

Gabriela Alexe · Sorin Alexe · Peter L. Hammer

Pattern-based clustering and attribute analysis

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Abstract The logical analysis of data (LAD) is a combinatorics, optimization and logic based methodology for the analysis of datasets with binary or numerical input variables, and binary outcomes. It has been established in previous studies that LAD provides a competitive classification tool comparable in efficiency with the top classification techniques available. The goal of this paper is to show that the methodology of LAD can be useful in the discovery of new classes of observations and in the analysis of attributes. After a brief description of the main concepts of LAD, two efficient combinatorial algorithms are described for the generation of all prime, respectively all spanned, patterns (rules) satisfying certain conditions. It is shown that the application of classic clustering techniques to the set of observations represented in prime pattern space leads to the identification of a subclass of, say positive, observations, which is accurately recognizable, and is sharply distinct from the observations in the opposite, say negative, class. It is also shown that the set of all spanned patterns allows the introduction of a measure of significance and of a concept of monotonicity in the set of attributes.

Keywords Logical Analysis of Data (LAD) · Patterns · Clustering · Feature analysis

Abbreviations LAD: Logical Analysis of Data

1 Introduction

The extraction of knowledge hidden in records of past observations is a common problem in practically every area of science, engineering and business, and is the central object of

study of classical disciplines, like statistics, and newer ones, like machine learning and data mining. Numerous methods have been developed to address this type of problems, and substantial success with their use is reported in the literature. One of the basic questions addressed by all the above mentioned areas is that of classification, e.g., that of recognizing – on the basis of similarities with already known observations in a given dataset Ω – whether a not-yet-seen observation (i.e., one not belonging to Ω) is positive or negative (or true or false, or sick or healthy, etc). We plan to show in this paper that the tools developed for classification can be successfully applied also for the extraction of other important information from datasets.

In order to clarify the concepts and the methods proposed in this paper we shall illustrate them on the breast cancer wisconsin (BCW) dataset – one of the most frequently quoted, publicly available datasets (<http://www1.ics.uci.edu/~mllearn/MLRepository.html>). This dataset includes 699 observations, of which we shall only use those 683 for which the values of all the nine attributes are specified. Of these 683 observations, 239 correspond to *positive* (i.e., malignant breast cancer) cases, while 444 correspond to *negative* (i.e., benign breast cancer) cases. The nine variables of the problem, clump thickness, uniformity of cell size, uniformity of cell shape, marginal adhesion, single epithelial cell size, bare nuclei, bland chromatin, normal nucleoli, and mitosis, take values from one to ten, and will be denoted in this paper by x_1, \dots, x_9 .

Various statistical and machine learning classification techniques are available for distinguishing the positive observations from the negative ones. Among the methods which are most frequently applied for the solution of such problems we mention logistic regression, Bayesian networks, nearest neighbors, linear (diagonal) discriminant, decision trees, artificial neural networks, support vector machines (see e.g., [19, 15]). The method we shall use in this study is the logical analysis of data (LAD), which was selected because of its double potential of answering the basic classification question on the one hand, and of providing on the other hand, novel types of information about the problems under study, e.g., the analysis

G. Alexe
Institute for Advanced Study, Princeton, NJ 08540, USA

S. Alexe · P.L. Hammer (✉)
RUTCOR-Rutgers Center for Operations Research,
Rutgers University, Piscataway, NJ 08854, USA
Tel.: +1-732-445-4812
Fax: +1-732-445-5472
E-mail: hammer@rutcort.rutgers.edu

Table 1 Number and generation time of prime patterns with prevalence $\geq 10\%$ in **bcw** dataset

Homogeneity	Degree 2			3			4		
	# positive patterns	# negative patterns	Time (s)	# positive patterns	# negative patterns	Time (s)	# positive patterns	# negative patterns	Time (s)
90%	45	56	0	45	105	1	45	110	43
95%	59	54	0	87	216	1	99	411	43
100%	39	7	0	194	68	1	464	201	43

of the role and nature of attributes, the discovery of new classes, etc.

The paper is structured as follows: the basic concepts of LAD will be presented in Sect. 2. Section 3 will deal with the algorithmic problems of generating different types of patterns. Section 4 will deal with various applications of the large collections of patterns generated by LAD, including a new type of clustering of the observations (aimed at discovering new classes of observations), and the analysis of the importance and role of features. The paper ends with some brief conclusions presented in Sect. 5.

2 Basic concepts of LAD

The Logical Analysis of Data (LAD), introduced in [13, 14], is a combinatorial optimization-based approach to the analysis of a dataset $\Omega = \Omega^+ \cup \Omega^-$, consisting of “positive” and “negative” observations, each of which is represented as a vector of n attribute values, each attribute x_i taking the values $\{0, 1, \dots, k_i\}$. It has been established in previous studies ([5, 12]) that LAD provides a competitive classification tool, comparable in efficiency with the best classification techniques available. The key concept used in LAD is that of *patterns*, which makes it in particular possible to provide clear justifications of the reasons for which a not-yet-seen observation should be considered positive or negative. As it will be seen in this paper, the set of patterns can provide numerous other important information about the data. The essence of LAD consists in the systematic and exhaustive generation of all the patterns satisfying certain limiting conditions, and the extraction of information from this set of patterns.

Let us first introduce some basic concepts. A set of bounding restrictions imposed on the values of several attributes is called a *conjunction*. A conjunction is called a *positive* (or *negative*) *pattern* if it is sufficiently “biased”, i.e., it satisfies at least a prescribed proportion of the positive (negative) observations, and at most a prescribed proportion of the negative (positive) observations. A positive (negative) pattern is called *pure* if every negative (positive) observation in the dataset violates at least one of its defining conditions. For illustration, the conditions “*uniformity of cell size*” ≥ 5 , “*marginal adhesion*” ≥ 2 , and “*normal nucleoli*” ≥ 3 imposed on the attribute values of the observations in **bcw** represent a pure positive pattern, say P , because they are simultaneously satisfied by 137 (57.3%) of the 239 positive cases, and by none of the negative cases.

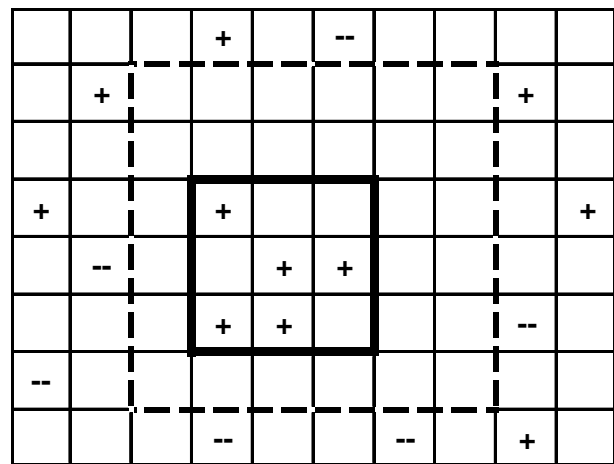


Fig. 1 An intuitive example of a prime and of a spanned pattern

It was shown in [12, 17] that the key role in knowledge extraction by LAD is played by two types of patterns, called “prime” and “spanned”. A *prime pattern* is in fact “minimal” with respect to the set of its defining conditions, i.e., it is a pattern such that if any of its defining conditions is *relaxed*, the remaining system of conditions defines a conjunction which is no longer a pattern. In the case of a positive (negative) pattern, this means that after the relaxation of any of its defining conditions, the proportion of negative (positive) observations satisfying the remaining conjunction violates the prescribed bias. For illustration, if we consider positive patterns to have a bias of 0% (i.e., no negative observation should be satisfied) then the pure positive pattern P is prime, since by relaxing any of its defining conditions allows some of the negative observations to satisfy its conditions; for instance, by relaxing the second condition to “*marginal adhesion* ≥ 1 ”, and leaving the other two unchanged, the new conjunction C obtained in this way will be satisfied by two negative observations. A *spanned pattern* is in fact also a “minimal” one, but in a different sense than in the prime case. More exactly, a spanned pattern is such that by *strengthening* any of its defining conditions, at least one of the observations *covered* by the pattern (i.e., satisfying its defining conditions) will no longer be covered. For illustration, if in the positive pure pattern discussed above we strengthen any of its defining conditions, some of the positive observations covered by it will be uncovered; for instance, by strengthening the second condition to “*marginal adhesion* ≥ 3 ”, the number of positive

Table 2 Generation time (in seconds) of spanned pure patterns in **bcw** dataset

Prevalence (%)	Number of spanned pure patterns produced			
	1000	5000	10000	16000
5	3	25	47	93
10	4	28	51	99

observations covered by the conjunction obtained in this way, say D , will drop from 137 to 123. An intuitive example of a prime and a spanned pattern in a fictitious example of a dataset with two variables is shown in Figure 1; the “box” enclosed by the dotted line represents a prime pattern, while that enclosed by a heavy line represents a spanned pattern.

There are five basic parameters $\sigma, \tau, \delta, \pi, \chi$ associated to a pattern. The *sign* σ of a pattern, can only take the values $+$ or $-$ to indicate whether it has a positive or a negative bias. The *type* of the pattern, τ , can take the values “prime” or “spanned”. The *degree* δ of a pattern indicates the number of variables used in its definition, for instance $\delta = 3$ for the pattern P mentioned above. The *prevalence* π of a pattern represents the proportion of observations covered within Ω^+ (in the case of positive patterns), or Ω^- (in the case of negative patterns) covered by it; e.g., the prevalence of P is $\pi = 57.3\%$. In the case of positive (negative) patterns, their *homogeneity* χ represents the proportion of those of the observations covered by them which are positive (respectively, negative). For instance the conjunction C mentioned before covers 143 positive and 2 negative observations; the corresponding positive pattern has a homogeneity χ of 98.62%.

Clearly, if n is the number of attributes of a dataset, then the set $I(P)$ of points of \mathbb{R}^n which satisfy the inequalities defining a pattern P form an interval of \mathbb{R}^n . If P^* is a prime pattern, then $I(P^*)$ is inclusionwise maximal in the family of all intervals $I(P)$ (i.e., no constraint of the type $x \leq a$ appearing in their definition can be relaxed to $x \leq a'$ with $a < a'$).

On the other hand, if maximality is defined in terms of the set of observations in Ω covered by a pattern, then neither the prime nor the spanned patterns are necessarily maximal. Because of the large number of possible patterns, we usually list only the coverage-wise maximal ones. In particular, Tables 5 and 6 only list the coverage-wise maximal patterns in the respective pandects.

Both prime and spanned patterns provide valuable information about the dataset. There are advantages and disadvantages associated both to the use of prime and to the use of spanned patterns. Prime patterns of low degree can be generated more efficiently than spanned patterns and are more easily comprehensible. In classification problems in which the primary criterion is to not leave any new observation “unclassified”, they are the preferred tool. On the other hand, spanned patterns usually have higher degrees, and are more “conservative” than the prime ones. It was shown in [6] that classifications based on models using spanned patterns are more “robust”, having usually fewer errors, at the cost of

Table 3 Dissimilarities for k -means clustering

	k -means clustering		
	$k = 2$	$k = 3$	$k = 4$
Attribute space	91.15%	95.28%	95.07%
Pattern space	95.95%	96.54%	97.29%

leaving somewhat larger numbers of observations unclassified. It will be seen below that prime patterns are the major tool used in the proposed approach to class discovery, while the proposed attribute analysis procedures are mostly based on information provided by spanned patterns.

It is clear that the “most interesting” patterns are those which have *low degrees* (i.e., high explicative power due to their intuitive nature), *high prevalences* (i.e., high reliability, due to the fraction of observations covered by them), and *high homogeneity* (i.e., highly informative, due to their strong bias). The set of all patterns of a given sign σ^* , type τ^* , degree at most δ^* , prevalence at least π^* , and homogeneity at least χ^* will be called the $(\sigma^*, \tau^*, \delta^*, \pi^*, \chi^*)$ -*pandect* of the dataset Ω . It should be noted that beside the positive and the negative pandects (for which σ^* is “+” or “-”, respectively), we shall also consider the pandect of all positive or negative patterns with the given characteristics; we shall use the symbol “ \pm ” to indicate this type of pandect.

It has been shown in [7,8] that the $(\sigma^*, \tau^*, \delta^*, \pi^*, \chi^*)$ -pandect can be generated (for a fixed δ^*) in polynomial time in the input size (i.e., the number n of variables and the number m of observations). If δ^* is not fixed, this set can still be generated in total polynomial time (i.e., in n, m and the number c of conjunctions). The generation algorithms of prime and spanned patterns will be briefly outlined in the next section.

In numerous case studies ([1,2,5,6,9,12,16,24], etc) it was noticed that the most informative pandects were those with δ^* equal 2 or 3, or (rarely) 4; usually $\delta^* \geq 5$ lead to a phenomenon resembling statistical overfitting. The values of π^* had substantial variations (5–80%) in the case studies examined, being usually in the 10–50% range. Finally, χ^* was usually restricted to the 90–100% range, reaching however, in the extreme case of “inseparable” and “unbalanced” data ([6,25]) values as low as 16.5%.

Since the patterns can be seen as new, synthetic attributes, the pandect defines a new way of representing observations. Each observation can be represented in the *pattern space* corresponding to a pandect as a binary vector, whose j th component indicates whether the observation is or is not covered by the j th pattern. Similarly, the attributes can be represented as ternary vectors in another pattern space corresponding to a pandect, the $(-1,0,1)$ component j of which indicates whether the attribute’s values are bounded from above/are unrestricted / are bounded from below in the definition of pattern j .

Pandect-based classification is one of the essential and well-known applications of LAD (see e.g., [2,5,6,12,15,25]). The purpose of this paper is to describe two other applications of LAD, one being a new *class discovery* technique

based on clustering in the binary pattern space of a pandect, and the other being an *attribute analysis technique*, based on the role of variables in the corresponding ternary pattern space.

3 Pandect generation

3.1 Generation of prime patterns

The algorithm evaluates the (positive and negative) prevalence, degree, and homogeneity of all possible conjunctions (intervals) in the dataset, and selects subsequently only those which satisfy the pandect-defining degree, prevalence, and homogeneity requirements.

The basic component of the algorithm is the calculation of the positive and of the negative prevalences of each interval in the discrete space. While the algorithm for calculating these prevalences is given in [9] for the general n -dimensional case, its basic principles will be illustrated here for the special case $n = 2$. The attributes are denoted X and Y , and take values in the sets $\{0, 1, \dots, p\}$ and $\{0, 1, \dots, q\}$, respectively. We shall denote an *interval* in the two dimensional discrete space as $I = [(i, j), (k, l)]$ ($i \leq k, j \leq l$), and shall indicate by $Cov^+(I)$ and $Cov^-(I)$ the number of positive, respectively negative, elements of the dataset contained in I .

We shall illustrate the way the algorithm calculates prevalences on the positive case. The algorithm starts by associating to Ω the matrix M , whose entries are $m_{ij} = Cov^+([(i, j), (i, j)])$, and aims at calculating a sequence of matrices leading to a matrix $R^{(0,0)}$ whose elements are the positive prevalences of each of the discrete intervals. In most cases, m_{ij} takes the values 0 or 1, since it is assumed that there is no duplication of observations.

For every pair of integers $k \in \{0, 1, \dots, p\}$ and $l \in \{0, 1, \dots, q\}$, the algorithm recursively constructs matrices $R^{(k,l)}$, where for each $i \leq k, j \leq l$, the entry (i, j) of $R^{(k,l)}$ is defined as $r_{i,j}^{(k,l)} = Cov^+([(i, j), (k, l)])$. The first matrix, $R^{(p,q)} = R$ can be calculated as follows:

```
R:=M;
For i:=p downto 0 do
For j:=q - 1 downto 0 do ri,j:=ri,j+1 + ri,j;
For j:=q downto 0 do
For i:=p - 1 downto 0 do ri,j:=ri+1,j + ri,j;
```

The recursive computation of $R^{(k,l)}$ is based on the enumeration of the pairs (k, l) , $k \in \{0, 1, \dots, p\}$ and $l \in \{0, 1, \dots, q\}$, by utilizing a generalized form of Gray code [23], which makes it possible: (a) to generate every pair between (0,0) and (p,q) exactly once, and (b) to assure that any two consecutive pairs differ in exactly one component, and by exactly one unit. As soon as the matrix $R^{(p,q)}$ is computed, the recursion can proceed to the next pair in the Gray sequence. Denoting the current pair by (k, l) , the next element if the Gray sequence is defined as one of pairs $(k+1, l)$, $(k-1, l)$, $(k, l+1)$, $(k, l-1)$. In the case when the next pair is $(k, l-1)$, the corresponding matrix is calculated as follows:

Table 4 Positive content of nearest neighborhood

R	Average proportion of positive cases in C^* (%)	Average proportion of positive cases in C' (%)
1.50	99	35
1.75	98	35
2.00	98	37
2.50	98	45
3.00	96	54
3.50	95	52
4.00	90	46

```
R := R(k,l);
For i:=0 to p do
{For j:=0 to l - 1 do ri,j:=ri,j - ri,l;
For j:=l to q do ri,j:=ri,j + ri,l-1;}

```

The calculation of the following matrix in the other three cases is defined in a similar way.

Example. Let $p = 3, q = 3$, and let Ω be a dataset. The number m_{ij} of positive elements (i, j) in Ω is shown in the matrix M . The Gray code defines the sequence: (3,3), (3,2), (3,1), (3,0), (2,0), (2,1), \dots , (0,0). The corresponding matrices are $R^{(3,3)}, R^{(3,2)}, \dots, R^{(0,0)}$. We start by calculating

$r_{i,j}^{(3,3)} = \sum_{s=i}^3 \sum_{t=j}^3 m_{st}$; for example, $Cov^+[(1, 1), (3, 3)] = r_{1,1}^{(3,3)} = 8$. In the following step we calculate the matrix $R^{(3,2)}$, etc.

$$M = \begin{pmatrix} m_{00} & m_{01} & m_{02} & m_{03} \\ m_{10} & m_{11} & m_{12} & m_{13} \\ m_{20} & m_{21} & m_{22} & m_{23} \\ m_{30} & m_{31} & m_{32} & m_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 \\ 2 & 2 & 2 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix},$$

$$R^{(3,3)} = \begin{pmatrix} 17 & 11 & 7 & 3 \\ 13 & 8 & 4 & 1 \\ 10 & 7 & 4 & 1 \\ 3 & 2 & 1 & 0 \end{pmatrix}, \quad R^{(3,2)} = \begin{pmatrix} 14 & 8 & 4 & 7 \\ 12 & 7 & 3 & 4 \\ 9 & 6 & 3 & 4 \\ 3 & 2 & 1 & 1 \end{pmatrix}, \dots,$$

$$R^{(0,0)} = \begin{pmatrix} 1 & 1 & 2 & 4 \\ 3 & 4 & 5 & 7 \\ 5 & 8 & 11 & 14 \\ 6 & 10 & 14 & 17 \end{pmatrix}.$$

Making a similar calculation for the negative prevalences of each interval, we have all the information necessary to enumerate all the positive patterns satisfying the prescribed requirements. The number of operations (additions) Op necessary to generate all the prime patterns satisfies $Op \leq 2^n c$, where c is the number of conjunctions. Clearly, if the number n of attributes is small, the algorithm is linear in the size of the output.

In order to illustrate the efficiency of the algorithm for generation of prime patterns, we present in Table 1 the number of patterns which are generated in the **bcw** dataset for $\delta^* = \{2, 3, 4\}$, $\pi^* = 10\%$ and $\chi^* = 90\%, 95\%$, and 100% , as well as their generation time on a Pentium III 1 GHz processor.

3.2 Generation of spanned patterns

An incremental polynomial time algorithm using a consensus-type approach was developed in [6] for the generation of all the spanned patterns in a dataset. The well-known method of consensus was proposed by Blake [11] and Quine [26] for finding prime implicants of a Boolean function. Malgrange [24] used a consensus-type approach to find all the maximal submatrices consisting of the 1s of a 0–1 matrix. Also, a consensus-type algorithm for finding all maximal bicliques of a graph was presented in [4].

Consensus-type methods enumerate the family of all maximal objects of a certain collection, by starting from a sufficiently large set of objects, and systematically completing it by the application of two simple operations. The operation of *consensus adjunction* associates to a pair of objects in the given collection, one or more new objects, and adds them to the collection. The operation of *absorption* removes from the collection those objects which are “dominated” by other objects in the collection. The two operations are repeated as many times as possible, leading eventually to a collection consisting exactly of all the maximal objects.

Below we describe the proposed algorithm [7] for the generation of all the positive spanned patterns in a dataset. The negative spanned patterns can be generated in a similar way.

We shall briefly present here a particular variant of the consensus method, which produces the complete collection of all its spanned positive patterns, restricting our attention only to the case of pure patterns. For any two integers a_i, b_i with $0 \leq a_i \leq b_i \leq k_i$, we denote by $[a_i, b_i]$ the interval of integers $\{a_i, a_i + 1, \dots, b_i\}$, and we represent an n -dimensional interval as $[a_1, b_1] \times \dots \times [a_n, b_n]$. Let $P = [a_1, b_1] \times \dots \times [a_n, b_n]$ and $P' = [a'_1, b'_1] \times \dots \times [a'_n, b'_n]$ be a pair of positive pure spanned patterns, and let P'' be the interval $[a''_1, b''_1] \times \dots \times [a''_n, b''_n]$, where $a''_i = \min\{a_i, a'_i\}$ and $b''_i = \max\{b_i, b'_i\}$, $i = 1, \dots, n$. If P'' is a positive pure pattern, then it is called the *consensus* of the pure patterns P and P' . Clearly, a pair of positive spanned pure patterns can have at most one consensus, which is the pure pattern spanned by the observations covered by P or P' . We say that the positive spanned pure pattern P *absorbs* the positive spanned pure pattern P' if $P = P''$.

The proposed algorithm for generating all positive spanned pure patterns runs as follows. Let us start with the collection $C := C_0$ of all those spanned patterns, which cover exactly one observation in Ω^+ . The collection C will be augmented by the inclusion of additional patterns. More precisely, at each stage, we shall select a pair of patterns P_0 in C_0 and P in C , whose consensus P' exists and is not already contained in C , and add P' to C . This operation will be repeated until the collection C cannot be enlarged anymore in this way. It was proved in [6] that at this stage, C will consist exactly of the collection of all spanned patterns.

Example. We shall illustrate the algorithm for the dataset Ω consisting of the four observations $\omega_1 = (1,0,2)$, $\omega_2 = (0,2,0)$, $\omega_3 = (3,1,1)$, $\omega_4 = (2,0,2)$, where ω_1, ω_3 , and ω_4 are positive, and ω_2 is negative. The input collection C_0 is $\{P_1 = [1,1] \times$

$[0,0] \times [2,2], P_3 = [3,3] \times [1,1] \times [1,1], P_4 = [2,2] \times [0,0] \times [2,2]\}$. Initialize $C := C_0$. Perform consensus adjunction for the pair of patterns P_1 in C_0 and P_3 in C : the candidate for consensus is $P_{1,3} = [1,3] \times [0,1] \times [1,2]$, covering the positive observations $\omega_1, \omega_3, \omega_4$; since $P_{1,3}$ is not contained in C , it is added to C . Perform consensus adjunction for the pair of patterns P_1 in C_0 and P_4 in C : the candidate for consensus is $P_{1,4} = [1,2] \times [0,0] \times [2,2]$, covering the positive observations ω_1, ω_4 ; since $P_{1,4}$ is not contained in C , it is added to C . Perform consensus adjunction for the pair of patterns P_3 in C_0 and P_4 in C : the candidate for consensus is $P_{3,4} = [2,3] \times [0,1] \times [1,2]$, covering the positive observations ω_3, ω_4 ; since $P_{3,4}$ is not contained in C , it is added to C . The consensus of any other pair of patterns from C and C_0 is contained in C . The algorithm stops and outputs the family of all positive pure spanned patterns $C = \{P_1, P_3, P_4, P_{1,3}, P_{1,4}, P_{3,4}\}$.

The proof of correctness of this algorithm (i.e. of the fact that it stops after a finite number of steps, coinciding at termination with the list of all pure spanned positive patterns), as well as its worst-case complexity, are presented in [6]. The algorithm runs in incremental polynomial time, its total running time being $O(\beta m_+(m + m_+n))$, where β is the number of positive spanned pure patterns, and m_+ is the number of positive observations in the dataset. In order to illustrate the efficiency of the proposed algorithm, we present in Table 2 the computational time when applying it to the **bcw** dataset.

In all real-life applications encountered, the number of spanned pure patterns was extremely high. In view of this fact, it was important to apply various filtering mechanisms to restrict the number of pure patterns produced, and to keep in this way both time and memory requirements at an acceptable level. The final list of pure spanned patterns is obtained from the list C , based on several selection criteria, which include restrictions on the number of pure patterns produced, and the total time allocation.

Applications of patterns

One of the most important applications of the collections of positive and negative patterns is the construction of classifiers (see [13, 10]). The basic idea of pattern-based classification is the following.

- (i) If a new observation (i.e., one which is not contained in Ω) satisfies the defining conditions of some of the positive (negative) patterns in the collection, but does not satisfy the defining conditions of any negative (positive) pattern in the collection, then this observation is classified as positive (negative).
- (ii) If an observation satisfies the defining conditions of some positive and some negative patterns, then a weighting criterion ([10]) is applied to determine the classification.
- (iii) In case that a new observation does not satisfy the defining conditions of any positive or negative pattern in the collection, the observation is left unclassified; it should

Table 5 Pandect of pure prime patterns having degrees ≤ 3 and positive (negative) prevalences $\geq 30\%$ (respectively, 50%)

Pattern		Pattern description									Prevalence (%)	
Name	Sign	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	Positive	Negative
P1	+		≥ 4					≥ 4			54	0
P2	+		≥ 4	≥ 4				≥ 4			52	0
P3	+		≥ 4		≥ 2				≥ 2		51	0
P4	+			≥ 2	≥ 5.5						46	0
P5	+		≥ 3		≥ 5.5						46	0
P6	+	≥ 6.5	≥ 4								44	0
P7	+		≥ 4			≥ 3			≥ 4.5		44	0
P8	+	≥ 3.5	≥ 2		≥ 5.5						42	0
P9	+	≥ 3.5			≥ 5.5			≥ 2			42	0
P10	+				≥ 5.5	≥ 3		≥ 2			41	0
P11	+			≥ 5.5	≥ 2				≥ 3.5		40	0
P12	+		≥ 2		≥ 5.5	≥ 3					40	0
P13	+	≥ 6.5		≥ 4			≥ 2.5				40	0
P14	+				≥ 5.5		≥ 4.5	≥ 2			39	0
P15	+		≥ 2		≥ 5.5		≥ 4.5				39	0
P16	+			≥ 4			≥ 4.5		≥ 4.5		38	0
P17	+			≥ 4	≥ 4				≥ 2		38	0
P18	+		≥ 4				≥ 4.5		≥ 4.5		38	0
P19	+				≥ 5.5			≥ 4			38	0
P20	+			≥ 5.5		≥ 3			≥ 4.5		37	0
P21	+				≥ 5.5		≥ 5.5				37	0
P22	+		≥ 4			≥ 5					36	0
P23	+	≥ 3.5			≥ 5.5				≥ 2		36	0
P24	+				≥ 5.5	≥ 3			≥ 2		36	0
P25	+		≥ 4							≥ 1.5	36	0
P26	+				≥ 5.5		≥ 4.5		≥ 2		34	0
P27	+			≥ 4						≥ 1.5	33	0
P28	+	≥ 6.5		≥ 4		≥ 3					33	0
P29	+	≥ 6.5		≥ 4					≥ 3.5		31	0
P30	+		≥ 3							≥ 2	30	0
N1	-		≤ 3				≤ 2.5		≤ 3.5		0	91
N2	-		≤ 3			≤ 3.5	≤ 2.5				0	90
N3	-		≤ 3	≤ 3			≤ 2.5				0	90
N4	-	≤ 6.5				≤ 3.5	≤ 2.5				0	89
N5	-			≤ 3			≤ 2.5			≤ 4	0	89
N6	-	≤ 6.5	≤ 2				≤ 4.5				0	89
N7	-		≤ 4				≤ 2.5		≤ 2		0	89
N8	-			≤ 4			≤ 2.5		≤ 2		0	88
N9	-	≤ 5	≤ 3				≤ 2.5				0	88
N10	-	≤ 5		≤ 3			≤ 2.5				0	86
N11	-		≤ 2				≤ 2.5			≤ 2.5	0	86
N12	-		≤ 2				≤ 2.5	≤ 4			0	85
N13	-		≤ 4			≤ 2.5	≤ 2.5				0	85
N14	-	≤ 5		≤ 2			≤ 4.5				0	85
N15	-			≤ 4		≤ 2.5	≤ 2.5				0	85
N16	-		≤ 2			≤ 2.5	≤ 4.5				0	84
N17	-					≤ 2.5	≤ 2.5	≤ 4			0	84
N18	-		≤ 2	≤ 2			≤ 4.5				0	83
N19	-	≤ 6.5			≤ 2.5	≤ 2.5					0	83
N20	-			≤ 2		≤ 2.5	≤ 4.5				0	80
N21	-	≤ 5		≤ 2	≤ 2.5						0	80
N22	-		≤ 4				≤ 4.5	≤ 2.5			0	66
N23	-			≤ 5.5			≤ 4.5	≤ 2.5			0	66
N24	-	≤ 6.5					≤ 4.5	≤ 2.5			0	66
N25	-		≤ 5.5				≤ 2.5	≤ 2.5			0	64
N26	-						≤ 2.5	≤ 2.5	≤ 5.5		0	64
N27	-					≤ 5	≤ 2.5	≤ 2.5			0	63
N28	-	≤ 6.5			≤ 2.5			≤ 2.5			0	61
N29	-	≤ 3.5	≤ 3	≤ 3							0	61
N30	-	≤ 3.5		≤ 3			≤ 5.5				0	61
N31	-	≤ 3.5	≤ 3				≤ 4.5				0	60
N32	-	≤ 3.5			≤ 5.5		≤ 4.5				0	60
N33	-	≤ 3.5		≤ 3		≤ 3.5					0	60
N34	-	≤ 3.5					≤ 5.5		≤ 2		0	59
N35	-	≤ 3.5		≤ 3				≤ 4			0	59

Table 5 (Continued)

Pattern		Pattern description									Prevalence (%)	
Name	Sign	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	Positive	Negative
N36	-	≤ 3.5	≤ 2								0	59
N37	-	≤ 3.5		≤ 4	≤ 2.5						0	58
N38	-	≤ 3.5		≤ 2							0	58
N39	-	≤ 3.5			≤ 2.5		≤ 5.5				0	58
N40	-	≤ 3.5				≤ 2.5			≤ 4.5		0	57
N41	-	≤ 3.5				≤ 2.5	≤ 4.5				0	55

be mentioned that this case is extremely rare, and that in practical applications the number of cases in this situation is usually less than 1%.

Numerous applications of this technique have shown it to be highly accurate ([1, 5, 6, 10, 24]), and to have sensitivities and specificities comparable to or somewhat better than those reported in the literature.

3.3 Pattern-based clustering

In their original form, the observations in the dataset $\Omega = \Omega^+ \cup \Omega^-$ appear as numerical and binary vectors in the n -dimensional discrete space. The similarities and dissimilarities existing between the observations represented in this way are frequently explored ([18, 27]) by using various clustering techniques, by partitioning Ω into subsets, or “clusters”, in such a way that the pairs of observations grouped into a common cluster have a high “degree of similarity” (according to various metrics), and the pairs of observations belonging to different clusters have high “degrees of dissimilarity”.

The representation of observations in pattern space, discussed at the end of Sect. 1, makes it possible to use clustering techniques for the exploration of similarities between observations which are covered by similar sets of patterns. Given the pandect $\Pi = \{P_1, P_2, \dots, P_r, N_1, N_2, \dots, N_s\}$, each observation in $\omega \in \Omega$ is represented as an $(r + s)$ -dimensional binary vector, which indicates the patterns in Π which cover ω . The interest in clustering Ω in the space of patterns comes from the fact that patterns can be viewed as synthetic attributes which reflect more closely the positive or negative nature of an observation than the original attributes. Therefore, it can be expected that observations covered by the same (or almost the same) sets of patterns may have high degrees of similarity.

In order to compare the usefulness of clustering in pattern space vs. clustering in the original discrete space, we have carried out several k -means clustering experiments (for $k = 2, 3$ and 4) using the two representations of the observations; the results of these experiments are reported in Table 3.

In each experiment we measured the percentage of those pairs of observations x, y , (with $x \in \Omega^+, y \in \Omega^-$) which were assigned to different clusters; the results of these experiments are reported in Table 3.

It is clear that clustering in pattern space produces consistently a better separation of positive and negative points than clustering in the original discrete space of the attributes.

Based on this conclusion, we have carried out a series of pattern space-based clustering experiments on several publicly available datasets. We shall illustrate the type of results found in such applications on the bcw dataset, using the $(+, p, 3, 30\%, 100\%)$ – and the $(-, s, 3, 50\%, 100\%)$ – pandects (see Tables 5, 6). Because of space limitation, we shall only present here conclusions concerning the set Ω^+ of positive observations, although similar conclusions were also found for Ω^- . For these experiments we have applied three of the most frequently used clustering techniques: k -means clustering, partitioning k -medoids, and hierarchical agglomerative clustering (see e.g., [22] for a description of these techniques). The reason for not limiting these experiments to the well-known k -means clustering technique is the fact that other methods (e.g., partitioning k -medoids) may be less sensitive to outliers and may work effectively for small datasets, or are independent of the selection of the number k of classes (e.g., hierarchical agglomerative clustering). It would be interesting to extend these experiments to other clustering techniques, including those of Huang [20] and of Jollois and Nadif [21].

(a) Stability Applying three-means clustering to Ω , we find that one of the three clusters, say C , contains 105 positive observations and no negative ones, while the remaining observations are clustered into a set D consisting of 404 negative observations, and no positive ones, and a set E containing both positive and negative observations.

The repeated application of k -means clustering produces usually partitionings which differ from one experiment to the other. This is a consequence of the way k -means clustering works. It starts with a random partition of the original set into k subsets, and is followed by a sequence of transfers of elements between the subsets. In view of this fact, it is surprising that the set C turns out to be very “stable”. Indeed, by repeating the same clustering 20 times, we find that the cluster C reappears without any changes in every single experiment.

Even more unexpected is the fact that a two-means clustering of Ω^+ splits the set of positive observations into two clusters, one of which, say C^* , is almost exactly the set C , differing from it only by the addition of one single supplementary observation. Again, 20 repetitions of this experiment, produce invariably C^* as one of the two clusters.

Applying the more robust *partitioning k -medoids* clustering technique [22], the same property reappears: in each of

Table 6 Pandect of pure spanned patterns having positive (negative) prevalences $\geq 35\%$ (respectively, 85%)

Pattern		Pattern description									Prevalence (%)	
Name	Sign	x ₁	x ₂	x ₃	x ₄	x ₅	x ₆	x ₇	x ₈	x ₉	Positive	Negative
P1	+		>4					>4			54	0
P2	+		>2	>4				>4			52	0
P3	+		>4	>4	>2.5			>2.5	>2		51	0
P4	+		>2	>2	>5.5						46	0
P5	+		>3		>5.5						46	0
P6	+	>6.5	>4								44	0
P7	+		>4			>2.5			>4.5		44	0
P8	+	>2.5			>5.5			>2.5			42	0
P9	+	>2.5		>4	>2.5				>2.5		42	0
P10	+		>2	>4	>2.5		>4.5		>2		42	0
P11	+	>2.5	>2		>5.5						42	0
P12	+				>5.5	>2.5		>2.5			41	0
P13	+		>2	>5.5	>2.5	>2.5		>2.5	>2.5		40	0
P14	+	>6.5		>4			>2.5				40	0
P15	+		>2		>5.5	>2.5		>2.5			40	0
P16	+		>2		>5.5		>4.5				39	0
P17	+				>5.5		>4.5	>2.5			39	0
P18	+		>2	>5.5	>2.5	>2.5		>2.5	>2		39	0
P19	+		>2	>5.5	>2.5	>2.5	>2.5	>2.5	>2		39	0
P20	+		>4	>2	>2.5	>2.5	>4.5		>4.5		38	0
P21	+		>2	>4	>4			>2.5	>2		38	0
P22	+		>2	>4			>4.5		>4.5		38	0
P23	+				>5.5			>4			38	0
P24	+		>2	>5.5		>2.5			>4.5		37	0
P25	+				>5.5		>5.5				37	0
P26	+		>4			>5					36	0
P27	+	>2.5			>5.5				>2		36	0
P28	+				>5.5	>2.5		>2.5	>2		36	0
P29	+		>4							>1.5	36	0
P30	+	>5	>4			>2.5			>2		35	0
N1	-		≤3				≤2.5		≤3.5		0	91
N2	-	≤6.5	≤3				≤2.5		≤3.5		0	90
N3	-		≤3			≤3	≤2.5				0	90
N4	-		≤3				≤2.5		≤3.5	≤2	0	90
N5	-		≤4			≤3	≤2.5			≤4	0	90
N6	-		≤3	≤3			≤2.5				0	90
N7	-	≤6.5			≤4		≤2.5		≤3.5		0	89
N8	-	≤6.5				≤3	≤2.5				0	89
N9	-	≤6.5	≤2				≤4.5				0	89
N10	-		≤3	≤3			≤2.5			≤4	0	89
N11	-		≤3				≤2.5	≤4	≤3.5		0	89
N12	-		≤3	≤4		≤3	≤2.5			≤4	0	89
N13	-	≤5	≤4				≤4.5		≤2		0	89
N14	-	≤6.5	≤3	≤3			≤2.5				0	89
N15	-	≤5		≤4			≤4.5		≤2		0	89
N16	-	≤6.5		≤3	≤4		≤2.5				0	89
N17	-		≤3				≤2.5		≤2		0	89
N18	-	≤6.5		≤3		≤5	≤2.5				0	89
N19	-	≤5			≤4		≤4.5		≤2		0	89
N20	-		≤3	≤4			≤2.5		≤2		0	88
N21	-		≤4			≤3	≤2.5	≤4		≤4	0	88
N22	-	≤6.5		≤3			≤2.5		≤3.5		0	88
N23	-	≤5	≤3	≤3			≤2.5				0	88
N24	-		≤2	≤3		≤5	≤4.5				0	88
N25	-	≤5	≤4		≤4		≤2.5				0	88
N26	-	≤6.5		≤3			≤2.5	≤5			0	88
N27	-	≤6.5	≤3				≤2.5		≤2		0	88
N28	-		≤2	≤3			≤4.5	≤5			0	88
N29	-		≤2	≤4		≤5	≤4.5		≤2		0	87
N30	-		≤3				≤2.5	≤4	≤2		0	87
N31	-	≤5				≤3	≤4.5		≤2		0	87
N32	-		≤4		≤4	≤2.5	≤4.5		≤3.5		0	87
N33	-	≤5			≤4	≤5	≤2.5				0	87
N34	-		≤4	≤4	≤4	≤2.5	≤4.5		≤3.5		0	87
N35	-	≤5			≤4		≤2.5			≤2	0	87

Table 6 (Continued)

Pattern		Pattern description									Prevalence (%)	
Name	Sign	x ₁	x ₂	x ₃	x ₄	x ₅	x ₆	x ₇	x ₈	x ₉	Positive	Negative
N36	-		≤3			≤5	≤2.5	≤4	≤2		0	87
N37	-		≤2	≤4			≤4.5	≤4	≤2		0	87
N38	-	≤6.5				≤2.5	≤4.5		≤3.5		0	87
N39	-		≤3		≤4		≤2.5	≤4	≤2		0	87
N40	-	≤5			≤4		≤2.5	≤4			0	87
N41	-	≤5		≤3			≤2.5				0	86
N42	-	≤5			≤2		≤5.5			≤2	0	86
N43	-		≤2	≤4			≤2.5			≤2	0	86
N44	-		≤2	≤4			≤2.5	≤4			0	85
N45	-		≤3		≤4	≤2.5	≤2.5				0	85

Table 7 Accuracies of models using high/low ranked attributes

k	Accuracy (%) of model built on	
	Top ranked k attributes	Bottom ranked k attributes
3	81.2	62.9
4	92.5	86.3
5	93.9	94.0
6	95.3	93.2
7	95.7	94.0
8	95.5	93.4
9	95.5	95.5

20 experiments, the set C* turns out to be one of the clusters appearing among the final clusters.

Finally, applying now a third clustering technique, called hierarchical agglomerative clustering with average linkage [22], in which the number of subsets in the partition is not fixed *a priori*, the set C* reappears again.

(b) Strong positivity Within the set of positive observations Ω⁺, the subset C* displays a series of powerful characteristics indicating the positive nature of its observations, distinguishing it clearly from C' = Ω⁺ \ C*.

First, the proportion of positive observations in the neighborhood of each observation in C* is much higher than in the neighborhood of observations in C'. In order to see this, the original data were “normalized”, i.e., the measurement x_{ij} of each attribute j in observation i was replaced by (x_{ij} - μ_j)/σ_j, where μ_j and σ_j are respectively the mean and the standard deviation of attribute j in Ω. The average proportions of positive observations contained in the spheres centered in the points of C*, respectively C' are reported in Table 4. The radius R of each sphere is calculated in the Euclidean metric applied to the normalized data (as described above). Since we are only interested in the distribution of positive and negative observations within the neighborhood of points in C* and C', we taken into account those spheres whose radius is at most 4 (i.e., about 30% of the maximum distance between most of the pairs of observations).

Clearly, the proportion of positive points in the neighborhoods of the points in C* exceeds substantially that of the points in the neighborhoods of points in C', regardless to the choice of the neighborhood defining radius. Moreover, the disproportion increases rapidly when the radius decreases.

Second, the points in C* have a much stronger coverage by positive patterns than those in C'. Indeed, the proportion

of positive patterns in Π covering an average point in C* is 3 times higher (57%) than in C' (19%). Moreover, the average prevalence of the patterns covering the points in C* is significantly higher (40%) than in C' (32%).

(c) Separation The observations in C* can be separated from the other observations in Ω by the interval hull [C*] of C*, i.e., the unique minimum n-dimensional interval which includes C* in the original discrete space. Indeed, the set [C*] consists of C*, 9 addition points in Ω⁺, and 1 point in Ω⁻.

In fact, [C*] can be viewed as a spanned pattern of high prevalence (48.12%), and homogeneity (99.14%). Using the variables x₁, . . . , x₉ defined in Section 1, this pattern can be described by the system of inequalities “x₃ ≥ 2, x₄ ≥ 6, x₅ ≥ 2, and x₇ ≥ 2”. It should be remarked that after the elimination of redundancies, the resulting prime pattern “x₃ ≥ 2, x₄ ≥ 6” covers the same points as [C*]. Finally, the Fisher linear discriminant

$$y = 38.7x_1 - 9.6x_2 + 29.3x_3 - 49x_4 + 5.4x_5 - 22.4x_6 + 14x_7 - 9.7x_8 + 1.9x_9 + 2334$$

separates the entire interval [C*] from Ω \ C* with an accuracy of 99.4%.

(d) High predictability The most important consequence of the stability, the strong positivity, and the separability of [C*] is that the classification by LAD of the positive points belonging to this set is extremely accurate. Indeed, the application of 20 cross-validation experiments by two-folding, produced 4.35% errors in the set Ω⁺ \ [C*], but only 0.67% errors in [C*].

The underlying principles of the approach presented in this section bear certain similarities with the approach taken by Vrac et al. [28] in combining rule-based reasoning with clustering techniques. We are grateful to an anonymous referee who has kindly called our attention to this reference, and has also pointed out the potential of the Vrac et al. [28] approach to handle problems with more complex types of data.

3.4 Attribute analysis

An interesting application of the availability of the pandect is the possibility it offers for measuring the relative importance of the various attributes, as well as for identifying monotone

attributes. We shall illustrate this possibilities on the nine attributes of the **bcw** dataset.

3.4.1 Importance of attributes

The degree of participation of a variable in the patterns appearing in the pandect offers a valuable measure of its importance. Clearly, this analysis has to be based on spanned, rather than prime patterns, since the description of a prime pattern “hides” the implicit bounding conditions on some of the variables.

Assuming that the set of spanned patterns in the pandect $\Pi^* = \{P_1^*, P_2^*, \dots, P_u^*, N_1^*, N_2^*, \dots, N_v^*\}$, we shall define the role ρ_j of variable x_j as $w_j/(u + v)$, where w_j is the number of patterns in Π^* which include a bounding condition on x_j . The values of ρ_j for the 9 variables x_1, x_2, \dots, x_9 in **bcw** are 65%, 43%, 43.5%, 33.5%, 31.5%, 52%, 43.5%, 35.5% and 23.5%, showing that their respective ranks are 1, 5, 3, 8, 6, 2, 4, 7 and 9.

An indication of the significance of this frequency-based ranking of the variables, is shown in the following experiment. We have removed from the dataset the top ranked k variables, constructed a LAD model on the remaining variables and evaluated through cross-validation the accuracy of the classification provided by the model. After this, the experience was repeated by removing this time the bottom ranked k variables. The resulting accuracies are shown in Table 7. The results clearly demonstrate the consistently superior performance of the models built on the high ranking variables compared to those built on the low ranking ones.

3.4.2 Monotonicity of attributes

A variable x_j with the properties that: (i) no positive pattern in the pandect includes a bounding condition of the form $x_j \leq \alpha$, and (ii) no negative pattern in the pandect includes a bounding condition of the form $x_j \geq \beta$, is called a *contributor*. Similarly, a variable x_j with the properties that: (1) no negative pattern in the pandect includes a bounding condition of the form $x_j \leq \alpha$, and (2) no positive pattern in the pandect includes a bounding condition of the form $x_j \geq \beta$, is called a *blocker*. Contributors and blockers are called *monotone variables*. Clearly, if x_i is a contributor, $\omega = (x_1^*, x_2^*, \dots, x_{i-1}^*, x_i^*, x_{i+1}^*, \dots, x_n^*) \in \Omega^+$ and if $x_i^{**} \geq x_i^*$, then

$$\omega' = (x_1^*, x_2^*, \dots, x_{i-1}^*, x_i^{**}, x_{i+1}^*, \dots, x_n^*) \in \Omega^+.$$

A similar observation holds, of course, for blockers. For illustration, we mention that in the **bcw** dataset, all the nine variables are contributors.

4 Conclusions

While much of the statistical, data mining, and machine learning literature is focused on problems of classification and clustering, computational techniques can reveal important

structural characteristics of datasets. This study is aimed at describing some ways of discovering such characteristics of datasets by examining the set of its combinatorial patterns.

After defining two types of patterns (prime and spanned), and outlining some efficient enumerative algorithms for the generation of significant subclasses of such patterns, we briefly describe the possibility of using these families of patterns for classification purposes. The paper is focused on two other uses of the large families of patterns generated by the above mentioned algorithms.

The first major application described in this paper shows that a combination of classic clustering algorithms with the pattern-space representation of the observations in the dataset can lead to the discovery of new classes of observations. In particular, it is shown that the frequently analyzed breast cancer wisconsin **BCW** contains a subclass of 104 cancer patients with markedly different characteristics from those of all the other patients.

A second major application described in this paper identifies a new ranking of features which takes into account their impact on distinguishing positive cases from negative ones. An application to the **bcw** dataset shows that the accuracy of models using top-ranked features is superior to that of models using features of lower ranks. It is also shown that the family of patterns hidden in a dataset can be used for identifying features which contribute or inhibit a certain condition. It turns out that all the 9 features considered in the **bcw** dataset are contributors, i.e., an increase in their values increases the chances of a patient to have breast cancer. It should be remarked however, that in general, only a subset of the features have a contributing or inhibiting nature, while the nature of the remaining features can vary according to the particular values taken by other features.

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