Mining Low-Support Discriminative Patterns from Dense and High-Dimensional Data

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Abstract—Discriminative patterns can provide valuable insights into data sets with class labels, that may not be available from the individual features or the predictive models built using them. Most existing approaches work efficiently for sparse or low-dimensional data sets. However, for dense and high-dimensional data sets, they have to use high thresholds to produce the complete results within limited time, and thus, may miss interesting low-support patterns. In this paper, we address the necessity of trading off the completeness of discriminative pattern discovery with the efficient discovery of low-support discriminative patterns from such data sets. We propose a family of antimonotonic measures named *SupMaxK* that organize the set of discriminative patterns into nested layers of subsets, which are progressively more complete in their coverage, but require increasingly more computation. In particular, the member of *SupMaxK* with $K = 2$, named *SupMaxPair*, is suitable for dense and high-dimensional data sets. Experiments on both synthetic data sets and a cancer gene expression data set demonstrate that there are low-support patterns that can be discovered using *SupMaxPair* but not by existing approaches. Furthermore, we show that the low-support discriminative patterns that are only discovered using *SupMaxPair* from the cancer gene expression data set are statistically significant and biologically relevant. This illustrates the complementarity of *SupMaxPair* to existing approaches for discriminative pattern discovery. The codes and data set for this paper are available at http://vk.cs.umn.edu/SMP/.

Index Terms—Association analysis, discriminative pattern mining, biomarker discovery, permutation test.

1 Introduction

For data sets with class labels, association patterns [2], [43] that occur with disproportionate frequency in some classes versus others can be of considerable value in many applications. Such applications include census data analysis that aims at identifying differences among demographic groups [14], [5] and biomarker discovery, which searches for groups of genes or related entities, that are associated with diseases [8], [39], [1]. We will refer to these patterns as discriminative patterns[1] in this paper, although they have also been investigated under other names [35], such as emerging patterns (EPs) [14] and contrast sets (CSETs) [5]. In this paper, we focus on two-class problems, which can be generalized to multiclass problems as described in [5].

Discriminative patterns have been shown to be useful for improving the classification performance for data sets where combinations of features have better discriminative power than the individual features [9], [13], [47], [10], [15], [30]. More importantly, as discussed in [5], discriminative pattern mining can provide insights beyond classification models. For example, for biomarker discovery from case-control data (e.g., disease versus normal samples), it is important to identify groups of biological entities, such as genes and single-nucleotide polymorphisms (SNPs), that are collectively associated with a certain disease or other phenotypes [1], [50], [38]. Algorithms that can discover a comprehensive set of discriminative patterns are especially useful for domains like biomarker discovery, and such algorithms are the focus of this paper.

The algorithms for finding discriminative patterns usually employ a measure for the discriminative power of a pattern. Such measures are generally defined as a function of the pattern's relative support[2] in the two classes, and can be defined either simply as the ratio [14] or difference [5] of the two supports, or other variations, such as its information gain [9], Gini index, odds ratio [43], etc. In this paper, we use the measure that is defined as the difference of the supports of an item set in the two classes (originally proposed in [5] and used by its extensions [24], [25]). We will refer to this measure as *DiffSup* (formally discussed in Section 2). Given a data set with 0-1 class labels and a *DiffSup* threshold r, the patterns with $DiffSup \geq r$ can be considered as valid discriminative patterns.

To introduce some key ideas about discriminative patterns and make the following discussion easier to follow,

1. The terms "pattern" and "item set" are used interchangeably in this paper.

2. Note that, in this paper, unless specified, the support of a pattern in a class is relative to the number of transactions (instances) in that class, i.e., a ratio between 0 and 1, which can help handle the case of skewed class distributions.

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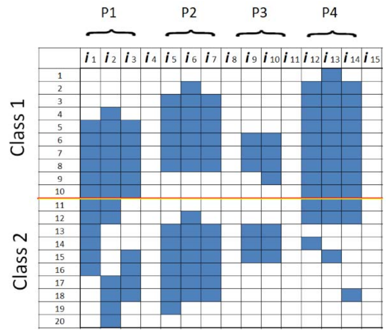

Fig. 1. A sample data set with interesting discriminative patterns (P_1, P_4) and uninteresting patterns (P_2, P_3).

consider Fig. 1, which displays a sample data set[3] containing 15 items (columns) and two classes, each with 10 instances (rows). In the figure, four patterns (sets of binary variables) can be observed: $P_1 = \{i_1, i_2, i_3\}$, $P_2 = \{i_5, i_6, i_7\}$, $P_3 = \{i_9, i_{10}\}$, and $P_4 = \{i_{12}, i_{13}, i_{14}\}$. P_1 and P_4 are interesting discriminative patterns that occur with different frequencies in the two classes, whose *DiffSup* is 0.6 and 0.7, respectively. In contrast, P_2 and P_3 are uninteresting patterns with a relatively uniform occurrence across the classes, both having a *DiffSup* of 0. Furthermore, P_4 is a discriminative pattern whose individual items are also highly discriminative, while those of P_1 are not. Based on support in the whole data set, P_2 is a frequent nondiscriminative pattern, while P_3 is a relatively infrequent nondiscriminative pattern.

Note that the discriminative measures discussed above are generally not antimonotonic as shown by [14], [5], [9]. Take *DiffSup* for instance (while other measures like support ratio, information gain, and odds ratio are not antimonotonic either): although the *DiffSup* of the three items in P_1 are 0, 0, and 0.2, respectively, P_1 has a *DiffSup* of 0.6 as an item set. Due to the lack of antimonotonicity, these measures cannot be directly used in an Apriori framework [2] for exhaustive and efficient pattern mining as can be done for measures like support [2], h-confidence [53], etc. To address this issue, many approaches [29], [28], [55], [11], [9] adopt a two-step strategy (denoted as Group A), where first, a frequent pattern mining algorithm is used to find all (closed) frequent patterns that satisfy a certain support threshold $minsup$ either from the whole data set or from only one of the classes. The patterns found can be further refined using other interestingness measures (e.g., [7], [23], [44]). Then, as postprocessing, *DiffSup* is computed for each of these patterns, based on which discriminative patterns are selected. Note that, in general, these two-step approaches can work even with a very low $minsup$ threshold [49], [9] on relatively sparse or low-dimensional data sets.

However, since these approaches ignore class-label information in the mining process, many frequent patterns discovered in the first step may turn out to have low discriminative power in the second step. For instance, in Fig. 1, the relative supports of P_2 and P_3 in the whole data set are 0.6 and 0.3, respectively, and will be considered as frequent patterns if the support threshold is 0.2. However,

3. The discussion in this paper assumes that the data are binary. Nominal categorical data can be converted to binary data without loss of information, while ordinal categorical data and continuous data can be binarized, although with some loss of magnitude and order information.

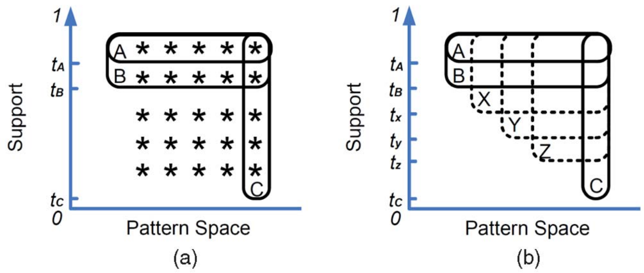

Fig. 2. An Illustration of the coverage of the space of discriminative patterns by different approaches given the same amount of time. The t's on the y-axis represent the lowest support of the patterns that are, respectively, covered by the corresponding approaches (represented by boxes), given the same and fixed amount of time. (a) Box A, B, and C represent the set of patterns discovered by the corresponding approaches in group A, B, and C, respectively. (b) Illustration of the trade-off between the capability to search low-support discriminative patterns in dense and high-dimensional data and the completeness of the pattern discovery. Boxes X, Y, and Z represent three conceptual low-support discriminative pattern mining approaches that discover patterns not found by the approaches in groups A, B, and C. Note that, in this figure, the set of interesting discriminative patterns is the same as that in (a), but the corresponding $*$'s are not shown for the sake of clarity. (a) The limitation of existing approaches. (b) The motivation of the proposed work.

P_2 and P_3 are not discriminative since they both have a *DiffSup* of 0. In particular, in data sets with relatively high density[4] and high dimensionality, a huge number of nondiscriminative patterns like P_2 and P_3 in Fig. 1 may exist. Such patterns may meet the $minsup$ threshold and would be discovered in the first step, but would be found as nondiscriminative patterns in the second step. If a low $minsup$ is used, a huge number of such patterns can reduce the efficiency of both the two steps as discussed in [10]. In such a situation, the two-step approaches have to use a sufficiently high $minsup$ in order to generate the complete set of results within an acceptable amount of time, and thus may miss a large number of highly discriminative patterns that fall below the $minsup$ threshold.

A possible strategy for improving the performance of the two-step approaches is to directly utilize the support of a pattern in the two classes for pruning some nondiscriminative patterns in the pattern mining stage. Indeed, several approaches have been proposed [5], [9], where the antimonotonic upper bounds of discriminative measures, such as *DiffSup*, are used for pruning some nondiscriminative patterns in an Apriori-like framework [2]. This strategy, like the two-step approaches, also guarantees to find the complete set of discriminative patterns with respect to a threshold, although in a more efficient manner. However, in data sets with relatively high density and high dimensionality, there can be a large number of frequent nondiscriminative patterns like P_2 in Fig. 1. Such patterns may not be pruned by these approaches because the upper bounds of the discriminative measures may be weak (technical details in Section 3). Thus, as illustrated in Fig. 2a, these approaches (referred to as group B in the rest of this paper) are able to discover a larger fraction of the interesting discriminative patterns as compared to the two-step approaches. However, they may still miss a lot of highly discriminative patterns, particularly those at low-support levels, given the same

4. The density of a transaction matrix is the percentage of 1s in the transaction-by-item matrix.

fixed amount of time. These low-support patterns are supported by a relatively small number of samples but can still be highly discriminative according to their *DiffSup* value, especially in the case of data sets with skewed class size distributions.

Yet another strategy for discovering a significant subset of the discriminative patterns is to directly use a measure of discriminative power for pruning nondiscriminative patterns [56]. As an instance of such an approach, *DiffSup* can be computed for each candidate pattern α, and if $DiffSup(\alpha) < r$, then α and all its supersets can be pruned in an Apriori-like algorithm [2]. This strategy is computationally more efficient than the two-step approaches, because no patterns with $DiffSup(\alpha) < r$ are generated during the mining process. However, this improved efficiency comes at the cost of not discovering the complete set of discriminative patterns, since *DiffSup* is not antimonotonic [5]. More specifically, the algorithms in this group (referred to as group C in the rest of this paper) may miss interesting discriminative patterns whose individual items are not discriminative (e.g., P_1 in Fig. 1). With respect to the coverage of the set of interesting discriminative patterns, the approaches in this group may be able to discover low-support patterns at the expense of missing a large number of interesting patterns, as illustrated by the stars not included in box C in Fig. 2a. This observation is also reflected in our experimental results (Section 6.2.2).

As can be seen from the discussion above, which is summarized in Fig. 2a, the current approaches face an inherent trade-off when discovering discriminative patterns from a dense and high-dimensional data set. The approaches in groups A and B face challenges with discovering low-support patterns due to their focus on the complete discovery of discriminative patterns satisfying the corresponding thresholds. On the other hand, the approaches in group C sacrifice completeness for the ability of discovering low-support discriminative patterns. This trade-off is expected to be faced by any algorithm for this complex problem, particularly due to the restriction of fixed computational time. In such a scenario, an appropriate approach to discover some of the interesting discriminative patterns missed by the current approaches is to formulate new measures for discriminative power and corresponding algorithms that can progressively explore lower support thresholds for discovering patterns, while trading off completeness to some extent. Such a design is illustrated in Fig. 2b, where boxes X, Y, and Z represent three approaches, which can discover patterns with progressively lower thresholds ($t_x > t_y > t_z$). However, the cost associated with this ability is that of potentially missing some patterns that are at higher support levels. Still, X, Y, and Z can all discover several patterns that are exclusive to only one of them, and can thus play a complementary role to the existing approaches by expanding the coverage of the set of interesting discriminative patterns.

Corresponding to the motivation discussed above, we propose a family of antimonotonic measures of discriminative power named *SupMaxK*. These measures conceptually organize the set of discriminative patterns into nested layers of subsets, which are progressively complete in their coverage, but require increasingly more computation for their discovery. Essentially, *SupMaxK* estimates the *DiffSup* of an item set by calculating the difference of its support in one class and the maximal support among all of its size-K subsets in the other class. The smaller the value of K, the more effective *SupMaxK* is for finding low-support discriminative patterns by effectively pruning frequent nondiscriminative patterns. Notably, due to the antimonotonicity property of all the members of *SupMaxK*, each of them can be used in an Apriori-like framework [2] to guarantee the discovery of all the discriminative patterns with $SupMaxK \geq r$, where r is a user-specified threshold. Given the same (limited) amount of time, the members of this family provide a trade-off between the ability to search for low-support discriminative patterns and the coverage of the space of valid discriminative patterns for the corresponding threshold, as illustrated by the three conceptual approaches X, Y, and Z in Fig. 2b. In particular, we find that a special member with $K = 2$ named *SupMaxPair* is suitable for dense and high-dimensional data. We have designed a framework, named SMP, which uses *SupMaxPair* for discovering discriminative patterns. Carefully designed experiments with both synthetic data sets and a cancer gene expression data set are used to demonstrate that SMP can serve a complementary role to the existing approaches by discovering low support yet highly discriminative patterns from dense and high-dimensional data, when the latter fail to discover them within an acceptable amount of time.

1.1 Contributions of This Paper

The contributions of this paper can be summarized as follows:

1. We address the necessity of trading off the completeness of discriminative pattern discovery with the ability to discover low-support discriminative patterns from dense and high-dimensional data within an acceptable amount of time. For this, we propose a family of antimonotonic measures named *SupMaxK* that conceptually organize the set of discriminative patterns into nested layers of subsets, which are progressively more complete in their coverage, but require increasingly more computation for their discovery.
2. In particular, *SupMaxK* with $K = 2$, named *SupMaxPair*, is a special member of this family that is suitable for dense and high-dimensional data, and can serve a complementary role to the existing approaches by helping to discover low-support discriminative patterns, when the latter fail to discover them within an acceptable amount of time. We designed a framework, named SMP, which uses *SupMaxPair* for discovering discriminative patterns.
3. A variety of experiments with both synthetic data sets and a cancer gene expression data set are presented to demonstrate that there are many patterns with relatively low support that can be discovered by SMP but not by the existing approaches. In particular, these experiments rigorously demonstrate that the low-support discriminative patterns discovered only by SMP from the cancer gene expression data set are statistically significant (via permutation test [18], [42]) and biologically relevant (via comparison with a list of cancer-related genes [21] and a collection of biological gene sets [42] (e.g., pathways)). These are the recognized methods for evaluating the utility of

such patterns for applications such as biomarker discovery [42], [8], [22].

The source codes and data set used in this paper are available at http://vk.cs.umn.edu/SMP/.

2 Basic Terminology and Problem Definition

Let D be a data set with a set of m items, $I = \{i_1, i_2, \dots, i_m\}$, two class labels S_1 and S_2, and a set of n labeled instances (item sets), $D = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$, where $\boldsymbol{x}_i \subseteq I$ is a set of items and $y_i \in \{S_1, S_2\}$ is the class label for $\boldsymbol{x}_i$. The two sets of instances that, respectively, belong to the class S_1 and S_2 are denoted by D^1 and D^2, and we have $|D| = |D^1| + |D^2|$. For an item set $\alpha = \{\alpha_1, \alpha_2, \dots, \alpha_l\}$ where $\alpha \subseteq I$, the set of instances in D^1 and D^2 that contain α are, respectively, denoted by D^1_α and D^2_α. The relative supports of α in classes S_1 and S_2 are $RelSup^1(\alpha) = \frac{|D^1_\alpha|}{|D^1|}$ and $RelSup^2(\alpha) = \frac{|D^2_\alpha|}{|D^2|}$, respectively. $RelSup$ is antimonotonic since the denominator is fixed and the numerator is support of the item set, which is antimonotonic.

The absolute difference of the relative supports of α in D^1 and D^2 is defined originally in [5] and denoted in this paper as *DiffSup*:

$$DiffSup(\alpha) = |RelSup^1(\alpha) - RelSup^2(\alpha)|. \tag{1}$$

An item set α is $r - discriminative$ if $DiffSup(\alpha) \geq r$. The problem addressed by discriminative pattern mining algorithms is to discover all patterns in a data set with $DiffSup \geq r$.

Without loss of generality, we only consider discriminative patterns for the binary-class problem. Our work can be extended to multiple classes as described in [5].

3 Computational Limitations of Current Approaches

As discussed in Section 1, in dense and high-dimensional data, the approaches in groups A and B have to use a relatively high threshold in order to provide the complete result within an acceptable amount of time. In this section, we will show that this limitation is essentially due to the ineffective pruning of frequent nondiscriminative patterns (e.g., P_2 in Fig. 1). Generally, the approaches in group B are relatively more efficient than those in group A, as discussed in Section 1. We use the measure originally proposed in CSET [5] as a representative of group B for this discussion, while a similar discussion also holds for other approaches in group B [9], [34]. In CSET, an upper bound of *DiffSup* is defined as the bigger of the relative supports of a pattern α in D^1 and D^2. In this paper, we denote it as *BiggerSup*:

$$BiggerSup(\alpha) = max(RelSup^1(\alpha), RelSup^2(\alpha)). \tag{2}$$

Lemma 1. *BiggerSup is antimonotonic.*

Proof. Follows from the antimonotonicity of $RelSup$ and the property of the max function. □

Since *BiggerSup* is an upper bound of *DiffSup* [5], and it is also antimonotonic (Lemma 1), CSET [5] uses *BiggerSup* as a pruning measure in a Apriori-like framework, and can discover, given sufficient time and computing resources, the complete set of discriminative patterns (w.r.t a *BiggerSup* threshold). However, by using the bigger one to estimate the difference of the two supports, *BiggerSup* is a weak upper bound of *DiffSup*. For instance, if we want to use CSET to search for $0.4 - discriminative$ patterns in Fig. 1, P_3 can be pruned, because it has a *BiggerSup* of 0.3. However, P_2 cannot be pruned ($BiggerSup(P_2) = 0.6$), even though it is not discriminative ($DiffSup(P_2) = 0$). More generally, *BiggerSup*-based pruning can only prune infrequent nondiscriminative patterns with relatively low support, but not frequent nondiscriminative patterns. Therefore, in dense and high-dimensional data, where a large number of frequent nondiscriminative patterns are expected to exist, CSET with a relatively low *BiggerSup* threshold can often fail to produce the complete results in a reasonable amount of time. Thus, CSET has to set the *BiggerSup* threshold high and may not discover discriminative patterns at lower support that may be of interest. Similar discussion on the limited ability of pruning frequent nondiscriminative patterns also holds for other approaches in groups A and B, i.e., all the two-step approaches, and those based on the information gain upper bound [9], and other statistical metric-based pruning [5], [34].

4 Proposed Approach

As shown above, the limitation of existing approaches is essentially the ineffectiveness of pruning frequent nondiscriminative patterns. Conceptually, to prune frequent nondiscriminative patterns, a new measure should be designed such that a pattern's support in one class can be effectively limited to a relatively smaller number compared to its support in the other class. In this section, we start with such a measure $SupMax1$ in Definition 1, and then extend it to a family of measures *SupMaxK*. Then, we will discuss the relationships between $DiffSup$, *BiggerSup*, and *SupMaxK*. Finally, we will focus on a special member of this family *SupMaxPair* that is suitable for high-dimensional data. Note that, for an item set α, two cases can happen: $RelSup^1(\alpha) \geq RelSup^2(\alpha)$ or $RelSup^1(\alpha) < RelSup^2(\alpha)$. In the following discussion, without loss of generality, we assume $RelSup^1(\alpha) \geq RelSup^2(\alpha)$ for simplicity.

4.1 SupMax1: A Simple Measure to Start with

Definition 1. *The $SupMax1$ of an item set α in D^1 and D^2 is defined as*

$$SupMax1(\alpha) = RelSup^1(\alpha) - max_{a\in\alpha}(RelSup^2(\{a\})).$$

$SupMax1$ of an item set α is computed as the difference between the support of α in D^1, and the maximal individual support of the items in α in D^2. $SupMax1$ approximates $DiffSup$ by using the maximal individual support in D^2 to estimate $RelSup^2(\alpha)$. Clearly, the maximal individual support is quite a rough estimator for $RelSup^2(\alpha)$, because a pattern can have very low support in class S_2 but the items in it can still have very high individual supports in this class. However, an alternative way to interpret $SupMax1$ is that a pattern with large $SupMax1$ has relatively high support in one class and all the items in it have relatively low support in the other class. P_4 is such an example whose $SupMax1$ is $0.9 - max(0.3, 0.3, 0.3) = 0.6$ as shown in Fig. 1. Thus, given a $SupMax1$ threshold, say 0.4, $SupMax1$ discovers a subset of $0.4 - discriminative$ patterns but not all, e.g., it will miss patterns like P_1 in Fig. 1, which has relatively high *DiffSup* (0.6) but zero $SupMax1$.

4.2 *SupMaxK*

Following the rationale of $SupMax1$, the maximal support of size-k subsets of a pattern in D^2 can be used to estimate $RelSup^2(\alpha)$ instead of using maximal individual support in class S_2 to estimate $RelSup^2(\alpha)$. This can provide a better estimation of $RelSup^2(\alpha)$. In such a manner, $SupMax1$ can be generalized into a family of measures *SupMaxK*, which is formally defined in Definition 2. Note that in the following discussion, *SupMaxK* will be used to refer to this family as well as one of its general members, for the clarity of presentation.

Definition 2. *The* SupMaxK *of an item set* α *in* D^1 *and* D^2 *is defined as*

$$SupMaxK(\alpha) = RelSup^1(\alpha) - \max_{\beta \subseteq \alpha}(RelSup^2(\beta)),$$
$$where\ |\beta| = K.$$

So, *SupMaxK* of an item set α is computed as the difference between the support of α in D^1, and the maximal support among all the size-K subsets of α in D^2. Note that, in this paper, *SupMaxK* is defined with respect to *DiffSup*, while similar concept can also be applied to other discriminative measures such as the ratio-based measure [14].

4.3 Properties of the *SupMaxK* Family

In the following sections, we discuss three properties of the *SupMaxK* family.

4.3.1 *The Subset-Superset Relationship among* SupMaxK *Members*

Based on the definition of *SupMaxK*, the following two lemmas show the relationship among *SupMaxK* members.

Lemma 2. *If we use* $\mathrm{MaxSup}(\alpha, K)$ *to denote the second component of* $\mathrm{SupMaxK}(\alpha)$, *i.e.,* $max_{\beta \subseteq \alpha}(\mathrm{RelSup}(\beta))$ *with* $|\beta| = K$, *then* $\mathrm{MaxSup}(\alpha, K)$ *is a lower bound of* $\mathrm{MaxSup}(\alpha, K-1)$ *for integer* $K \in [2, |\alpha|]$.

Proof. For every size-$(K-1)$ subset of α (say β, $|\beta| = K-1$), there exists a size-K subset of α (say β', $|\beta'| = K$) such that $\beta \subset \beta'$, e.g., by adding any i to β, where $i \in \alpha$ and $i \notin \beta$. Based on the antimonotonicity property of $RelSup$, it is guaranteed that $RelSup(\beta') \leq RelSup(\beta)$. Then, from the properties of the max function, $max_{\beta' \subseteq \alpha}(RelSup(\beta')) \leq max_{\beta \subseteq \alpha}(RelSup(\beta))$. Thus, $MaxSup(\alpha, K)$ is a lower bound of $MaxSup(\alpha, K-1)$. □

Lemma 3. $SupMax(K-1)$ *of an item set* α *is a lower bound of its* SupMaxK, *or alternatively* SupMaxK *of an item set* α *is an upper bound of its* $\mathrm{SupMax}(K-1)$, *for integer* $K \in [2, |\alpha|]$.

Proof. Follows directly from Definition 2, Lemma 2. □

From Lemma 3, we know that, given the same threshold r and sufficient time, the set of patterns discovered with $SupMax(K-1)$ in an Apriori framework is a subset of the set of patterns discovered with *SupMaxK*. This means that

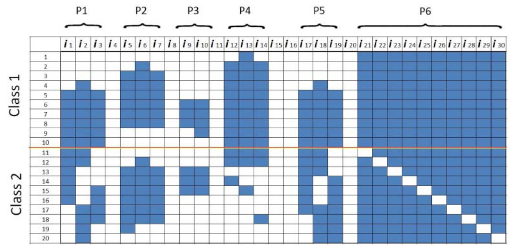

Fig. 3. An extended version of the data set shown in Fig. 1 containing 15 addition items ($i_{16} - i_{30}$) and two patterns P_5 and P_6, the rest being identical to Fig. 1.

SupMaxK can find more and more discriminative patterns as K increases from 1 (*SupMax1*), to 2 (*SupMax2*), to 3 (*SupMax3*), and so on. The patterns that are discovered by $SupMaxK$ but not by $SupMax(K-1)$ are those with $SupMaxK \geq r$, but with $SupMax(K-1) < r$. Fig. 3 shows an extended version of the data set shown in Fig. 1 containing 15 addition items ($i_{16} - i_{30}$) and two patterns P_5 and P_6, the rest being identical to Fig. 1. In this data set, given the same threshold $r = 0.4$, *SupMax1* can find P_4, but not P_1 and P_5, both of which have $DiffSup = 0.6$, but zero *SupMax1*; *SupMax2* can find P_1 in addition to P_4; furthermore, *SupMax3* can find P_5 in addition to P_4 and P_1. This illustrates that *SupMax3* can find all the patterns found using *SupMax1* and *SupMax2*, but not vice versa, as discussed above. Furthermore, *SupMax10* will be able to discover pattern P_6 in addition to the patterns found using *SupMax1*, *SupMax2*, and *SupMax3*.

4.3.2 *The Exactness of the* SupMaxK *Family*

Lemmas 2 and 3 lead to Theorem 1, which shows the relationship between *SupMaxK* and *DiffSup*.

Theorem 1. SupMaxK *is a lower bound of* DiffSup, *for integer* $K \in [1, |\alpha| - 1]$.

Proof. Since *DiffSup(α)* is equivalent to *SupMaxK(α)* with $K = |\alpha|$ (we assumed $RelSup^1(\alpha) \geq RelSup^2(\alpha)$ for simplicity earlier this section), this theorem follows from Lemma 3. □

Theorem 1 guarantees that the patterns discovered by any *SupMaxK* members with threshold r also have $DiffSup \geq r$. Therefore, *SupMaxK* members with threshold r discover only $r - discriminative$ patterns.

4.3.3 *The Increasing Completeness of the* SupMaxK *Family*

The max function together with the antimonotonicity of $RelSup$ yields the following result about the antimonotonicity of each member of *SupMaxK*.

Theorem 2. *Each member of* SupMaxK *is antimonotonic.*

Proof. Let $\alpha \subseteq I$ be an item set, and $\alpha' \subseteq I$ be a superset of α, such that $\alpha' = \alpha \cup \{i\}$, where $i \in I$ and $i \notin \alpha$. First, from the antimonotonicity of $RelSup$, we have $RelSup^1(\alpha') \leq RelSup^1(\alpha)$. Then, based on the property of the max function,

$$\max_{\beta' \subseteq \alpha'}(RelSup^2(\beta')) \geq \max_{\beta \subseteq \alpha}(RelSup^2(\beta)),$$

where $|\beta| = K$ and $|\beta'| = K$. Finally, we have the following:

$$\begin{aligned} SupMaxK(\alpha') &= RelSup^1(\alpha') - \max_{\beta' \subseteq \alpha'}(RelSup^2(\beta')) \\ &\leq RelSup^1(\alpha) - \max_{\beta \subseteq \alpha}(RelSup^2(\beta)) \\ &= SupMaxK(\alpha). \end{aligned}$$

□

Based on Theorem 2, given a threshold r, any member of the *SupMaxK* family can be used within an Apriori-like framework [2] to discover the complete set of patterns with $SupMaxK \geq r$. Note that *SupMaxK* could be alternatively defined using the min function, thus providing a better estimation of *DiffSup*. However, this version of *SupMaxK* will not be antimonotonic and thus cannot be used in the Apriori framework for the systematic search of discriminative patterns.

Since there are a finite number of discriminative patterns in a data set given a *DiffSup* threshold, and *SupMaxK* finds more and more discriminative patterns as K increases (Lemma 3), the set of patterns discovered with *SupMaxK* and threshold r within an Apriori-like framework is increasingly more complete with respect to the complete set of $r - discriminative$ patterns.

4.3.4 *Summary of the Three Properties of the* SupMaxK *Family*

From the subset-superset relationship among *SupMaxK* members, and the exactness and increasing completeness of the *SupMaxK* family, *SupMaxK* members conceptually organize the complete set of discriminative patterns into nested subsets of patterns that are increasingly more complete in their coverage with respect to $r - discriminative$ patterns. This yields interesting relationships between *DiffSup*, *BiggerSup*, and the *SupMaxK* family, which are discussed below.

4.4 Relationship between *DiffSup*, *BiggerSup*, and the *SupMaxK* Family

To understand relationship among *DiffSup*, *BiggerSup*, and *SupMaxK*, Fig. 4 displays the nested structure of the *SupMaxK* family together with *DiffSup* and *BiggerSup* from the perspective of the search space of discriminative patterns in a data set. L_{All} is the complete set of $r - discriminative$ patterns given a *DiffSup* threshold r. L_{CSET} is the search space explored by CSET in order to find all the patterns in L_{All}. Note that L_{CSET} is a superset of L_{All}, because *BiggerSup* is an upper bound of *DiffSup*. Note that, L_{CSET} can be much larger than L_{All} for dense and high-dimensional data sets, especially when a relatively low *BiggerSup* threshold is used. In such cases, CSET may not be able to generate complete results within an acceptable amount of time. For instance, on the cancer gene expression data set used in our experiments, the lowest *BiggerSup* threshold for which CSET can produce the complete results within 4 hours is 0.6. With a lower threshold 0.4, CSET cannot produce the complete results within 24 hours.

Members of the *SupMaxK* family help address this problem with *BiggerSup* by stratifying all the $r - discriminative$ patterns into subsets that are increasingly more complete (Set $L_1, L_2, \ldots, L_k, L_{k+1}, \ldots, L_{All}$), as shown in Lemma 3 and the subsequent discussion, and illustrated in Fig. 4. However, note that these superset-subset relationships among *SupMaxK* members and between *SupMaxK* and *BiggerSup* (used by CSET) hold only when the same threshold is used for *BiggerSup* and all the *SupMaxK* members, and unlimited computation time is available. In practice, given the same fixed amount of time, progressively lower thresholds can be used for *SupMaxK* members as K decreases. This trade-off was illustrated earlier in Fig. 2b.

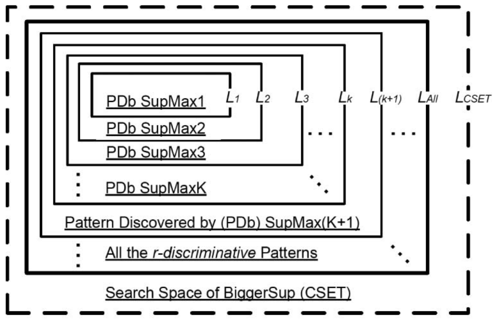

Fig. 4. Nested layers ($L_1, L_2, L_3, \ldots, L_k, L_{k+1}, \ldots, L_{All}, L_{CSET}$) of patterns defined by *SupMaxK*, and relationship with the complete set of discriminative patterns (layer L_{All}), and the search space of *BiggerSup* used by CSET (layer L_{CSET}). (PDb stands for "Patterns Discovered by.") $PDbSupMaxK$ is a subset of $PDbSupMax(K+1)$. Note that this figure only shows the subset-superset relationship, while the size of each rectangle does not the imply number of patterns in each set.

Since the focus of this paper is on dense and high-dimensional data, another practical factor should be considered, that is, the computational efficiency of the *SupMaxK* members. In the next section, we will introduce a special member of the *SupMaxK* family that is computationally suitable for dense and high-dimensional data.

4.5 *SupMaxPair:* A Special Member Suitable for High-Dimensional Data

In the previous discussion, we showed that as K increases, the set of patterns discovered with *SupMaxK* and threshold r in an Apriori framework is increasingly more complete with respect to the complete set of $r - discriminative$ patterns. Thus, in order to discover as many $r - discriminative$ patterns as possible, an as large as possible value of K should be used given the time limit. However, it is worth noting that the time and space complexity to compute and store the second component in the definition of $SupMaxK$, i.e., $MaxSup(\alpha, K) = max_{\beta \in \alpha}(RelSup^2(\beta))$ with $|\beta| = K$ are both $O(m^K)$ (the exact times of calculation are $\binom{M}{K}$), where M is the number of items in the data set. In high-dimensional data set (large M), $K > 2$ is usually infeasible. For instance, if there are 10,000 items in the data set ($M = 10{,}000$), even *SupMaxK* with $K = 3$ will require the computation of the support of all $\binom{10000}{3} \approx 1.6 \times 10^{11}$ size-3 patterns. Therefore, due to our emphasis on dense and high-dimensional data, we will focus on *SupMaxK* with $K = 2$, i.e., *SupMaxPair*, to balance the accurate estimation of *DiffSup* and computational efficiency. Note that, based on the definition of *SupMaxPair*, the computational complexity of the second component of *SupMaxPair* (maximal pairwise support in class S_2) for an item set $\alpha = \{\alpha_1, \alpha_2, \ldots, \alpha_l\}$ with size greater than 2 is $O(l^2)$. However, according to the Apriori framework [2], $MaxSup(\alpha, 2)$ only depends on three terms that will have been computed before the computation of $MaxSup(\alpha, 2)$ itself: $MaxSup(\{\alpha_1, \alpha_2, \ldots, \alpha_{l-1}\}, 2)$ and $MaxSup(\{\alpha_1, \alpha_2, \ldots, \alpha_{l-2}, \alpha_l\}, 2)$, and $MaxSup(\{\alpha_{l-1}, \alpha_l\}, 2)$, and thus the computational complexity for $MaxSup(\alpha, 2)$ is $O(1)$ per item set α.

As shown in Fig. 4, *SupMaxPair* can perform a complete search of the $r-discriminative$ patterns in the first two layers, even for a low value of r. Indeed, we will demonstrate in our experimental results on a cancer gene expression data set (Section 6) that searching these two layers itself can enable SupMaxPair to discover many low-support patterns that may not be discovered by CSET within an acceptable amount of time. Furthermore, these patterns are statistically significant and biologically relevant.

Before we discuss these results, we lay out the complete framework that we use for discovering discriminative patterns from dense and high-dimensional data.

5 Framework for Discriminative Pattern Mining

In this section, we explain the major steps in the framework used for discriminative pattern mining in our experiments:

- **Step 1.** This is an algorithm-specific step. For example, for *SupMaxPair*, all the item-pair supports are computed and stored in a matrix, whose (i, j) entry is the item-pair support of items i and j. The complexity of this step is $O(nm^2)$, where n is the number of transactions, and m is the number of unique items. No such precomputation has to be done for CSET.
- **Step 2.** The Apriori framework [2] is used in this step for discriminative pattern mining using the antimonotonic measures *BiggerSup* and *SupMaxPair*. For SMP, discriminative patterns are first mined from one class and then mined from the other, while CSET discovers patterns once from the whole data set.
- **Step 3.** To facilitate further pattern processing and pattern evaluation, we selected only the closed item sets [37] from the complete set of item sets produced.

For clarity, we refer to the version of this framework where *BiggerSup* is used for discovering patterns as **CSET**, while the version using *SupMaxPair* is referred to as **SMP** in the subsequent discussion. Our analysis of the quality of the patterns and the computational time requirements are presented with respect to the patterns produced by these complete pipelines.

6 Experimental Results

In order to evaluate the efficacy of different discriminative pattern mining algorithms, particularly CSET (a representative of the approaches in group B discussed in Section 1) and our proposed algorithm SMP, we designed two sets of experiments. The first set of experiments utilize synthetic data sets with varying density and dimensionality to study the properties of CSET and SMP. The second set of experiments involve the application of CSET and SMP to a breast cancer gene expression data. The second set aims at a systematic evaluation of the statistical significance and biological relevance of the resultant patterns, thus validating the effectiveness of CSET and SMP for knowledge discovery from real data. All the experiments presented here were run on a Linux machine with 8 Intel(R) Xeon(R) CPUs (E5310 @ 1.60 GHz) and 16 GB memory.

TABLE 1
Number of Type-I and Type-II Discriminative Patterns of Size-2, 4, 6, 8, and 10

	size-2	size-4	size-6	size-8	size-10
type-I patterns	3	6	5	8	7
type-II patterns	7	4	5	2	3
Total patterns of each size	10	10	10	10	10

6.1 Experiments on Synthetic Data Sets with Varying Density and Dimensionality

In the first set of experiments, we study the performance of SMP and CSET on synthetic binary data sets whose background can be fully controlled. Specifically, we created two collections of synthetic data sets, respectively, with 1) varying density and fixed dimensionality, and 2) varying dimensionality and fixed density. We first describe the approach we used to create these two collections of data sets and then present the performance of SMP compared to CSET.

6.1.1 Methodology for Generating Synthetic Data Sets

Each synthetic data set has two major components: discriminative and nondiscriminative patterns. Discriminative patterns are the target of the mining algorithms, while nondiscriminative patterns are obstacles. As discussed in Section 1, an effective discriminative pattern mining algorithm should be able to prune the nondiscriminative patterns at early stage while discovering discriminative patterns.

Ten discriminative patterns each of sizes 2, 4, 6, 8, and 10 were embedded in each synthetic data set, resulting in a total of 50 discriminative patterns per data set. To reflect the distribution of different types of discriminative patterns in real data, for each of the five sizes, we randomly determined a number of patterns (out of 10) that can be discovered by CSET but not SMP (type-I), and the remaining patterns that can be discovered by SMP but not CSET (type-II). Specifically, type-I patterns are those that have *DiffSup* greater than 0.2, but *SupMaxPair* below 0.2. As discussed in Section 4, SMP cannot find type-I patterns due to the fact that *SupMaxPair* is a lower bound of *DiffSup*. In contrast, type-II patterns are those that have *BiggerSup* below the lowest threshold (0.2) that CSET can finish within an acceptable amount of time (we use 4 hours as the representative acceptable amount of time). SMP can find these type-II patterns if it can effectively prune nondiscriminative patterns and can search at lower support levels (0.1). Table 1 displays the number of type-I and type-II discriminative patterns of different sizes embedded in each of the synthetic data sets. Note that these numbers are kept the same for all the synthetic data sets to ensure that results across different data sets are comparable. Note that in practice, there may be other types of patterns that can be discovered by both CSET and SMP. In this analysis, we do not embed these other types of patterns and focus only on the effectiveness of CSET and SMP for discovering different types of discriminative patterns.

For all the synthetic data sets, we fix the number of samples at 700, in which half are of class 1 and the other half are of class 2. Two collections of data sets were generated as follows:

Varying density with fixed dimensionality. For this collection of data sets, we fix the dimensionality at 4,000. After we embed the 50 discriminative patterns, we have the first data set of density 10 percent. Next, we keep adding nondiscriminative patterns of size-10 and support greater than 0.2, and create four more data sets with densities of 0.13, 0.16, 0.19, and 0.22, respectively.

Varying dimensionality with fixed density. For this collection of data sets, we fix the density of the data set at 0.2. After we embed the 50 discriminative patterns (density 10 percent), we further add nondiscriminative patterns to make the density equal to 0.2 and use this data set as the first data set (the dimensionality is 350). Next, we further add nondiscriminative patterns of size-10 and support greater than 0.2 and simultaneously increase the dimensionality of the data set to maintain the density at 0.2. In this way, we create another four data sets with dimensionalities of 500, 2,000, 4,000, and 6,000.

Note that the supporting transactions of both the discriminative and nondiscriminative patterns are selected randomly to avoid their combination into patterns of larger sizes. To simulate practical situations, for each data set generated in the above process, we add an additional 10 percent noise by flipping 10 percent of the 0s to 1s and 1s to 0s.

6.1.2 Performance of SMP and CSET on Synthetic Data Sets

For both the collections of data sets, we use a *BiggerSup* threshold of 0.2 for CSET and a *SupMaxPair* threshold of 0.1 for SMP. These thresholds agree with the definitions of type-I and type-II patterns for the following experiments (Section 6.1.1). The questions we want to answer in these experiments are: Which level of the item set lattice can CSET and SMP reach when mining these synthetic data sets given the time limit of 4 hours, and correspondingly, how many of the discriminative patterns at each level can be discovered by the two algorithms?

Figs. 5a and 5b display the levels that CSET and SMP reach on each of the five synthetic data sets of varying density and varying dimensionality, respectively. Note that the highest level is 10, which is the size of the largest discriminative and nondiscriminative patterns. Several observations can be made from Fig. 5a. First, when the density is 10 percent, both CSET and SMP can reach all the 10 levels. Thus, CSET can discover all the 29 type-I patterns (but none of the type-II patterns) and SMP can discover all the 21 type-II patterns (but none of the type-I patterns). Second, when the density increases to 13 percent, CSET only reaches level 3 and thus can only discover its three type-I patterns of size-2. In contrast, SMP can complete all the 10 levels and discovers all the 21 type-II patterns. Similar observation also holds for densities 0.16 and 0.19.

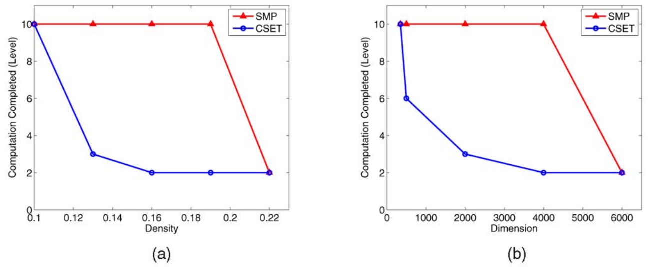

Fig. 5. Levels that can be reached by CSET and SMP in the two series of synthetic data sets (varying density and varying dimensionality). (a) Data sets with varying density and fixed dimensionality (4,000). (b) Data sets with varying dimensionality and fixed density (0.2).

This illustrates that even for reasonably high levels of density, SMP can discover type-II patterns with lower support that cannot be discovered by CSET, even though it can miss some type-I patterns that can be discovered by CSET. Finally, when density increases to 0.22, both SMP and CSET only reach level 2, i.e., CSET discovers its three type-I patterns and SMP discovers its seven type-II patterns. This indicates that for relatively very high levels of density, both CSET and SMP can face challenges in discovering the embedded patterns that they are supposed to discover (i.e., type-I patterns for CSET and type-II patterns for SMP). However, it should be noted that this deterioration in the performance of SMP is due to the expense of the $O(N^2)$ time complexity in the generation of level 2 candidates. Indeed, even at this density (0.22), SMP can again finish all the 10 levels in only an additional 0.5 hour (total 4.5 hours). However, CSET is still unable to generate all the level 3 candidates even in another 4 hours (total more than 8 hours). In summary, these results show that SMP is more effective for searching for low-support discriminative patterns on dense data sets.

Similar observations can also be made from Fig. 5b. First, at the dimensionality 350, both CSET and SMP can complete all the 10 levels and discover all the patterns they are supposed to find. Second, at dimensionality 500, 2,000, and 4,000, CSET can only reach up to levels 6, 3, and 2, respectively, while SMP still reaches all the 10 levels. Finally, at dimensionality 6,000, both SMP and CSET can only complete level 2. Again, SMP can finish all the 10 levels in another half an hour, but CSET is still generating level 3 candidates in another 4 hours. These results show that SMP is more effective for searching for low-support discriminative patterns from high-dimensional data sets.

From the above experimental results on the two collections of synthetic data sets with varying density and varying dimensionality, we demonstrated the efficacy of SMP for mining low-support discriminative patterns from dense and high-dimensional data sets. Next, we will use a real gene expression data set to study the practical utility of SMP for discovering low-support discriminative patterns.

6.2 Experiments on a Breast Cancer Gene Expression Data Set

In the second set of experiments, we used CSET and SMP to discover discriminative patterns from a breast cancer gene expression data set. Only closed patterns are used in these experiments. The details of this data set are provided in

TABLE 2
Details of Patterns Discovered by CSET at Various *BiggerSup* Thresholds

$BiggerSup$ Threshold	Time (sec)	# Closed Patterns	Pattern Size(s)	Highest $NegLogP$
0.4*	617	64942	2	12.09
0.55*	1454	84840	2-3	9.65
0.6	1558	90637	2-10	8.78

Expansion of the set of patterns to patterns of larger sizes could not finish in over 12 hours, and thus, their results are not included here.

TABLE 3
Details of Patterns Discovered by SMP at Various *SupMaxPair* Thresholds

$SupMaxPair$ Threshold	Time (sec)	# Closed Patterns	Pattern Size(s)	Highest $NegLogP$
0.18	2401	45982	2-7	12.09
0.2	1187	21285	2-5	12.09
0.25	332	3007	2-4	12.09
0.3	186	283	2-3	12.09

Section 6.2.1. We first present a global analysis of these patterns in Section 6.2.2. Subsequently, we perform an extensive statistical and biological evaluation of these patterns, the results of which are presented in Sections 6.2.3 and 6.2.4. In particular, we highlight the statistical significance and biological relevance of low-support patterns discovered by SMP but not CSET, thus illustrating the complementarity that SMP can provide to the existing approaches discussed in Section 1.

6.2.1 Data Set Description

A breast cancer gene expression data set [45] is used for evaluating the efficacy of discriminative pattern mining algorithms on complex, real data sets. This data set contains the expression profiles of about 25,000 genes in 295 breast cancer patients, categorized into two classes corresponding to whether the patient survives the disease (0) or not (1). Using preprocessing methodologies suggested by the authors [46], we only considered 5,981 genes that showed evidence of significant up- or down-regulation (at least a twofold change), and whose expression measurements were accurate (p-value ≤ 0.01) for at least five patients. Furthermore, to make the data set usable for binary pattern mining algorithms, each column pertaining to the expression of a single gene is split into two binary columns. Since the data have been properly normalized to eliminate between-gene variations in the scale of their expression values, we adopt a simple discretization method, as used in other studies [32], [12]: a 1 is stored in the first column if the expression of the gene is less than -0.2, while a 1 is stored in the second column if the expression of the gene is greater than 0.2. Values between -0.2 and 0.2 are not included, since genes showing an expression around 0 are not expected to be interesting, and may add substantial noise to the data set. The resulting binary data set has 11,962 items and 295 transactions, with a density of 16.62 percent.

For this data set, discriminative pattern mining can help uncover groups of genes that are collectively associated with the progression or suppression of cancer, and our experiments are designed to evaluate the effectiveness of different algorithms for this task.

6.2.2 General Analysis of the Patterns Discovered

We ran CSET and SMP at the lowest parameter thresholds for which they would finish in about 4 hours.[5] Only closed patterns are used in our experiments. Due to the weaker pruning of *BiggerSup* and the resulting large number of discriminative patterns, we were forced to use relatively higher thresholds for CSET and restrict the computation to patterns of a limited size to obtain the patterns necessary for our evaluation. Table 2 shows that the lowest *BiggerSup* threshold for which CSET can produce the complete results within 4 hours is 0.6. The lowest *BiggerSup* threshold for which CSET can discover size-2 and size-3 patterns within 4 hours is 0.55. At a lower threshold of 0.4, CSET can only discover size-2 patterns before running out of time. In contrast, SMP is able to run at a much lower *SupMaxPair* threshold of 0.18 and finds patterns of size as high as 7 in about 40 minutes. See Table 3 for the details of the patterns found by SMP at different thresholds. For the evaluation of pattern quality, we combine the patterns discovered by CSET at the 0.4, 0.55, and 0.6 $BiggerSup$ thresholds as the collection of all patterns that can be discovered by CSET, while for SMP, we only use the patterns discovered at the single *SupMaxPair* threshold 0.18. Indeed, even with this setup that is slightly biased toward CSET, there are still high quality low-support patterns that can only be discovered by SMP, the details of which are provided later.

In addition to analyzing the characteristics of the patterns discovered by SMP and CSET, we also examined the value of DiffSup for each individual gene constituting these patterns. Specifically, Fig. 6 displays the distribution of the *DiffSup* of individual genes in the patterns discovered only by *SMP* at a SupMaxPair threshold of 0.18, but not by CSET. Among the 332 genes covered by these patterns, almost 60 percent (198) of the genes have *DiffSup* lower than the 0.18. Based on the discussion of approaches that directly utilize $DiffSup$ or other measures of discriminative power for finding discriminative patterns (group C) in Section 1, it can be seen that these approaches cannot discover any of these genes, and thus cannot discover the patterns that include them. Since one of our major foci is on algorithms that can discover patterns whose individual genes may not be discriminative, we discuss only the results of CSET and SMP, which can find such patterns, in the rest of this section.

6.2.3 Statistical Evaluation

There are various ways to evaluate the importance of discriminative patterns. We are interested in patterns that occur disproportionately between the two classes. However, in real-world data sets, particularly those with small

5. Some time period needed to be chosen for the experiments. The duration of 4 hours is, although slightly arbitrary, generally reasonable for most data analysis operations.

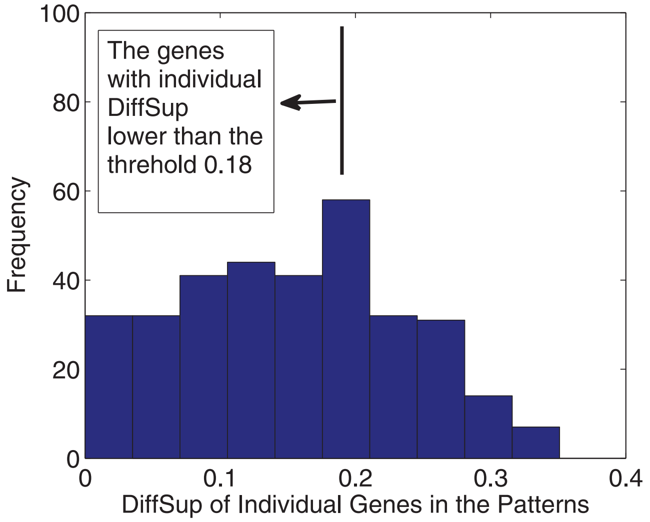

Fig. 6. Histogram of the *DiffSup* of individual genes in the patterns discovered only by SMP, but not by CSET.

number of instances in the two classes, even patterns that occur with similar support across classes will show some deviation from perfect balance in data sets with relatively small sample size. Thus, to ensure that the patterns found are not just a result of random fluctuation, a statistical test is commonly used to ensure that any deviation from equal support is statistically significant. In this section, we will perform this type of evaluation for the patterns from CSET and SMP.

We use the Fisher exact test [16] for this evaluation, whose result is a p-value (probability). If the p-value is below some user-defined threshold, e.g., 0.05 or 0.01, then the pattern is regarded as authentic. Note that p-values are often expressed as their negative log_{10} value for convenience (the higher this $-log_{10}$ value (denoted as ***NegLogP***), the more reliable the discriminative pattern is expected to be). We will refer to this measure as ***NegLogP***. If there are multiple patterns, the $NegLogP$ threshold needs to be adjusted. By using a randomization test, as discussed below, we were able to determine that a $NegLogP$ of 8 is unlikely to arise from a random pattern. We give the technical details of this a bit later.

In Fig. 7, we show plots of $NegLogP$ versus global support for the patterns discovered by both CSET and SMP. For CSET, patterns discovered by using *BiggerSup* thresholds 0.4, 0.55, and 0.6 were combined as described in Section 6.2.2, while for SMP, a 0.18 threshold was used. Several conclusions can be drawn from this figure. First, CSET finds more patterns than SMP, particularly for patterns with higher support (the ones with support greater than 0.4). This is not surprising since SMP sacrifices completeness to find lower support patterns. Second, CSET finds many patterns with $NegLogP$ less than 2, while all the patterns discovered by SMP have $NegLogP$ higher than 2. This demonstrates the exactness of *SupMaxPair* (Theorem 1), i.e., because *SupMaxPair* is a lower bound of *DiffSup*, all the patterns discovered with r are $r - discriminative$. Last and the most important, SMP finds many patterns at low-support level that are not found by CSET, especially the ones with $NegLogP$ higher than the significance threshold 8. Also, these patterns are constituted by many genes that are not covered by the patterns discovered by CSET, as will be discussed in Section 6.2.4.

We now come back to the details of how we determined a significance threshold for $NegLogP$, both for the completeness of the above discussion and to further illustrate the quality of the patterns found by SMP but not found by CSET. Because of the issues of low sample size and high-dimensionality for data sets used for problems such as biomarker discovery, many patterns may be falsely associated with the class label. This raises the multiple-hypothesis testing problem [40], [18], which is addressed by various approaches, such as Bonferroni correction [33], false discovery rate control [48], and permutation test [33], [52], [18]. Permutation tests based on row-wise, column-wise, and swap randomization [18] have been used to assess the statistical significance of the results of unsupervised pattern discovery and clustering algorithms. While in the context of labeled transactions, class-label permutation tests [42], [50] are often an effective option. In this approach, a reference distribution for evaluation measures like $NegLogP$ is generated by randomly shuffling the class labels (permutations). Specifically, for each iteration, the class labels are randomly shuffled and reassigned to patients, discriminative patterns

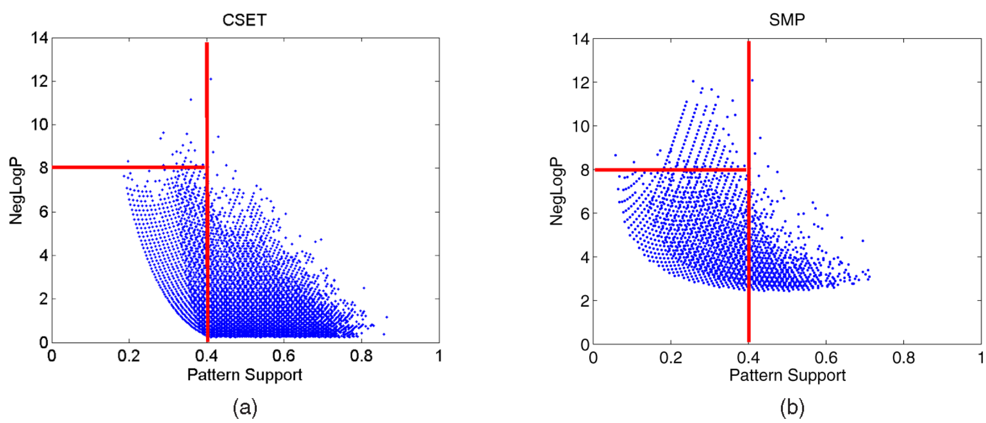

Fig. 7. Plot of $NegLogP$ versus global support for patterns from CSET and SMP, where the support is relative to the whole data set. (a) $NegLogP$ versus global support for CSET patterns. (b) $NegLogP$ versus global support for SMP patterns.

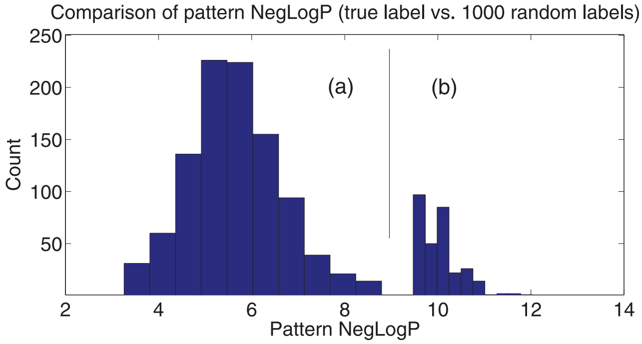

Fig. 8. Histogram of $NegLogP$ values: (a) the maximum $NegLogP$ for each of the 1,000 permutation tests where randomized labels are used by SMP. (b) The top $300 NegLogP$ values of the patterns discovered only by SMP but not by CSET.

are found, and the $NegLogP$ values are computed for these patterns using the same method as for the patterns discovered with the true labels. The $NegLogP$ values from the random runs can be used to generate an empirical distribution for the $NegLogP$ values, which can be displayed as a histogram as in Fig. 8. (Sometimes, only the extreme (maximum) $NegLogP$ values are used as in this figure.) If a $NegLogP$ of a pattern derived from the true labels falls outside the main concentration of $NegLogP$ values from the random labels, then the $NegLogP$ very likely indicates a discriminative pattern with a "more than random" variation from equal frequency across classes.

Fig. 8 summarizes the results of such a permutation test for the data set being used in these experiments. The right-hand side shows the top $300 NegLogP$ of the patterns discovered only by SMP but not by CSET, while the left-hand side displays the maximum $NegLogP$ for each of the 1,000 permutation tests where randomized labels are used for pattern mining. We observe that the $NegLogP$ values with random labels rarely exceed 8 (less than 8.72 in each of the 1,000 permutation tests). Thus, we can use 8 as a relaxed threshold for significance, since only a few percent of the random patterns are above this value. The $NegLogP$ values of the top-300 patterns discovered by SMP but not by CSET with true label are much higher (all larger than 9.67). In contrast, only 34 patterns discovered by CSET have a $NegLogP$ greater than 8. This shows that SMP can discover additional statistically significant low-support patterns. In the next section, we illustrate the biological significance of these patterns and how they can be used to discover cancer-related genes.

6.2.4 Biological Relevance of Patterns Based on a List of Cancer-Related Genes

There are various ways to determine the biological relevance of discriminative patterns. Since the application we consider is that of discovering biomarkers for cancer, we measured the biological relevance of the patterns using a list of about 2,400 human genes known to be involved in the induction, progression, and suppression of various types of cancers [21]. Of these 2,400 genes, 611 were included in the set of 5,981 genes in our processed gene expression data set. If the discriminative patterns found by CSET and SMP, which are just small sets of genes, tend to disproportionately contain these 610 cancer-related genes as opposed to the non-cancer-related genes, then this indicates that these patterns contain information that may be of significance to a biological researcher. To make this idea concrete for the purposes of evaluation, two evaluation approaches were designed.

1. **Pattern-based biological relevance.** For each pattern generated by CSET or SMP, we matched the genes in the pattern with the set of 611 validated cancer genes, giving us a measure of the "precision" of the pattern. For instance, if a pattern contains three genes, of which two are found to match the list of cancer genes, then the precision of this pattern is $2/3 = 66.67\%$. Note that if a pattern with N genes is randomly chosen from our set of 5,981 genes, one would expect a precision of $[N*(611/5981)]/N = 10.2\%$.
2. **Gene collection-based biological relevance.** Since patterns may overlap with each other (pattern redundancy), and do not directly show how many cancer genes can be discovered by SMP in addition to CSET, we also designed a gene collection-based evaluation methodology. Here, we collect the set of genes covered by all the patterns discovered by CSET(SMP), and compare this set of genes with the set of 611 validated cancer genes just as for pattern-based evaluation. For instance, if a set of 100 patterns covers 300 genes, of which 50 are found to match the list of cancer genes, then the precision of the set of patterns is $50/300 = 16.67\%$ and the recall is $50/611 = 8.18\%$. To compare, if we select 300 genes randomly from the 5,981 genes, then the expected precision is $[300*(611/5981)]/300 = 10.2\%$, and the expected recall is $[300*(611/5981)]/611 = 5.02\%$.

This section details the results obtained from with these evaluation methodologies.

Brief preview of results. From the pattern-based biological relevance evaluation, we observed that CSET can discover patterns with good precision at relatively high-support level, while SMP can further discover good quality patterns at relatively low-support level, among which, there are some patterns with 100 percent precision with respect to the cancer gene list. From the gene collection-based biological relevance evaluation, we observed that both the techniques discovered substantially more cancer genes than expected by random chance, especially among the higher $NegLogP$ patterns. In particular, SMP was able to discover more cancer genes as compared to CSET due to its ability of discovering low-support patterns. This result further indicates the potential usefulness of recovering low-support patterns and discovering biomarkers that may be examined and utilized by the biology community. The following discussion provides additional details of these results.

Results from pattern-based relevance. Fig. 9a shows the distribution of pattern-based precision of those patterns discovered only by SMP but not by CSET. For comparison, we generated a sequence of size-k patterns exactly according to the sizes of the patterns corresponding to Fig. 9a. The distribution of precision of these random patterns is shown in Fig. 9b. We can make the following observations from a comparison of Figs. 9a and 9b: 1) these patterns that are discovered exclusively by SMP include

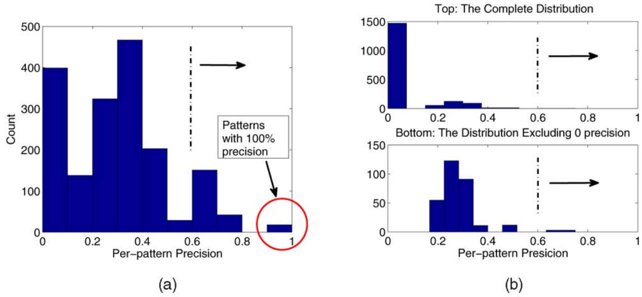

Fig. 9. Comparison of the distributions of pattern-based precision between (a) the patterns discovered by SMP but not CSET and (b) random generated patterns.

many that have a relatively high precision. Specifically, about 200 patterns have precisions above 0.6, among which there are 18 with a precision of 100 percent. 2) The pattern-based precision of randomly generated patterns is mostly (about 1,500 times) 0, and sometimes (about 300 times) falls into the range of 0.2 and 0.3, but rarely (less than 20) goes beyond 0.4, and never goes beyond 0.8. Interestingly, some of the SMP patterns with 100 percent precision play similar roles in cancer processes.

Results from gene collection-based relevance. To investigate how many cancer genes can be discovered using CSET and SMP, we summarized the gene collection-based evaluation results for them in Tables 4 and 5, respectively. These tables include the number of cancer genes discovered, precision, recall, and expected recall for randomly selected group of genes of the same size. Note that, the expected precision for a random collection of genes is 10.2 percent as calculated earlier, and thus we do not include this in these tables. The following observations can be made from these tables:

1. Both CSET and SMP usually find very precise patterns for reasonably high levels of the $NegLogP$ measure, and this precision is much higher than that expected from a set of randomly selected gene collection of the same size (10.2 percent). Similarly, the recall values for the genes covered by these patterns are much higher than those expected from the same type of randomly selected gene collection, as shown by a comparison with the last column of these tables.

TABLE 4
Precision-Recall Results of CSET Patterns with *BiggerSup* ≥ 0.4

NegLogP Threshold	# Patterns	# Genes Covered	# Cancer Genes	Pre (%)	Rec (%)	ERec (%)
12	2	3	2	66.7	0.3	0.052
11	2	3	2	66.7	0.3	0.052
10	2	3	2	66.7	0.3	0.052
9	10	12	3	25.0	0.5	0.21
8	34	31	7	22.6	1.1	0.54

Pre: precision, Rec: Recall, Expected precision for random gene collections is 10.2 percent, ERec: Expected recall of random gene collections with the same size.

TABLE 5
Precision-Recall Results of SMP Patterns with $SupMaxPair \geq 0.18$

NegLogP Threshold	# Patterns	# Genes Covered	# Cancer Genes	Pre (%)	Rec (%)	ERec (%)
12	2	4	2	50.0	0.3	0.067
11	6	7	3	42.9	0.5	0.12
10	200	36	11	30.6	1.8	0.60
9	541	57	17	29.8	2.8	0.95
8	1502	103	26	25.2	4.3	1.72

Pre: Precision, Rec: Recall, Expected precision for random gene collections is 10.2 percent, ERec: Expected recall of random gene collections with the same size.

2. For similar values of cancer gene discovery precision, SMP generally finds more cancer genes than CSET. For instance, at a precision of about 25 percent, the recall of CSET is only 0.5 percent (three cancer genes), while SMP has a recall 4.3 percent (26 cancer genes).

Note that the highlight of the second observation is not that SMP discovers more cancer genes, but that SMP can discover cancer genes from discriminative patterns with low support in addition to the ones discovered by CSET, thus indicating the complementarity of SMP to existing approaches like CSET. Because of such complementarity, even if SMP discovered less cancer genes than CSET, SMP still complement CSET as long as additional genes are exclusively discovered by SMP. Indeed, from the specific example in the second observation, at least 23 cancer genes are discovered by SMP in addition to CSET.

6.2.5 Biological Relevance of Patterns Based on Biological Gene Sets

An alternative way of evaluating the biological relevance of the patterns discovered only by SMP but not by CSET is to estimate how well they capture the 5,452 known biological gene sets (e.g., pathways) in the Molecular Signature database [42][6] (MSigDB). MSigDB is widely used collection of gene groups containing genes with similar biological functions. The methodology we adopt for this evaluation is one of calculating the enrichment of one pattern with these gene groups. This enrichment is measured as the probability of a random pattern of the same size having the same or better annotations by a given gene group by random chance, and the lower this probability, the more enriched a pattern is with a given gene group. Specifically, for a pattern of size k and a gene set of size m which share x common genes, we use the hypergeometric cumulative distribution function[7] to compute the probability that there are greater or equal to x common genes between the pattern and the gene set by random chance given that the total number of genes in the data set is N [3]. The $-log$ value of this probability can be considered as an enrichment score between a pattern and a gene set (denoted by

6. Specifically, MSigDB (version 2.1, Feb. 2007) contains 386 positional gene sets, 1,892 curated gene sets, 837 motif gene sets, 883 computational gene sets, and 1,454 annotations in Gene Ontology. http://www.broad institute.org/gsea/msigdb/.

7. $p(x|k, m, N) = 1 - \sum_{i=0}^{x-1} \frac{\binom{N-i}{k-i}\binom{m}{i}}{\binom{N}{k}}$.

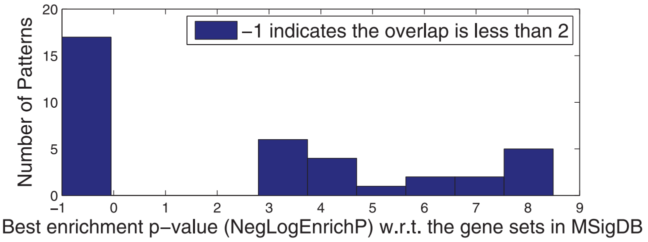

Fig. 10. Histogram of the best enrichment *NegLogEnrichP* values w.r.t. the gene sets in MSigDB, for the patterns discovered by SMP but not by CSET. An enrichment p-value is computed only if a pattern and a gene set have at least two genes in common.

NegLogEnrichP), and the larger this score, the more significant the biological relevance of the pattern. For each pattern, we use the best *NegLogEnrichP* with the 5,452 gene sets as a measure of its biological relevance.

Instead of directly applying the above enrichment methodology to all the patterns that are discovered only by SMP but not by CSET, we first select a subset in which no pairs of patterns have greater than 25 percent overlap of genes. This selection helps reduce the effect of the redundancy between these patterns on the enrichment results. The resultant set has 37 patterns. Fig. 10 shows the distribution of the best *NegLogEnrichP* values of these 37 patterns with respect to the gene sets in MSigDB. It can observed that more than half of the patterns (20) have at least two genes overlapping with one or more gene sets, and some patterns even have a *NegLogEnrichP* value as high as 8 (original p-value as low as 10^{-8}). Interestingly, some of the patterns in this collection are enriched with several gene sets that are clearly related to breast cancer such as *BREAST-DUCTAL-CARCINOMA-GENES* ($NegLogEnrichP = 8.02$) and *BREAST-CANCER-PROGNOSIS-NEG* ($NegLogEnrichP = 6.73$), as well as several gene sets that are related to general cancer-related biological processes such as the cell-growth-related gene set *IRITANI-ADPROX-LYMPH* [42] ($NegLogEnrichP = 6.67$) and the proliferation-related gene set *HOFFMANN-BIVSBII-BI-TABLE2* [42] ($NegLogEnrichP = 6.15$). These results further support the biological relevance of the patterns discovered only by SMP but not by CSET, and thus demonstrate the benefits of using SMP to search for low-support discriminative patterns in addition to existing approaches.

6.2.6 Comparison of the Scalability of the Algorithms

In Section 6.1, we compared the effectiveness of CSET and SMP for discovering low-support patterns from synthetic data sets with varying density and dimensionality. In this part of the study, we test the scalability of CSET and SMP with varying thresholds on the real gene expression data. In addition, we also test the FPClose (FPC) [19] algorithm (plus pattern selection) as the baseline as used by other studies [10], [15]. Note that, as mentioned in Section 6.2, the gene expression data set was discretized with ± 0.2 as thresholds, into a binary matrix with density 16.62 percent and dimension 11,962, to preserve most of the information in the data. This data set is quite dense, due to which CSET can only generate complete results at a threshold larger than 0.6. In order to obtain a more complete picture of the scalabilities of FPC, CSET, and SMP, we discretized the gene expression data set using ± 0.3 as the discretization threshold in this section, which yields a binary matrix with density 8.71 percent.

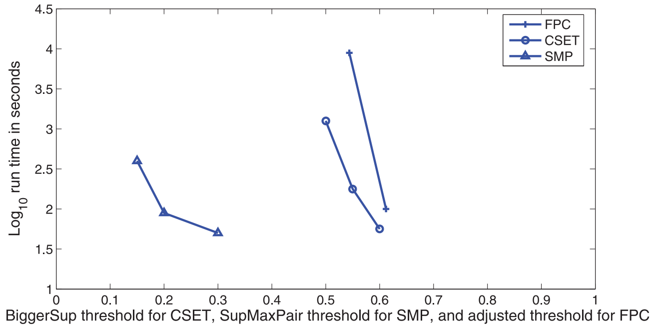

Fig. 11. Scalability of different discriminative pattern mining algorithms on the gene expression data.

Fig. 11 shows the results of these comparisons. The X-axis in this plot is the threshold used for discriminative pattern mining, while the Y-axis denotes the $\log_{10}$ (runtime in seconds) value. Note that runtimes are recorded for any algorithm only if it can produce output within 4 hours. The relative $minsup$ threshold used in FPC is defined on the whole data set (both classes), while *BiggerSup* for CSET and *SupMaxPair* for SMP take into account the support in each of the classes individually. Therefore, for a fair comparison, FPC's $minsup$ is adjusted according to the size ratio of the two classes (divided by the percentage of the majority class in the whole data set (0.74)) and then plotted together with *BiggerSup* and *SupMaxPair*.

Several observations can be made from these plots: 1) the FPC-based two-step approach can search for discriminative patterns at high-support levels (above 0.55), 2) by using *BiggerSup*, CSET is able to search at slightly lower support levels (above 0.5) compared to FPC; and for the same threshold, CSET is more efficient than FPC, and 3) *SupMaxPair* can explore pattern space with substantially lower support levels (0.1-0.3). Thus, FPC and CSET can be used to discover patterns at higher thresholds, while SMP is able to find lower support patterns missed by the other approaches.

6.3 Summary of Results

Based on the experimental results on both the synthetic data sets and the cancer gene expression data set presented in this section, we have demonstrated that on dense and high-dimensional data, there are patterns with relatively low support that can only be discovered by *SupMaxPair* but not by the existing approaches. Specifically, on the cancer gene expression data set, the low-support discriminative patterns discovered only by SMP are statistically significant and biologically relevant.

We also did another set of experiments for studying how well the members of *SupMaxK* approximate *DiffSup* as K increases. We selected several UCI data sets [4], on which all the discriminative patterns (given a relatively low DiffSup threshold) can be discovered and used for the study. The experimental results show that: 1) *SupMax1* generally provides very poor approximation of *DiffSup*; 2) the approximation is improved substantially when K goes to 2, i.e., SupMaxPair; and 3) when K is increased further to 3 and 4, the computation time increases exponentially, but the approximation improves much slower compared to the improvement obtained when K goes from 1 to 2. These experimental results indicate that *SupMaxPair* provides a good balance between the approximation of *DiffSup* and the computational expense. The detailed results are discussed as a supplementary material (available at http://vk.cs.umn.edu/SMP/).

7 Related Work

Over the past decade, many approaches have studied discriminative pattern mining and related topics. Dong and Li [14] defined *emerging patterns* as item sets with a sufficiently large growth rate (support ratio) between two classes. A two-step algorithm is proposed to discover EPs, which first finds frequent item sets with the Max-Miner algorithm [6] for each of the two classes, and then compares these item sets to find EPs. Emerging patterns were the first formulation of discriminative patterns and have been extended further to several special cases such as jumping emerging patterns [26] and minimal emerging patterns [31], [27]. Here, the discriminative power of a pattern is measured with support ratio [14], or simply with the two supports of the pattern in the two classes and two corresponding thresholds [31]. As discussed in [5], these emerging pattern mining algorithms must mine the data multiple times given a certain threshold for support ratio (or two thresholds for the two supports). In [5], a new formulation of discriminative patterns, contrast sets, is proposed along with an algorithm to mine them. CSET is the first technique that formulates discriminative pattern mining within an Apriori-like framework [2], [6], in which different pruning measures can be used to perform a systematic search on the item set lattice [2]. In [51], contrast set mining is shown to be a special case of a more general task, namely, rule learning, where a contrast set can be considered as an antecedent of a rule whose consequent is a group. Notably, CSET has also be used in some biomedical applications [25]. The upper bounds of statistical discriminative measures have also been studied for discriminative pattern mining, e.g., information gain [9], $\chi^2 - test$ [5], and several others [34].

Next, we also briefly discuss other research work related to discriminative pattern mining, although they are not the focus of the paper. Many existing approaches have studied the use of frequent patterns in classification. Associative classifiers [29], [28], [55], [11], [49] are a series of approaches that focus on the mining of high-support, high-confidence rules that can be used in a rule-based classifier. Cheng et al. [9] recently conducted a systematic evaluation of the utility of frequent patterns in classification. Several pattern-based classification frameworks have also been proposed, in which a small number of discriminative patterns are selected, which can achieve comparable classification accuracy with respect to the whole set of discriminative patterns [10], [15], [54], [30]. Discriminative pattern mining from multiple classes has been studied in [5], [27], [25], while mining complex discriminative patterns has been studied in [31]. Although traditional pattern summarization approaches [20] can be adopted to control the redundancy among discriminative patterns, closeness and redundancy are specially studied for in the context of discriminative patterns, respectively, in [17] and [41].

8 Conclusions

In this paper, we addressed the necessity of trading off the completeness of discriminative pattern discovery, with the ability to discover low-support discriminative patterns from dense and high-dimensional data within an acceptable amount of time. For this, we proposed a family of antimonotonic measures of discriminative power named *SupMaxK* that conceptually organize the set of discriminative patterns into nested layers of subsets, and are progressively more complete in their coverage, but require increasingly more computation for their discovery. Given the same and fixed amount of time, the *SupMaxK* family provides a trade-off between the ability to search for low-support discriminative patterns and the coverage of the space of valid discriminative patterns for the corresponding threshold. In particular, *SupMaxK* with $\mathrm{K} = 2$ named *SupMaxPair* is a special member of this family that is suitable for dense and high-dimensional data. We designed a framework, named SMP, which uses *SupMaxPair* for discovering discriminative patterns from dense and high-dimensional data. A variety of experiments on both synthetic data sets and a breast cancer gene expression data set demonstrated that there are patterns with relatively low support that can be discovered using SMP but not by the existing approaches. In particular, the low-support discriminative patterns discovered only by SMP from the gene expression data set are statistically significant and biologically relevant. In summary, SMP can complement existing algorithms for discovering discriminative patterns by finding patterns with relatively low support from dense and high-dimensional data sets that other approaches fail to discover within an acceptable amount of time. Thus, in practice, it is recommended that CSET and other existing approaches should be used to discover medium-to-high support patterns from such data sets within an acceptable amount of time, and then SMP could be used to further discover low-support discriminative patterns that existing approaches may not discover.

Our work can be extended in several directions. As discussed in Section 4.4, the members of *SupMaxK* induce a hierarchy of subsets of the complete set of discriminative patterns. This hierarchy motivates further research that focuses on the mining of discriminative patterns from the other layers that are not covered by *SupMaxPair*. It is also interesting to study the quality of the discriminative patterns in the different layers of this hierarchy, which may provide insights into different priorities for discriminative pattern mining from these layers. Note that, the use of measures from the *SupMaxK* family is only one possible method for trading off the completeness of pattern discovery with the ability to discover low-support discriminative patterns from high-dimensional data. Indeed, other approaches that adopt a different strategy for handling this trade-off are also possible and should be studied. Also, most existing discriminative pattern mining algorithms (as well as SMP) are designed for binary data, and have to rely on discretization for continuous data. It will be useful to design approaches that can directly handle continuous data for discriminative pattern mining, as has been done for discovering patterns in an unsupervised manner [36].

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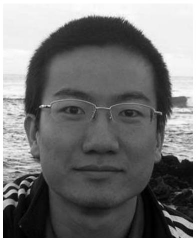

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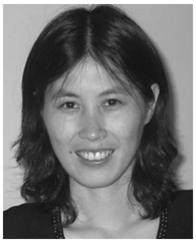

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