	ute error ($\times 10^{4}$)	
k	$\frac{\varepsilon}{4} \times 10^4$	Min.	1 st Q.	Median	3 rd Q.	Max
	125	< 0.01	0.32	0.76	1.87	25.50
10	50	0.01	1.14	2.48	4.50	8.20
10	25	0.66	2.69	3.44	5.10	10.78
	18.75	0.01	0.77	1.88	2.61	4.45
	125	< 0.01	0.32	0.76	1.88	25.50
50	50	< 0.01	0.13	0.30	0.74	8.20
	25	< 0.01	0.95	1.81	2.87	10.78
	18.75	< 0.01	0.56	1.13	2.07	4.45
	125	< 0.01	0.32	0.76	1.88	25.50
100	50	< 0.01	0.14	0.32	0.72	8.20
100	25	< 0.01	0.46	0.99	1.89	10.78
	18.75	< 0.01	0.43	0.84	1.46	4.98
	125	< 0.01	0.32	0.76	1.88	25.50
200	50	< 0.01	0.14	0.32	0.72	8.20
200	25	< 0.01	0.06	0.14	0.42	10.78
	18.75	< 0.01	0.26	0.60	1.09	4.98
	125	< 0.01	0.32	0.76	1.88	25.50
500	50	< 0.01	0.14	0.32	0.73	8.20
300	25	< 0.01	0.07	0.15	0.36	10.78
	18.75	< 0.01	0.05	0.11	0.26	4.98
	125	< 0.01	0.32	0.76	1.88	25.50
1000	50	< 0.01	0.14	0.32	0.73	8.20
1000	25	< 0.01	0.07	0.15	0.36	10.78
	18.75	< 0.01	0.05	0.11	0.26	4.98
	125	< 0.01	0.32	0.76	1.88	25.50
2000	50	< 0.01	0.14	0.32	0.73	8.20
2000	25	< 0.01	0.07	0.15	0.36	10.78
	18.75	< 0.01	0.05	0.11	0.26	4.98

the sample sizes are actually quite larger than those used by MiSo-SouP-1 and UB-1, due to the different dependency on ε . When comparing the runtimes, it is now even clearer than in the case for p=1 how the runtime improvement converges fast to the improvement in the sample size.

D.2.2 Accuracy. On the six rightmost columns of Table 9 we present statistics on the absolute error in the estimation of the 2-quality of the subgroups in the output of MiSoSouP-2 for k=1000. Additional results, qualitatively similar, are available in App. D. A comparison of the Max. and the $\varepsilon/4$ columns reveals that MiSoSouP-2 is between 4 and 13 times more accurate than guaranteed, even more than MiSoSouP-1. The whole distribution of the error is actually more concentrated towards zero than it was the case for p=1. This fact can be explained by the additional looseness in the derivation of the sample size used by MiSoSouP-2.

D.2.3 Output properties. We report the results on the False Positives included in the output of MiSoSouP-2 in Table 10 for the Car dataset. In this dataset, the distribution of the FP is denser than in the Mushroom dataset presented in Table 3, therefore the

Table 5: Accuracy (absolute error) evaluation – Mushroom – p = 1

					4.	
			Absol	ute error (
k	$\frac{\varepsilon}{4} \times 10^4$	Min.	1 st Q.	Median	3 rd Q.	Max
	125	18.72	22.96	29.99	35.95	39.19
10	50	7.29	7.70	13.51	15.96	16.37
10	25	0.16	0.55	0.74	1.06	2.32
	18.75	4.46	5.30	5.41	5.64	6.09
	125	5.82	14.92	20.23	25.12	39.19
50	50	2.16	8.73	13.49	15.98	18.83
30	25	0.16	0.93	2.32	2.91	4.7
	18.75	3.01	3.95	5.00	6.09	6.4
	125	3.79	12.90	20.23	26.09	44.3
100	50	1.36	4.86	9.14	13.89	18.83
100	25	0.05	1.37	2.53	3.76	4.7
	18.75	2.44	3.85	4.54	5.30	6.79
	125	2.07	8.60	17.17	23.29	45.7
200	50	1.36	4.14	6.76	11.36	19.9
200	25	0.05	1.47	2.87	3.76	5.3
	18.75	2.44	3.76	4.46	5.20	8.5
	125	2.07	8.14	12.56	20.77	45.7
500	50	0.40	5.31	6.56	8.41	22.5
300	25	0.05	1.81	3.27	4.31	5.53
	18.75	0.86	3.56	4.10	4.88	8.8
	125	0.17	8.22	13.35	21.09	45.7
1000	50	0.40	5.63	6.56	8.45	22.8
1000	25	0.05	2.53	4.27	4.63	7.4
	18.75	0.05	3.41	3.77	4.43	8.8
	125	0.01	6.15	11.67	17.09	45.7
2000	50	0.02	4.14	6.56	9.10	22.8
2000	25	0.02	1.73	3.28	4.38	7.45
	18.75	< 0.01	2.59	3.56	4.30	8.8

percentages are often high. It is in such cases that the choice of k reveals its arbitrary nature w.r.t. the qualities of the subgroups considered of interest, and this nature is made visible but not caused by the properties of MiSoSouP-2.

-p = 1

Table 6: Accuracy (absolute error) evaluation - Tic-Tac-Toe

-			Absol	ute error (×10 ⁴)	
k	$\frac{\varepsilon}{4} \times 10^4$	Min.	1 st Q.	Median	3 rd Q.	Max.
	125	0.03	3.95	8.59	16.19	48.88
10	50	< 0.01	2.17	4.66	9.38	28.58
10	25	0.43	1.37	2.46	4.43	5.91
	18.75	0.09	0.48	1.35	1.75	5.14
	125	< 0.01	0.82	1.93	3.90	48.88
50	50	< 0.01	1.73	3.68	6.70	28.58
30	25	0.01	1.03	1.73	3.02	6.01
	18.75	0.04	0.56	1.18	1.73	5.14
	125	< 0.01	0.85	1.99	3.95	48.88
100	50	< 0.01	1.65	3.31	5.91	28.58
100	25	0.01	0.80	1.36	2.44	6.01
	18.75	0.04	0.66	1.18	1.95	5.14
	125	< 0.01	0.86	2.04	4.07	48.88
200	50	< 0.01	1.11	2.29	3.92	28.58
200	25	0.01	0.73	1.35	2.29	6.01
	18.75	< 0.01	0.49	1.01	1.66	5.14
	125	< 0.01	0.87	2.04	4.11	48.88
500	50	< 0.01	0.32	0.74	1.52	28.58
300	25	< 0.01	0.41	0.87	1.63	6.01
	18.75	< 0.01	0.35	0.79	1.36	5.14
	125	< 0.01	0.87	2.04	4.11	48.88
1000	50	< 0.01	0.34	0.77	1.53	28.58
1000	25	< 0.01	0.32	0.68	1.21	7.86
	18.75	< 0.01	0.29	0.64	1.11	5.14
	125	< 0.01	0.87	2.04	4.11	48.88
2000	50	< 0.01	0.34	0.78	1.56	28.58
2000	25	< 0.01	0.17	0.39	0.76	7.86
	18.75	< 0.01	0.21	0.44	0.80	5.14

Table 7: Output evaluation for Car – p = 1

				% of Acceptable
ε	k	$ TOP_1(k,\mathcal{D}) $	False Pos.	False Positives
	10	10	3218	99.41
	50	54	3188	99.84
	100	105	3139	99.90
0.05	200	211	3034	99.93
	500	549	2696	99.93
	1000	1340	1905	99.90
	2000	2357	888	99.78
	10	10	74	2.35
	50	54	2599	81.58
	100	105	3051	97.26
0.02	200	211	2970	97.99
	500	549	2679	99.48
	1000	1340	1900	99.74
	2000	2357	883	99.44
	10	10	15	20.00
	50	54	157	6.04
	100	105	551	18.06
0.01	200	211	2392	80.54
	500	549	2604	97.20
	1000	1340	1841	96.89
	2000	2357	824	93.32
	10	10	11	40.74
	50	54	77	13.25
	100	105	301	11.81
0.0075	200	211	609	20.69
	500	549	2376	90.27
	1000	1340	1816	96.19
	2000	2357	799	91.73

Table 8: Output evaluation for Tic-Tac-Toe -p = 1

Table 9: Sample size, runtime, and accuracy (absolute error) evaluation for MiSoSouP-2

							Absolute error ($\times 10^4$) (for $k = 1000$)				
Dataset	ε	$ \mathcal{S} $	Reduction w.r.t. UB-2	Runtime (s)	Reduction w.r.t. UB-2	Min.	1 st Q.	Median	3 rd Q.	Max.	$\varepsilon/4$
	0.05	213873	-29.49%	2.19	-8.07%	< 0.01	0.20	0.45	1.10	38.30	125
O	0.02	1331733		5.86	-20.20%	< 0.01	0.07	0.17	0.41	9.30	50
Car	0.01	5320295		17.46	-28.43%	< 0.01	0.04	0.09	0.20	6.97	25
	0.0075	9455351		30.30	-25.10%	< 0.01	0.03	0.07	0.16	5.46	18.75
	0.05	419951	-15.15%	573.03	-13.29%	< 0.01	0.04	0.09	0.26	20.21	125
Mushroom	0.02	2614931		3446.71	-15.11%	0.01	0.18	0.42	1.60	4.72	50
Mushroom	0.01	10446693		13562.23	-14.85%	0.01	0.42	0.60	0.68	2.02	25
	0.0075	18566105		23857.04	-15.03%	0.03	1.03	1.09	1.15	1.74	18.75
	0.05	291152	-21.34%	11.52	-18.04%	< 0.01	< 0.01	0.01	0.02	10.77	125
Tic-Tac-Toe	0.02	1812932		65.82	-20.50%	< 0.01	< 0.01	< 0.01	0.01	3.73	50
	0.01	7242694		244.89	-20.02%	< 0.01	< 0.01	< 0.01	< 0.01	1.87	25

Table 10: Output evaluation for MiSoSouP-2 on Car

Table 11: Output evaluation for Mushroom – p = 2

ε	k	$ TOP_1(k,\mathcal{D}) $	FP	% of all Acceptable FP	ε	k	$ TOP_1(k,\mathcal{D}) $	False Pos.	% of Acceptable False Positives
	10	10	6195	98.95		10	10	140	22.01
	50	54	6212	99.92		50	51	386	21.53
	100	105	6161	99.92		100	103	490	5.59
0.05	200	211	6058	99.97	0.05	200	201	672	0.67
	500	500	5769	99.97		500	501	4191	4.21
	1000	1019	5250	99.96		1000	1010	412867	417.08
	2000	2808	3461	99.94		2000	2000	422868	431.50
	10	10	60	0.97		10	10	24	32.88
	50	54	5623	90.55		50	51	54	18.82
	100	105	6075	98.60		100	103	235	65.10
0.02	200	211	5995	99.01	0.02	200	201	209	62.02
	500	500	5752	99.76		500	501	837	44.22
	1000	1019	5245	99.90		1000	1010	856	11.41
	2000	2808	3456	99.86		2000	2000	9503	9.70
	10	10	17	22.67		10	10	19	79.17
	50	54	164	2.92		50	51	18	38.30
	100	105	789	12.99		100	103	108	41.70
0.01	200	211	5420	90.42	0.01	200	201	99	47.60
	500	500	5677	98.70		500	501	145	17.32
	1000	1019	5161	98.40		1000	1010	486	55.16
	2000	2808	3397	98.29		2000	2000	1482	15.70
	10	10	11	40.74		10	10	19	100.00
	50	54	74	11.42		50	51	12	37.50
	100	105	306	5.49		100	103	102	63.75
0.0075	200	211	1030	17.26	0.0075	200	201	33	18.13
	500	500	5448	95.50		500	501	97	25.94
	1000	1019	5156	98.53		1000	1010	442	71.64
	2000	2808	3372	97.91		2000	2000	952	23.29

Table 12: Output evaluation for Tic-Tac-Toe -p = 2

ε	k	$ TOP_1(k,\mathcal{D}) $	False Pos.	% of Acceptable False Positives
	10	13	38343	100.00
	50	51	38305	100.00
	100	107	38249	100.00
0.05	200	213	38143	100.00
0.03	500	515	37841	100.00
	1000	1001	37355	100.00
	2000	2045	36311	100.00
	10	13	38317	99.93
	50	51	38301	99.99
	100	107	38245	99.99
0.02	200	213	38139	99.99
	500	515	37839	99.99
	1000	1001	37355	100.00
	2000	2045	36311	100.00
	10	13	40	0.10
	50	51	38273	99.93
	100	107	38233	99.97
0.01	200	213	38127	99.97
	500	515	37827	99.97
	1000	1001	37343	99.97
	2000	2045	36299	99.97

Table 13: Accuracy (absolute error) evaluation – Mushroom – p=2

					45	
			Absol	ute error (
k	$\frac{\varepsilon}{4} \times 10^4$	Min.	1 st Q.	Median	3 rd Q.	Max
	125	2.20	10.17	12.86	14.45	20.21
10	50	0.05	0.96	1.48	2.41	4.27
10	25	0.01	0.21	0.36	0.43	0.58
	18.75	0.22	0.44	0.68	0.83	1.17
	125	1.08	8.19	12.80	13.69	20.2
50	50	0.05	1.47	2.41	3.08	4.4
30	25	0.01	0.09	0.36	0.49	1.6
	18.75	0.22	0.45	0.71	1.00	1.6
	125	1.08	5.60	10.68	13.41	20.2
100	50	0.05	1.41	1.97	2.71	4.7
100	25	0.01	0.30	0.51	0.80	1.6
	18.75	0.22	0.74	1.07	1.29	1.7
	125	1.08	4.75	5.89	12.88	20.2
200	50	0.05	1.48	1.97	2.65	4.7
200	25	0.01	0.23	0.49	0.68	1.6
	18.75	0.22	0.76	1.07	1.29	1.7
	125	< 0.01	1.43	2.57	4.81	20.2
500	50	0.01	0.17	0.32	1.68	4.7
300	25	0.01	0.24	0.51	0.88	2.0
	18.75	0.05	0.79	1.08	1.25	1.7
	125	< 0.01	0.04	0.09	0.26	20.2
1000	50	0.01	0.18	0.42	1.60	4.7
1000	25	0.01	0.42	0.60	0.68	2.0
	18.75	0.03	1.03	1.09	1.15	1.7
	125	< 0.01	0.04	0.09	0.26	31.2
2000	50	< 0.01	0.09	0.28	0.50	4.7
2000	25	< 0.01	0.19	0.44	0.64	2.0
	18.75	< 0.01	0.31	0.55	1.09	1.7

Table 14: Accuracy (absolute error) evaluation – Car – p = 2

		Absolute error (×10 ⁴)							
k	$\frac{\varepsilon}{4} \times 10^4$	Min.	1 st Q.	Median	3 rd Q.	Max.			
10	125	< 0.01	0.20	0.45	1.07	38.30			
	50	0.02	1.27	2.85	5.47	9.30			
	25	0.18	1.15	1.99	3.10	5.80			
	18.75	0.24	0.69	1.78	2.94	5.46			
50	125	< 0.01	0.20	0.45	1.10	38.30			
	50	< 0.01	0.07	0.16	0.38	9.30			
	25	< 0.01	0.56	1.33	2.14	6.97			
	18.75	0.01	0.59	1.34	2.06	5.46			
100	125	< 0.01	0.20	0.45	1.10	38.30			
	50	< 0.01	0.07	0.17	0.40	9.30			
100	25	< 0.01	0.30	0.68	1.29	6.97			
	18.75	0.01	0.35	0.75	1.48	5.46			
200	125	< 0.01	0.20	0.45	1.10	38.30			
	50	< 0.01	0.07	0.17	0.41	9.30			
200	25	< 0.01	0.04	0.08	0.18	6.97			
	18.75	< 0.01	0.20	0.45	0.86	5.46			
	125	< 0.01	0.20	0.45	1.10	38.30			
500	50	< 0.01	0.07	0.17	0.41	9.30			
	25	< 0.01	0.04	0.09	0.20	6.97			
	18.75	< 0.01	0.03	0.07	0.15	5.46			
	125	< 0.01	0.20	0.45	1.10	38.30			
1000	50	< 0.01	0.07	0.17	0.41	9.30			
	25	< 0.01	0.04	0.09	0.20	6.97			
	18.75	< 0.01	0.03	0.07	0.16	5.46			
	125	< 0.01	0.20	0.45	1.10	38.30			
2000	50	< 0.01	0.07	0.17	0.41	9.30			
	25	< 0.01	0.04	0.09	0.20	6.97			
	18.75	< 0.01	0.03	0.07	0.16	5.46			

Table 15: Accuracy (absolute error) evaluation – Tic-Tac-Toe – p=2

k		Absolute error (×10 ⁴)					
	$\frac{\varepsilon}{4} \times 10^4$	Min.	1 st Q.	Median	3 rd Q.	Max	
10	125	< 0.01	< 0.01	0.01	0.02	10.77	
	50	< 0.01	< 0.01	< 0.01	0.01	3.73	
	25	0.01	0.13	0.24	0.39	1.87	
50	125	< 0.01	< 0.01	0.01	0.02	10.77	
	50	< 0.01	< 0.01	< 0.01	0.01	3.73	
	25	< 0.01	< 0.01	< 0.01	< 0.01	1.87	
100	125	< 0.01	< 0.01	0.01	0.02	10.77	
	50	< 0.01	< 0.01	< 0.01	0.01	3.73	
	25	< 0.01	< 0.01	< 0.01	< 0.01	1.87	
200	125	< 0.01	< 0.01	0.01	0.02	10.77	
	50	< 0.01	< 0.01	< 0.01	0.01	3.73	
	25	< 0.01	< 0.01	< 0.01	< 0.01	1.87	
500	125	< 0.01	< 0.01	0.01	0.02	10.77	
	50	< 0.01	< 0.01	< 0.01	0.01	3.73	
	25	< 0.01	< 0.01	< 0.01	< 0.01	1.87	
1000	125	< 0.01	< 0.01	0.01	0.02	10.77	
	50	< 0.01	< 0.01	< 0.01	0.01	3.73	
	25	< 0.01	< 0.01	< 0.01	< 0.01	1.87	
2000	125	< 0.01	< 0.01	0.01	0.02	10.77	
	50	< 0.01	< 0.01	< 0.01	0.01	3.73	
	25	< 0.01	< 0.01	< 0.01	< 0.01	1.87	