

Multiple Instance Learning with MultiObjective Genetic Programming for Web Mining

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Abstract—This paper introduces a multiobjective grammar based genetic programming algorithm to solve a Web Mining problem from multiple instance perspective. This algorithm, called MOG3P-MI, is evaluated and compared with other available algorithms which extend a well-known neighborhood based algorithm (k-nearest neighbour algorithm) and with a monoobjective version of grammar guided genetic programming G3P-MI. Computational experiments show that, the MOG3P-MI algorithm obtains the best results, solves problems of k-nearest neighbour algorithms, such as sparsity and scalability, adds comprehensibility and clarity in the knowledge discovery process and overcomes the results of monoobjective version.

I. INTRODUCTION

Multiple instance learning, or multi-instance learning (MIL) introduced by Dietterich et al. [1] is a recent learning framework which has attracted interest in the machine learning community. In this learning, the teacher labels examples that are sets (also called bags) of instances. The teacher does not label whether an individual instance in a bag is positive or negative. The learning algorithm needs to generate a classifier that will correctly classify unseen examples (i.e. bags of instances).

Numerous real-world applications have found in MIL a natural way of being represented. Among these tasks we can cite text categorization [2], content-based image retrieval [3], [4], [5], drug activity prediction [6], [7] and image annotation [8], [9], [10]. In this paper, we focus on web index page recommendation problem, a specific application of web mining from a multiple-instance perspective [11]. Web index pages are pages that contain references or brief summaries of other pages. The goal is to identify whether a new web index page will interest a user or not through analyzing the web index pages that the user has browsed. The difficulty added in this learning lies in that the available information about the user is whether he or she is interested in an index page, instead of specifying the concrete links that he or she is really interested in.

This problem has been resolved both from a traditional perspective with several techniques such as k-nearest neighbour [12] and inverse document frequencies [13], and from multiple-instance perspective adapting k-nearest neighbour algorithm [11] and a monoobjective grammar guided genetic programming algorithm [14]. Here we propose, MOG3P-MI [15], a multiobjective grammar guided genetic programming

algorithm. Our main motivations to introduce multiobjective genetic programming into this field are two mainly:

- First, grammar guided genetic programming (G3P) is considered a robust tool for classification in noisy and complex domains that overcomes the drawbacks of k-nearest neighbor (k-NN) algorithms. Although k-NN algorithms have been extensively used and have achieved an important acknowledgement in this area, these algorithms become hard to scale them to a large number of items, maintaining reasonable prediction performance and accuracy. This is due to they require computations that grows linearly with the number of items. Moreover the discovered knowledge is not understandable, they give no information about the user preferences. On the contrary, G3P not only obtains competitive results, but also adds comprehensibility and clarity in the knowledge discovery process, expressing the information in the form of IF-THEN prediction (classification) rules.
- Second, genetic programming with multiobjective strategy allows us to obtain a set of optimal solutions that represent a trade-off between different rule quality measurements, where no one can be considered to be better than any other with respect to all objective functions. Then, we could introduce preference information to select between this set of optimal solutions, the solution which offers the best classification guarantee with respect to new data sets.

Experimental results for solving this problem show that this approach obtains the best results in terms of accuracy, recall and precision. MOG3P-MI allows to discover user preferences in web page recommendation tasks and generates a simple rule based classifier that increases generalization ability, includes interpretability and clarity in the discovery knowledge providing information about user's interest and classifies new examples (web pages) quickly.

The rest of this paper is organized as follows. Section 2 presents Web Index Recommendation problem. Section 3 describes the proposed MOG3P-MI algorithm. Section 4 reports experimental results. Finally, section 5 presents the conclusions and future works.

II. WEB INDEX RECOMMENDATION PROBLEM

Web Index Pages are pages that provide titles or brief summaries of other pages. These pages contain plentiful

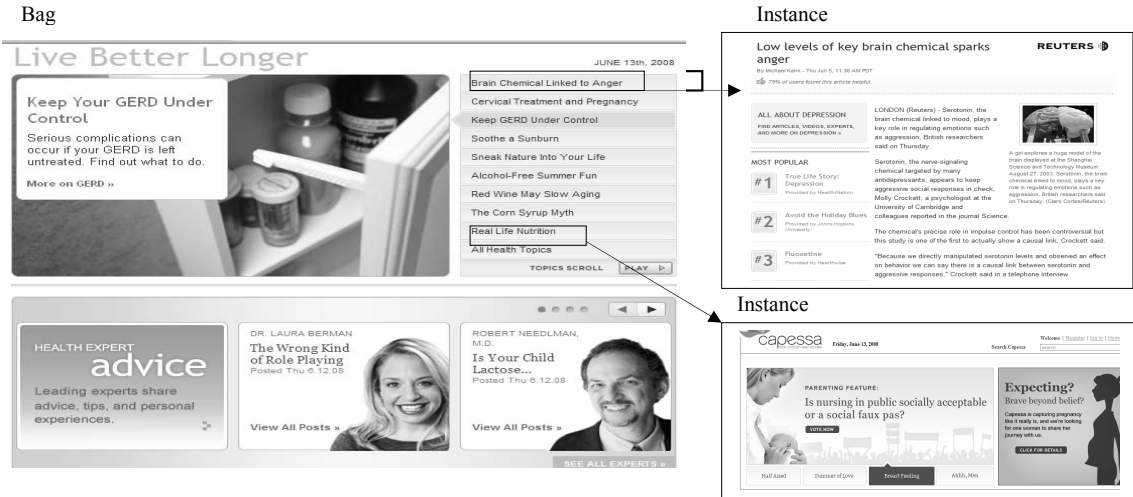


Fig. 1. Web index page and its multi-instance representation

information by means of references, leaving the detailed presentation to their linked pages. An example of a web index pages is the health entry of Yahoo (<http://health.yahoo.com>), it is shown in Figure 1.

There are many web index pages on Internet. Some of these pages may contain issues interesting to the web user while some may not. It would be interesting to analyze automatically these pages and to show to the user only the pages which contain issues interesting for him or her. To do that, it is necessary to identify the users' interests through analyzing the web index pages that the user has browsed and decide on if a new web index page will interest the user or not. This problem, called web index recommendation, is a specific web usage mining task whose goal is to label unseen web index pages as positive (the page is interesting for user) or negative (the page is not interesting for user). The main difficulty is that the user only specifies whether he or she is interested in an index web page, instead of specifying the concrete links that he or she is really interested in or the number of interesting links.

This idea can be particularly well represented as a multi-instance problem. A positive web index page is such a page that the user is interested in at least one of its linked pages. A negative web index page is such a page that none of its linked pages interested the user. To do this, we choose to represent an index web page as a set of vectors (i.e. a bag), each vector describes one of its linked pages and represents an instance in the bag. A linked page could be described by means of any of the representations used habitually in text categorization [16]. We use a bag of terms appearing on the page along with its frequency in the page. The number of terms considered is fixed and represents the most frequent terms appearing on the corresponding linked page without taking account trivial terms.

Thus, formally, each instance is represented by feature vectors, $T = [t_1, t_2, \dots, t_n]$, where t_i ($i = 1, 2, \dots, n$) is one

of the n most frequent terms appearing in the corresponding linked page. T is obtained accessing the linked page and then counting the occurrence of different terms.

For different bags, since their corresponding web index pages may contain different number of links, the number of instances in the bags may be different. A web index page linking to m pages, i.e. a bag containing m instances, can be represented as $[t_{11}, t_{12}, \dots, t_{1n}], [t_{21}, t_{22}, \dots, t_{2n}], \dots, [t_{m1}, t_{m2}, \dots, t_{mn}]$.

III. MULTI-OBJECTIVE MULTIPLE-INSTANCE GENETIC PROGRAMMING

In this section we describe MOG3P-MI algorithm. Two important factors have motivated to design this algorithm. On the one hand, G3P allows to generate an understandable rule based classifier. It is well-known exceptional properties of these systems with respect to include understandable and clarity in the discovery knowledge [17], [18]. On the other hand, multiobjective strategies are especially appropriate for classification tasks because the several measures for evaluating the solutions are related, thus if we maximize the value of any of them, the value of others can be significantly reduce. Therefore, there is not a single solution that simultaneously minimizes/maximizes the different measures, but a set of them, called Pareto Front, that have the same performance for solving the problem. It is very interesting to obtain this set of solutions and analyze which of them could be more interesting for classifying new examples.

For this reason, multiobjective techniques for evolutionary computation have been widely used on classification topics where they have researched important improvements in results [19], [20], [21]. If we evaluate its use in Genetic Programming (GP) [22], we can find that it provides solutions comparable to or better than those attained using standard GP with lower computational cost [23], [24], [25].

In this section we specify different aspects which have been taken into account in the design of the MOG3P-MI algorithm,

<pre> <cond> = <comp> "OR" <cmp> <cond> "AND" <comp> <cond> <cmp> = <op> <term_name> <op> = "Contains" "NotContains" <term_name> = Any valid term name </pre>	<pre> <cond> = <comp> "OR" <cmp> <cond> "AND" <comp> <cond> <cmp> = <op> <term_name> <freq_value> <op> = "<" ">=" <term_name> = Any valid term name <term_freq> = Any valid frequency value for term </pre>
(a) Boolean representation of pages	(b) Numerical representation of pages

Fig. 2. Grammars used in the web index recommendation problem

such as individual representation, genetic operators, fitness function and evolutionary process.

A. Individual Representation

In the MOG3P-MI, as in G3P-MI, individuals represent rules that determine if a bag should be considered positive (that is, is an instance of the concept we want to represent) or negative (if it is not).

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if  $cond_B(\text{bag})$  then
     $\text{bag}$  is an instance of the concept.
else
     $\text{bag}$  is not an instance of the concept.
end if

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where $cond_B$ is a condition that is applied over the bag. Considering the multi-instance perspective, $cond_B$ can be expressed as:

$$cond_B(\text{bag}) = \bigvee_{\forall \text{instance} \in \text{bag}} cond_I(\text{instance})$$

where \bigvee is the disjunction operator, and $cond_I$ is a condition that is applied over every instance contained in a given bag¹.

Given that the only variable part in the last expressions is the condition that is applied to instances (that is, $cond_I$), the individuals genotype represents this part, while phenotype represents the whole rule that is applied over the bags.

Figure 2 shows the two grammars used to represent individual genotypes for the web index recommendation problem. The first one is applied when we use a boolean representation for web pages, and generate expressions that inform about the presence/absence of a term in the web pages (instances). The second grammar is applied in the case of using term frequency representation for web pages, and informs about if a term is present with a frequency more or less than a value.

B. Genetic Operator

The elements of the next population are generated by means of two operators: crossover and mutation.

1) *Crossover*: The crossover [27] is performed by swapping the subtrees of two parents for two compatible points randomly selected in each parent. Two tree nodes are compatible if their subtrees can be swapped without producing an invalid

¹This expression is equivalent to the one used to define the concept of multi-instance rule coverage in the RIPPER-MI algorithm [26].

individual according to the defined grammar. If any of the two offspring is too large, they will be replaced by one of their parents.

2) *Mutation*: The mutation operator [27] randomly selects a node in the tree and the grammar is used to derive a new subtree which replaces the subtree in this node. If the new offspring is too large, it will be eliminated to avoid having invalid individuals.

C. Fitness Function

The fitness function evaluates the quality of each individual according to two measures that are normally used to evaluate the accuracy of algorithms in supervised classification problems [28], [29]. These are sensitivity and specificity. Sensitivity is the proportion of cases correctly identified as meeting a certain condition and specificity is the proportion of cases correctly identified as not meeting a certain condition.

The adaptation of these measures to the MIL field needs to consider the bag concept instead of the instance concept. In this way, their expression would be:

$$sensitivity_{MI} = \frac{t_p}{t_p + f_n} \quad (1)$$

$$specificity_{MI} = \frac{t_n}{t_n + f_p} \quad (2)$$

where true positive (t_p) represents the cases where the rule predicts that the bag has a given class and the bag does have that class. True negative, (t_n), are cases where the rule predicts that the bag does not have a given class, and indeed the bag does not have it. False negative, (f_n) cases are where the rule predicts that the bag does not have a given class but the bag does have it. False positive, (f_p) cases are where the rule predicts that the bag has a given class but the bag does not have it. The evaluation involves a simultaneous optimization of these two conflicting objectives where a value of 1 in both measurements represents a perfect classification. Normally, any increase in sensitivity will be accompanied by a decrease in specificity. With this multiobjective algorithm, we want to find such solutions and then we use other considerations to choose one of them for implementation because none of these solutions can be said to be superior if we do not include preference information.

D. Evolutionary Algorithm

The main steps of our algorithm are based on the well-known Strength Pareto Evolutionary Algorithm 2 (SPEA2) [30]. This algorithm designed by Zitzler, Laumanns and Thiele is a Pareto Front based multi-objective evolutionary algorithm that introduces some interesting concepts, such as an external elitist set of non-dominated solutions, a nearest neighbour density estimation technique, a truncation method that guarantees the preservation of boundary solutions and a fitness assignment schema which takes into account how many individuals each individual dominates and is dominated by. The general outline of our algorithm is the following:

Algorithm 1 MOG3P-MI

- 1: Generate initial population of rules, P_0 and empty archive (external set) A_0 .
 - 2: Set $t = 0$.
 - 3: **repeat**
 - 4: Calculate fitness values of individuals in P_t and A_t .
 - 5: $A_{t+1} =$ nondominated individuals in P_t and A_t .
 - 6: **if** size of $A_{t+1} > N$ **then**
 - 7: Reduce A_{t+1} .
 - 8: **else if** size of $A_{t+1} < N$ **then**
 - 9: Fill A_{t+1} with dominated individuals in P_t and A_t .
 - 10: **end if**
 - 11: Fill mating pool with binary tournament selection with replacement on A_{t+1} .
 - 12: Apply recombination and mutation operators to the mating pool and set P_{t+1} to the resulting population.
 - 13: Set $t = t + 1$
 - 14: **until** acceptable classification rule is found or the specified maximum number of generations has been reached.
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IV. EXPERIMENTS AND RESULTS

To evaluate the suitability of MOG3P-MI in solving the web index recommendation problem, we have compare its results with G3P-MI [14] (a previous version of the algorithm with monoobjective fitness) and with the results reported by Zhou et al. [11] that analysed several variants of the kNN algorithm over these data sets. This section introduces data sets employed, explains some configuration aspects of the algorithms tested and analyzes the results obtained.

A. Dataset and Running Parameters

Experiments have been done in nine data sets, in each one of which one different volunteer labelled 113 web index pages according to his/her interests. For each data set, 75 web index pages are randomly selected as training bags while the remaining 38 index pages are used as test bags. We have followed exactly the same setup as Zhou et al. [11].

These data sets can be categorized into three categories. The first one comprises datasets 1 to 3, and corresponds to users that ignore a high percentage of pages (*selective users*); the second category (datasets 4 to 6) contains users that accept a

TABLE I
EXPERIMENTAL DATA SETS

Dataset	Training		Test	
	Pos	Neg	Pos	Neg
1	17	58	4	34
2	18	57	3	35
3	14	61	7	31
4	56	19	33	5
5	62	13	27	11
6	60	15	29	9
7	39	36	16	22
8	35	40	20	18
9	37	38	18	20

high percentage of received pages (*permissive users*). Finally, the third category, which we have called *balanced users*, is made up of users who accept and reject a similar percentage of pages. Table I shows a description of data sets evaluated. This categorization is interesting to notice and study the behaviour of algorithms when the information about users like and does not like is not balanced.

Both MOG3P-MI and G3P-MI algorithms have been implemented in the JCLEC framework [31]. The parameters used in all MOG3P-MI runs were: population size: 1000, generations: 100, crossover probability: 95%, mutation probability: 15%, selection method for both parents: tournament selection) and maximum tree depth 15. All experiments are repeated five times with different seeds, and average values were used in report performed in the next section.

B. Experimental Results

Table II shows results obtained over all available datasets. This table is splitted in two sections. The first one corresponds to the results obtained with a boolean page representation (see Figure 2a) while the lower section corresponds to a frequency-based numerical representation of pages (see Figure 2b).

TABLE II
GLOBAL EXPERIMENTAL RESULTS.

	Acc	Se	Sp
Fretcit-kNN	0.8103	0.7007	0.7803
Txt-KNN	0.7233	0.7380	0.4847
Citation-KNN	0.7577	0.6073	0.7407
G3P-MI	0.7810	0.7723	0.7297
MOG3P-MI	0.8480	0.7793	0.7567
Fretcit-kNN ¹	0.8043	0.7117	0.7420
Citation-KNN ¹	0.7357	0.7020	0.5283
Txt-KNN ¹	0.7630	0.6130	0.7207
G3P-MI ¹	0.7313	0.9403	0.4013
MOG3P-MI ¹	0.8420	0.8727	0.7037

¹ Using frequency of words

As we can see, MOG3P-MI achieves the most accurate, selective and specific results, obtaining the most accurate models both with boolean and numerical representations. G3P-MI algorithm gets worse results with a boolean representation. In the case of a numerical representation although it obtains slightly higher sensitivity values, decreases too much the

TABLE III
SUMMARY RESULTS

Algorithm	Selective users			Permissive users			Balanced users		
	Acc	Se	Sp	Acc	Se	Sp	Acc	Se	Sp
Txt-KNN	0.795	0.636	0.822	0.805	0.863	0.194	0.570	0.715	0.438
Citation-KNN	0.803	0.397	0.868	0.796	0.863	0.577	0.674	0.562	0.777
Fretcit-kNN	0.879	0.579	0.919	0.854	0.924	0.634	0.698	0.599	0.788
G3P-MI	0.807	0.690	0.919	0.825	0.877	0.628	0.711	0.750	0.642
MOG3P-MI	0.904	0.579	0.950	0.868	0.975	0.557	0.772	0.784	0.763
Txt-KNN ¹	0.795	0.519	0.843	0.812	0.851	0.264	0.600	0.736	0.478
Citation-KNN ¹	0.833	0.402	0.907	0.782	0.851	0.498	0.674	0.586	0.757
Fretcit-kNN ¹	0.870	0.615	0.904	0.811	0.916	0.470	0.732	0.604	0.852
G3P-MI ¹	0.845	0.821	0.904	0.823	1.000	0.201	0.526	1.000	0.099
MOG3P-MI ¹	0.895	0.774	0.919	0.860	1.000	0.466	0.771	0.844	0.726

¹ Using frequency of words

specificity values. This means that its models do not identify correctly what does not interests users and therefore they are not so dependable. With respect to the rest of techniques (kNN variants), all of them show worse results in all metrics studied. Therefore, we conclude that our algorithm is more reliable (that is, it achieves better balanced results both user interests and does not interest) getting in all cases the best results in global accuracy.

With regard to the study over different kinds of data sets, Table 3 shows the results grouped by the different types of users. As can be seen in the first column, MOG3P-MI gets competitive results in the case of selective users, with very accurate and specific profiles (better accuracy and specificity values) without an important losing of sensitivity values. This result is specially important, because in this case there is not enough information about the interests of users and learning correctly their preferences is a specially difficult task. The second column shows the results in the case of permissive users. As can be seen, MOG3P-MI obtains better results than other techniques with respect to the sensitivity measure and similar results for the specificity measure. This case, working in the MIL framework, have a greater difficulty because, although we have enough information about the interests of the user, we do not know which specific links are of interest; we only know that the page contains at least one link that interests to the user. Even so, our new algorithm obtains competitive results, improving the accuracy obtained with respect to the other algorithms. Finally, the last column shows the results for balanced users. In this case, our algorithm remains reliable, providing the best results in both specificity and sensitivity and predicting everyone's tastes very well.

Another advantage of our system is the ability to generate comprehensive rules that are easy to understand and provide representative information about the user's interest. This comprehensibility of rules is greater when we use a boolean representation, because the use of term frequencies is less friendly than a list of user preferences. This fact can be shown in the following examples:

Firstly, we show a rule obtained for the first user/dataset using boolean representation.

IF (*no_contain financial*) \vee
(contain violence \wedge *no_contain science*) \vee
(no_contain services \wedge *no_contain web*))
THEN *Recommend page to V1 user.*
ELSE *No recommend page to V1 user.*

by mean of this rule we can learn what topics can be recommended to the user. Thus, user 1 is interested in such topics as violence and is not interested in financial or services or web.

Secondly, we show a rule obtained for the first user/dataset using numerical representation.

IF (*french* $>$ 16) \vee (*house* $>$ 11) \vee
(science $>$ 2 \wedge *edt* $>$ 20) \vee
(aol $>$ 7) \vee (*online* $>$ 6))
THEN *Recommend page to V1 user.*
ELSE *No recommend page to V1 user.*

We can see that this rule is more complex because the words are limited by their frequency and it is more difficult to identify the user preferences. For this, although both representations obtain similar results, after this study we can conclude that numerical representation is less interesting because it obtains less comprehensive rules.

V. CONCLUSIONS AND FUTURE WORK

This paper describes the use of MOG3P-MI for web mining tasks from MIL perspective, specifically, for web index page recommendation problem. Its results are compared with other techniques applied over this problem. As have been proved, MOG3P-MI obtains significantly better results than other techniques in terms of accuracy, sensitivity and specificity and generates interpretable hypotheses with few terms. Also, this representation allows us to export easily acquired knowledge to new examples.

Although the results are interesting, there are still quite a few considerations that will surely increase the model results. Thus, it would be interesting to employ feature selection techniques that allow us to reduce the number of attributes considered and check if these techniques are useful in a MIL scenario. Another interesting aspect is the choice of a concrete solution to be selected from the Pareto optimal set. This set

of solutions can not determinate if one is better than another without some information about specific preferences. Thus, we are studying various measures that identify, within the set of rules obtained, which of them can be expected to be better at identifying new topics of interest for the user.

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