# A Multiobjective Genetic Programming-Based Ensemble for Simultaneous Feature Selection and Classification

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Abstract—We present an integrated algorithm for simultane-2 ous feature selection (FS) and designing of diverse classifiers 3 using a steady state multiobiective genetic programming (GP). 4 which minimizes three objectives: 1) false positives (FPs); 2) false 5 negatives (FNs); and 3) the number of leaf nodes in the tree. 6 Our method divides a c-class problem into c binary classifica- $_{7}$  tion problems. It evolves c sets of genetic programs to create c 8 ensembles. During mutation operation, our method exploits the 9 fitness as well as unfitness of features, which dynamically change 10 with generations with a view to using a set of highly relevant 11 features with low redundancy. The classifiers of ith class deter-12 mine the net belongingness of an unknown data point to the ith 13 class using a weighted voting scheme, which makes use of the 14 FP and FN mistakes made on the training data. We test our 15 method on eight microarray and 11 text data sets with diverse 16 number of classes (from 2 to 44), large number of features 17 (from 2000 to 49151), and high feature-to-sample ratio (from 18 1.03 to 273.1). We compare our method with a bi-objective GP 19 scheme that does not use any FS and rule size reduction strat-20 egy. It depicts the effectiveness of the proposed FS and rule size 21 reduction schemes. Furthermore, we compare our method with 22 four classification methods in conjunction with six features selec-23 tion algorithms and full feature set. Our scheme performs the 24 best for 380 out of 474 combinations of data sets, algorithm and 25 FS method.

26 Index Terms—Classification, ensemble, feature selection (FS), 27 genetic programming (GP).

#### I. INTRODUCTION

LASSIFICATION is one of the most important and frequently encountered problems in data mining and machine learning. A wide range of real world problems of different domains can be restated as classification problems. This includes diagnosis from microarray data, text categorization, medical diagnosis, software quality assurance, and many more. The objective of classification is to take an input vector  $\mathbf{x} = (x_1, \dots, x_d)^T$  and to assign it to one of the K classes  $C_k$ ,

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where k = 1, ..., K. A model, called classifier, is used to solve this problem. The classifier encodes a set of criteria. Bepending upon some features of the data point, these criteria assign the data point to a particular class [1]. Sometimes, ensembles of weak classifiers are used to obtain better classification accuracy. High dimensionality, high feature-to-sample ratio, and redundant and/or noisy features are some common sources of difficulties associated with classification.

Feature selection (FS) is a process to select a small but useful subset of features from the set of available features which
is adequate for solving the problem in an efficient manner.
Some available features may be redundant, not useful, and may
cause confusion during the learning phase. These unwanted
features needlessly increase the size and complexity of the feature space. It increases the computation cost for learning, and
may sometimes be responsible for finding suboptimal solutions of the problem. This makes FS techniques important for
the analysis of high dimensional data sets, especially when
feature-to-sample ratio is extremely high.

The microarray technology has made it possible to diagnose different types of cancers directly using the microarray data sets. One of the main difficulties we face to do this is the high feature-to-sample ratio of microarray data sets, which makes FS an important step. Finding keywords as well as contexts from text data is essential to detect (without human intervention) the context of web pages, emails, or questions/answers, etc. A large set of distinct words in large texts (high number of features) and many categories of texts (high number of classes) are the two complicated challenges that we face in this task.

Genetic programming (GP) [2]–[5] is a biological-evolution inspired methodology where each solution is a program or an equation that evolves with one or more objective functions to perform specific tasks. References [6]–[12] used GP to design classifiers or to generate rules for binary classification problems. Some researchers have also attempted to solve multiclass problems [13]–[17]. GP has also been used for simultaneous FS and classification [18]. Liu and Xu [19] vused GP to create ensembles of classifiers (genetic programs). They have used these ensembles to classify microarray data sets. Though GP is a powerful tool, it has a drawback: without special care each genetic program (equation) becomes huge. As an effect, they do not learn the patterns in the training data. Rather, memorizes them. It also makes genetic programs to be difficult to comprehend. Besides, though ensembles can

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<sub>82</sub> perform better than individual classifiers [20], to obtain better 83 performance, each ensemble should be diverse and each mem-84 ber of the ensemble should be accurate [20]-[22]. Without 85 special care, due to lack of explicit diversity preservation 86 mechanism, the solutions of single objective GP may lose

The objective of this paper is to find an embedded method-89 ology of simultaneous FS and classification employing GP as a 90 tool. Some of the novel contributions of our schemes are as fol-91 lows. We have introduced a new multiobjective GP (MOGP), 92 called archive-based steady state micro GP (ASMiGP). It 93 is enriched by several new operators. The mating selec-94 tion judicially uses Roulette wheel selection, instead of two 95 tire multiobjective selection scheme (where domination is 96 preferred over diversity). The crossover is new and uses male-97 female differentiation so that the off-spring is more likely to be 98 close to the female parent in the genotypic space. The mutation 99 is restrictive and performs less exploration in the hypothesis 100 space. Thus, it reduces disruption. For feature nodes, instead of fitness, mutation uses unfitness to select the mutation point. 102 Altering the fitness and unfitness of the features in different 103 stages of learning, we change the objective of searching in the 104 corresponding stages. We use ASMiGP to learn c diverse sets 105 of classifiers (equations) minimizing three objectives: 1) false 106 positive (FP); 2) false negative (FN); and 3) number of leaf 107 nodes of a tree to restrict the rule size. Throughout the learning 108 process, implicit FS is performed using MOGP, whereas sev-109 eral filter-based approaches are used in different stages of the 110 procedure. In this way, we obtain concise rules that involve only simple arithmetic operations. A weighted negative vot-112 ing is then used among the rules of each ensemble. These 113 weights are determined on the basis of the performance of 114 the binary classifiers on the training data set. A new measure of weighted negative voting, called net belongingness, is also 116 introduced.

The proposed method has been tested on eight multiclass 117 118 microarray data sets having large number of features, varying 119 from 2000 to 49 151, and high feature-to-sample ratio, vary-120 ing from 32.26 to 273.06. It has also been tested on eleven high dimensional (varying from 3182 to 26832) text data sets, where the number of classes (categories) vary from 6 to 44. 123 Experimental results reveal that our method can generate 124 ensembles of classifiers with concise rules that can do a good 125 job of classification with a small subset of features.

#### II. BACKGROUND AND RELATED WORKS

This section provides a background to GP, GP-based online 128 FS and classification, ensembles, voting schemes, and concise 129 rule finding. This section also includes some related works on 130 these topics.

#### 131 A. Concise Introduction to GP

GP [2]–[5] is an approach to find programs that can solve 133 a given problem. GP uses Darwinian principle of "survival of 134 the fittest." It evolves the programs using biologically inspired 135 genetic operations like reproduction, crossover, and mutation 136 in the search space to find such programs which would be able to solve the given problem [15], [23], [24]. The overall search 137 process of traditional single objective GP is quite similar to 138 traditional population-based genetic algorithm. The main dif- 139 ference among them is in the representation of solutions. The 140 usual steps of traditional single objective GP can be found 141 in [2], [15], and [24].

There exist several ways to encode a program. Probably, the 143 most popular one is to use a tree structure [25]-[27] which 144 we use. In tree-based GP, a program is represented by a 145 tree where the internal nodes are from a set of functions  $\mathcal{F}$ , 146 and the leaf nodes are from a set of terminals  $\mathcal{T}$ . The sub- 147 trees of a function node are the arguments of that function. 148 The sets  ${\mathcal F}$  and  ${\mathcal T}$  must satisfy the closure and sufficiency 149 properties [2], [15]. To satisfy the closure property,  $\mathcal{F}$  must 150 be well defined and closed for any combination of probable 151 arguments that it may encounter [15]. Again, to satisfy the 152 sufficiency property,  $\mathcal F$  and  $\mathcal T$  must be able to represent any 153 possible valid solution of the problem.

## B. FS: Why Embedded?

FS methods are generally divided into two main groups: 156 1) filter method and 2) wrapper method [28]. A filter method 157 does not use any feedback from the classifier or any mining 158 algorithm. It relies on the general characteristics of data. On 159 the contrary, to measure the goodness of features, a wrapper 160 method uses a predetermined classifier or mining algorithm, 161 which will finally use the selected features. Consequently, a 162 wrapper method exploits interactions among the subset of fea- 163 tures on which it is tested. But, to find an optimal set of 164 features, a wrapper method needs to measure performances 165 on all possible subsets of features. This becomes infeasible 166 for high dimensional data sets. To overcome this problem, 167 wrapper methods typically use a heuristic-based forward or 168 backward selection mechanism [28], which does not evaluate 169 all possible subsets. So, in this paper, we consider embed- 170 ded methods, where FS and designing of the classification 171 system are done together. Embedded methods do not need 172 to evaluate all possible subsets. Moreover, they can account 173 for interaction between features and the classifier that is used 174 to solve the problem [29]. Usually, embedded methods attain 175 comparable accuracy to wrapper methods as well as compara- 176 ble efficiency to filter methods. Though for every classification 177 tool it may not be easy to define such an integrated mecha- 178 nism, several attempts of FS using embedded methods have 179 already been made. These attempts include using single objec- 180 tive GP [18], neural networks [30], [31], and support vector 181 machines [32].

## C. GP in Classification and FS

Many researchers have used GP as a tool for classifi- 184 cation and FS. Some literature on this topic can be found 185 in [1] and [33]. It has been used in both filter [34]–[37] 186 and wrapper [38]-[41] approaches. GP has also been 187 used for extracting decision trees [42]–[47]. Among these 188 in [45] and [46], MOGP has been used. GP has also been 189 adopted for learning rule-based systems [7]-[9], [48]-[51]. 190 classification [6], [7], [10]-[12], [48] binary

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192 multiclass [8], [9], [13]–[17], [49]–[51] classification prob-193 lems have been addressed by GP-based (rule-based) 194 systems. have Even, researchers applied GP-based 195 (rule-based) system for binary classification of imbal-196 anced data [52], [53]. Discriminant functions (DFs)-based 197 GP for online FS and classification has been adopted 198 in [18] to solve multiclass problems. It is noteworthy 199 that GP has also been used in feature extraction for edge 200 detection [54].

Since, in this paper, we have used MOGP for learning DFs, 202 we discuss some relevant GP-based systems. In DFs-based GP, 203 each program is a mathematical equation, where the variables 204 are features of the data. Usually every program is associated 205 with a class. For every input data point, the program converts 206 it to a single output value. If this output value is more than 207 a predefined threshold (usually zero), the point belongs to the 208 class to which the program is associated with. Thus, a sin-209 gle equation is enough for binary classification problems. For 210 c-class problems, there are two common ways. The first and 211 more frequently used approach is to consider a c-class problem 212 as c binary classification problems [1]. Thus, c number of DFs 213 are used to discriminate c classes. The second and less popular <sup>214</sup> approach is to use a single DF with (c-1) threshold values to create c intervals. Each of these intervals is then assigned to a 216 particular class. For both categories, a common practice is to 217 evolve a population where each individual encodes either one 218 (for binary classification problems having single threshold, or 219 for multiclass problems having multiple thresholds) or multi-220 ple DFs each of which uses a single threshold. Such encoding schemes have been used in [15] and [18]. In another practice, 222 each solution encodes multiple DFs having a single threshold. The final output value in this case may be obtained using a (weighted) voting scheme among the output values of each 225 function of the same individual. An example of this scheme can be found in [19].

In the recent years, researchers have made some notable 227 attempts to solve classification problems using MOGP. Wang et al. [55] proposed a MOGP to obtain a group of nondominated classifiers, with which the maximum receiver operating characteristic convex hull (ROCCH) can be obtained. To achieve this, they have adopted four different multiobjec-233 tive frameworks into GP. For further improvement of each individual GPs performance, they have defined two local search strategies that have been especially designed for classification problems. The experimental results in [55] have 237 demonstrated the efficacy of the proposed memetic scheme in 238 their MOGP framework. Another convex hull-based MOGP, 239 called CH-MOGP, can be found in [56]. Wang et al. [56] 240 showed the differences between the conventional multiobjec-241 tive optimization problem and ROCCH maximization problem. Wang et al. introduced a convex hull-based sorting without 243 redundancy and a new selection procedure which are suitable 244 for ROCCH maximization problem. Again, Bhowan et al. [22] 245 proposed a MOGP-based approach that is especially designed 246 for unbalanced data sets. This approach [22] evolves diverse 247 and accurate ensembles of GP classifiers with good per-248 formance on both the majority and the minority classes. 249 The individual members of the evolved ensembles, that are composed of nondominated solutions, vote on class 250 membership.

#### D. GP, Bloating, and Concise Rules

During evolution of GP, variable length genomes gradually 253 start to increase its length without significant improvement in 254 fitness. This incident, called bloating [57], is a well known 255 phenomenon in GP. Bloating causes genetic programs: 1) to 256 keep reducible genome structures and 2) to memorize training 257 data points, rather than recognizing patterns hidden in them. 258 To find rules which are to some extent human interpretable and 259 can be analyzed, each of the genetic programs must be concise. 260 A plausible way to achieve this target is to control bloat- 261 ing. A popular way to handle bloating is to take into account 262 the program size [2], [58]-[61]. Some other methods include 263 spatially-structured populations [62], [63], island-based mod- 264 els to introduce spatial structure to the population [62], [63], 265 intron deletion [64], and dynamic population sizing [65], [66]. 266 Song et al. [67] attempted to understand the GP evolved solu- 267 tions; while Luna et al. [68] attempted to find comprehensible 268 rules in subgroup discovery.

## E. Ensemble Classifier

In classification, the basic task is to search through a 271 hypothesis space to find a suitable hypothesis that will 272 be able to classify the data points in a better way. An 273 ensemble combines multiple hypotheses to form a better 274 one [19], [21], [22], [53], [69], [70]. Empirically, an ensem- 275 ble performs better when each of the classifiers is highly 276 accurate (strong learner) and the members of the ensemble are 277 significantly diverse. The explanation behind the better perfor- 278 mance of ensemble classifiers than a single classifier has been 279 described in [20]. Normally, to decide the class label of a data 280 point, the member classifiers of an ensemble use (weighted) 281 voting. Ensembles are often used in bio-informatics [71].

#### III. PROPOSED WORK

#### A. Representation of Classifiers or Solutions

In this paper, we evolve c-populations of genetic programs. 285 Each individual of these populations is a binary classifier. Each 286 binary classifier is represented by a single tree. When a data 287 point is passed through an individual of the ith population, 288 if the output value is positive, the individual says that the 289 passed data point belongs to the ith class; otherwise it says that 290 the point does not belong to that class. The internal (nonleaf) 291 nodes of these trees are functions  $\mathcal{F}$ . The terminal nodes must 292 be either a feature or a constant from the set C. We have 293 imposed some constraint on the minimum size (architecture) 294 of the trees. In each tree there must be at least one function 295 node and two terminal nodes (with at least one feature node). 296 Though, a single feature (terminal) node might be enough to 297 determine the class label, this would rarely happen in practice. 298 The above restrictions make the trees more useful without any 299 loss of generalization capability. Again, after generation of any 300 tree throughout the learning phase (using mutation, crossover, 301 or random initialization), the largest subtree consisting of only 302

303 constants as its leaf nodes is replaced by a constant leaf node 304 having the equivalent constant value.

#### 305 B. MOGP for Learning

Larger genetic programs may memorize the training patterns 306 which, in turn, may increase the training accuracy and reduce 308 the understandability of the rules. Therefore, we aim to find smaller but accurate classifiers. Again, when c is high enough,  $_{310}$  even a balanced c-class data set may get converted to c number of highly imbalanced bi-classification data sets. Instead of 312 minimization of classification error, simultaneous minimiza-313 tion of FP and FN would be more appropriate in this regard. Suppose a classifier makes some mistakes  $m=m_p+m_n$  on a given training data set, where  $m_p$  and  $m_n$  are, respectively, the 316 number of FPs and FNs. Consider two classifiers, each making  $_{317}$  the same number of mistakes m on a given data set. Let for the 318 first classifier  $m_p = m_n$  and for the second classifier  $m_p \gg m_n$ or  $m_p \ll m_n$ . If the cost of an FP is the same as that of a FN, we would prefer the first classifier. Consequently, minimization of both FP and FN would be a better strategy than minimiza-322 tion of the total number of misclassification, particularly for 323 imbalanced data sets. Thus, we have three objectives, i.e., minimizations of: 1) FP; 2) FN; and 3) rule size. Moreover, when different classes are overlapped, minimization of FP is usually in conflict with the minimization of FN and vice versa. Multiobjective optimization is more suitable when we need to optimize more than one conflicting objective. Therefore, dur-329 ing the learning of each binary classifier, we minimize three 330 objectives using an MOGP: 1) FP; 2) FN; and 3) number of 331 leaf nodes in the tree. The third objective is used to reduce 332 the size of the tree which enhances the understandability and 333 reduces the pattern memorization capability. The algorithm, proposed in this paper, is called ASMiGP, which is presented 335 in Algorithm 1.

In an evolutionary search, it is desired to have as many generations as possible and steady state nature of an algorithm maximizes the number of generations when the number of function evaluations is fixed [72]. Due to maximization of generations, a steady state evolutionary search is more exploitative to enhance the searching in a region which is more likely to have or closer to the Pareto front and avoiding exploration in regions that are less likely to improve the solutions. It causes faster convergence. In other words, independent of the fitness evaluation process, steady state selection is more performant than discrete generational selection [73]. Therefore, we have used a steady state algorithm instead of a generational one.

#### 348 C. FS

In this paper, we have used the embedded model of FS. Explicit FS is performed during population initialization and mutation. Implicit FS is performed during crossover. Filtering is also performed at three different stages of the learning process; in particular, at the beginning and after 50% and after 55% of evaluations as described next in this subsection.

To facilitate the FS, following [74], we define an index that assesses the discriminating ability of a feature. Consider a two-class problem. Note that for a multiclass problem, the

#### **Algorithm 1:** ASMiGP

20 return first front of Fronts.

```
1 Initialize population using ramped-half-and-half method.
2 Initialize the archive solutions using initial solutions.
  while Evaluations^{Current} \leq Evaluations^{Maximum} do
       repeat
5
           operator = Select crossover or mutation.
           if operator = crossover then
6
              Select male and female parents (mating
              selection).
              Perform crossover.
8
9
           end
           else
10
              Select an individual (mating selection).
              Mutate the individual.
12
          end
       until the infix equation of off-spring is distinct from
       infix equation of any individual of the archive
       Evaluate the new off-spring.
15
       Evaluations^{Current} = Evaluations^{Current} + 1
16
       Update the archive using new offspring
17
       (multi-objective environmental selection).
18 end
  \mathcal{F}ronts = Perform fast-non-dominated-sort.
```

one-versus-all case can also be viewed as a two-class prob- 358 lem. Let there be  $n_p$  number of training points and the class 359 label for the *j*th data point be +1 if it belongs to class 1 and -1 360 if it belongs to class 2. Let the value of the fth feature for the 361 ith data point be  $f_i$ ;  $i = 1, ..., n_p$ . If the fth feature is a good 362 discriminatory feature then for all data points from class 1, 363 it should have high values and for all points from class 2, it 364 should have low values or vice-versa. Hence for a good dis- 365 criminatory feature, we can define an ideal feature vector with 366 values 1, if the data point is from class 1 and 0 otherwise; or 367 the feature value is 0, if it is from class 1, otherwise, it is 0. 368 Let  $S_f$  be the vector containing the ideal feature values for feature f and  $s_{fi}$  be the ideal feature value of the fth feature for  $_{370}$ the *i*th sample. Note that, there could other important features 371 that are not linearly related to the class structure. We are not 372 considering them in this preliminary filtering step. As in [74], 373 we compute the Pearson's correlation (or any other measure of 374 similarity) between f and s as a measure of feature relevance 375

$$C_f = \sum_{j=1}^{n_p} (s_{ji} - \bar{s}) (f_j - \bar{f}) / \sqrt{\sum_{j=1}^{n_p} (s_{ji} - \bar{s})^2 \sum_{j=1}^{n_p} (f_j - \bar{f})^2}.$$
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A higher value of  $|C_f|$  indicates a stronger discriminative power of feature f. For a multiclass problem, using the oneversus-all strategy, for the ith binary classification problem (class i versus the rest), the correlation for the fth feature is denoted by  $C_f^i$ .

Now, we describe the FS procedure. Let the set of all features be  $\mathcal{F}_{all}$ . We intend to incorporate only those features trom  $\mathcal{F}_{all}$  which are more likely to help the classifiers to 385

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386 decide the class label. We assign different fitness and unfit-387 ness measures to the features during the learning phase. To 388 remove a feature node from any tree (during mutation), we 389 select it using Roulette wheel selection on the unfitness vales of the features which are present in that tree. Similarly, when a new feature is inserted in the tree, it is selected using oulette wheel selection on the fitness values. During the first 50% evaluations, the fitness and unfitness features are defined as

$$F_{\text{fitness}}^{0\%,i}(f,i) = \begin{cases} \left(\frac{C_f^i}{C_{\text{max}}^i}\right)^2, & \text{if } \frac{\left|C_f^i\right|}{C_{\text{max}}^i} > 0.3 \\ 0, & \text{otherwise} \end{cases}$$
 (2)

$$F_{\text{unfitness}}^{0\%,i}(f,i) = 1.0 - F_{\text{fitness}}^{0\%,i} \tag{3}$$

 $_{^{397}}$  where  $C^i_{\max}=\max_{f\in\mathcal{F}_{\mathrm{all}}}|C^i_f|.$  Equation (2) sets the fitness of  $_{^{398}}$  very poor (poor with respect to its discriminating power) to 399 zero to eliminate their impact during the initial evolution. Let  $\mathcal{F}_{\text{eval}=0\%,i} \subseteq \mathcal{F}_{\text{all}}$  be the features with nonzero fitness values. 401 Basically, at this stage we are using a filter on the feature set 402  $\mathcal{F}_{all}$  to obtain a smaller feature set.

After completion of 50% evaluations for each population, 404 we find the features used in that population. Let the feature set be  $\mathcal{F}_{\text{eval}=50\%,i}$ . Then we make the fitness of all features in  $\mathcal{F}_{all} - \mathcal{F}_{eval=50\%,i}$  to zero. This is done with the assumption 407 that after 50% evaluations useful features have been used by 408 the collection of decision trees. Now, the fitness and unfitness 409 values of all features in  $\mathcal{F}_{\text{eval}=50\%,i}$  are modified according 410 to (4) and (5), respectively

$$F_{\text{fitness}}^{50\%,i}(f,i) = \begin{cases} \frac{|C_f^i|}{\sum_{\substack{f \neq g \\ g \in \mathcal{F}_{50\%,i}}} |\rho_{fg}|}, & \text{if } f \in \mathcal{F}_{\text{eval}=50\%,i} \\ 0, & \text{otherwise} \end{cases}$$

$$F_{\text{unfitness}}^{50\%,i}(f,i) = e^{-\frac{F_{\text{fitness}}^{50\%,i}\{F_{\text{fitness}}^{50\%,i}\} - \min_{f}\{F_{\text{fitness}}^{50\%,i}\} - \min_{f}\{F_{\text{fitness}}^{50\%,i}\} }$$
(5)

$$F_{\text{unfitness}}^{50\%,i}(f,i) = e^{-\frac{F_{\text{fitness}}^{50\%,i}(f,i) - \min_{f} \left\{F_{\text{fitness}}^{50\%,i}\right\} - \min_{f} \left\{F_{\text{fitness}}^{50\%,i}\right\}}$$
(5)

413 where  $\rho_{fg}$  is the Pearson's correlation between fth and gth features. Here, we try to select features with higher relevance but reducing the redundancy in the set of selected features. The fitness, defined in (4), increases when the feature is highly 417 correlated with class label. Similarly, it reduces when it is more 418 correlated with other existent features. This is done to achieve maximum relevance minimum redundancy.

After 75% function evaluations, again we take another 420 snapshot of the population. Let the existent features for the population be  $\mathcal{F}_{\text{eval}=75\%,i} \subseteq \mathcal{F}_{\text{eval}=50\%,i}$ . Then, the fitness and unfitness values of the features in  $\mathcal{F}_{\text{eval}=75\%,i}$  are defined 424 in (6) and (7), respectively

$$F_{\text{fitness}}^{75\%,i}(f,i) = \begin{cases} F_{\text{fitness}}^{0\%}(f,i), & \text{if } f \in \mathcal{F}_{\text{eval}=75\%,i} \\ 0, & \text{otherwise} \end{cases}$$
 (6)

$$F_{\text{unfitness}}^{75\%,i}(f,i) = 1.0 - F_{\text{fitness}}^{75\%,i}(f,i).$$
 (7)

#### D. Population and Archive Initialization

We initialize each population using ramped-half-and-half 428 method. While constructing the random trees, selection of ter- 429 minal nodes has been made with a probability  $p_{\text{var}}$ . To insert a 430 terminal node in a tree, a random number  $r_n$  is drawn in [0, 1]. 431 If  $r_n < p_{\text{var}}$  then a feature node is added, otherwise a constant node is added. The function nodes are chosen from the 433 set  $\mathcal{F}$ , with equal probability of inclusion for all functions. The 434 feature nodes are selected using Roulette wheel selection on 435 fitness  $F_{\text{fitness}}^{0\%}$ , defined in (2).

To initialize the archive from the initial population, we have 437 used the multiobjective archive initialization scheme present 438 in [72] and [75]. It requires two parameters: 1) maximum 439 archive size  $(N_{\text{max}})$  and 2) minimum archive size  $(N_{\text{min}})$ .

#### E. Selection of Crossover or Mutation

Since ASMiGP is a steady state MOGP, in each generation 442 we generate only one offspring. We use either crossover or 443 mutation to do that. A random number  $r_c$  is drawn in [0, 1]. 444 if  $r_c < p_c$  then crossover operator is selected otherwise the 445 mutation operator is selected for that generation.

## F. Mating Selection

ASMiGP uses crossover with male and female differenti- 448 ation which needs one male and female parent. We perform 449 Roulette wheel selection using classification accuracy of the 450 binary classifiers as fitness to select the female parent. Then 451 the male parent is selected randomly from the remaining 452 archive. The only condition to be satisfied is that the male 453 and female parents must be distinct. For mutation, we need 454 only one individual and it is selected in the same way as done 455 for the female parent in case of crossover operator.

A choice of mating selection could have been the use 457 of some bi-level selection operator, where Pareto dominance 458 is preferred over diversity. In that case, solutions along the 459 whole Pareto optimal solution set with good diversity would 460 have been selected as the primary (female) parents. Note that, 461 we have used crossover with male-female differentiation that 462 tries to generate an off-spring near the primary parent in the 463 hypothesis space. Consequently, this might cause generation of 464 Pareto optimal binary classifiers along the whole Pareto opti- 465 mal solution set. Though they are Pareto optimal, these binary 466 classifiers may have poor accuracies. This is because of the 467 implicit imbalance nature of the binary classification problems 468 (due to conversion from multiclass classification problems) 469 and different classifier sizes. An ensemble classifier, however, 470 performs better when individual members of the ensemble 471 are more accurate. Therefore, we use classification accuracy- 472 based mating selection. It guides the search to generate more 473 accurate binary classifiers.

### G. Crossover

In this paper, we have used crossover operation with male 476 and female differentiation. We want the off-spring to be near 477 the female (acceptor) parent in the hypothesis space. The 478 male (donor) parent is used to make the off-spring diverse 479

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 $^{480}$  from its mother. To do this, two random points (nodes) are  $^{481}$  selected from each of the parents. The probabilities of selection of terminal nodes and function nodes as a crossover point  $^{482}$  (node) are, respectively,  $p_t^c$  and  $(1-p_t^c)$ . Then, the subtree  $^{484}$  rooted at the selected node of the mother tree is replaced with  $^{485}$  a similarly selected subtree from the father tree. If the off- $^{486}$  spring is identical to any of its parents, the whole procedure  $^{487}$  is repeated (before evaluation/learning of the off-spring).

#### 488 H. Mutation

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In most of the GP-based systems, for mutation a subtree rooted at a randomly selected node is replaced by a new randomly generated subtree. Though this kind of mutation explores more in the hypothesis space, it may be too disruptive in nature. Therefore, we intend to use less exploration by keeping the tree structure unaltered. During mutation we perform the following operations on a tree.

- 1) Each constant of the tree is replaced by another random constant with probability  $p_c^m$ .
- 2) Each function node of the tree is replaced by anther random function node with probability  $p_f^m$ .
- Only one feature node of the tree is replaced by another feature node.

For feature nodes, to select the mutation point Roulette wheel selection is performed on the unfitness of the features which are present in the tree. Similarly, to insert a new feature at the mutation point, we select a feature using Roulette wheel selection based on the fitness values (probability proportional to fitness) of the features.

This restricted mutation scheme ensures that the tree struc-509 ture of an equation remains the same. It also ensures that the 510 variables in an equation do not change drastically—changing 511 more than one variable would shift the solution (equation) in 512 the hypothesis space by a larger amount.

#### 513 I. Environmental Selection

ASMiGP uses the archive truncation strategy used 515 in [72] and [75]. This multiobjective archive truncation strat-516 egy uses Pareto-based fitness function, i.e., fitness is Pareto 517 dominance rank. This scheme maintains an archive (ensemble) 518 which has an adaptive and dynamic size. It does not allow the archive to fall below a minimum size ensuring diversity in the 520 genotypic space. Moreover, the environmental selection dimin-521 ishes the exploration in areas of objective space that are less 522 likely to yield improved solutions [72], ensuring diversity in 523 phenotypic space. Furthermore, we have made the following 524 difference in the environmental selection. ASMiGP ensures 525 that the infix expression of every off-spring (after mutation or 526 crossover) is distinct from every member of the archive. To 527 achieve this, before evaluating the offspring, ASMiGP converts it to its infix expression and then compares the expression with that of each individual of the archive. Only if the expression is unique, the off-spring is evaluated and added to the archive. Otherwise it is discarded and a new off-spring is gen-532 erated. Another noticeable difference is that here the number of objectives is three. Note that the diversity maintenance in each 534 ensemble both in phenotypic space and in genotypic space finds a diverse set of trees (bi-classifiers). Trees, being diverse, 595 enhance the performance of the corresponding ensemble. In 596 this context, it is worth mentioning that the archive, along 597 with the archive truncation strategy, helps to realize a good 598 Pareto front by explicitly maintaining diversity among the fit 699 (according to rank) solutions. However, the archive alone is not 540 sufficient to evolve a good Pareto front along all the objectives. 541

#### J. Decision Making

To determine the class label, we find the net belongingness 543 of a point to each class. The net belongingness lies in [0, 1]. 544 A higher value indicates more net belongingness to that class. 545 A data point is assigned to that class for which it has the 546 highest net belongingness. 547

After the learning, we obtain a set of c archives,  $\mathcal{A} = {}^{548}\{\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_c\}; \ \forall i, 1 \leq |\mathcal{A}_i| \leq N_{\text{max}}, \ \text{where } c \ \text{is the num-} \ \text{ber of classes, and } \mathcal{A}_i \ \text{is the set of all binary classifiers for the } \ \text{550} \ \text{ith class.}$  To determine the net belongingness of a data point  $\mathbf{p}$  551 to class m,  $\mathcal{B}_m^{\text{net}}(\mathbf{p})$ , it is passed through all genetic programs 552 of set  $\mathcal{A}_m$ . The net belongingness,  $\mathcal{B}_m^{\text{net}}(\mathbf{p})$ , of the point  $\mathbf{p}$  for 553 class m is computed using

$$\mathcal{B}_{m}^{\text{net}}(\mathbf{p}) = \frac{1}{2} \left( \frac{1}{|\mathcal{A}_{m}|} \sum_{i=1}^{|\mathcal{A}_{m}|} \mathcal{B}_{m}^{i}(\mathbf{p}) + 1.0 \right)$$
(8) 555

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where  $\mathcal{B}_{m}^{i}$  is defined as

$$\mathcal{B}_{m}^{i}(\mathbf{p}) = \begin{cases} +\left(1.0 - \frac{\mathrm{FP}_{m}^{i}}{\mathrm{FP}_{m}^{\mathrm{max}}}\right), & \text{if } \mathcal{A}_{m}^{i}(\mathbf{p}) > 0\\ -\left(1.0 - \frac{\mathrm{FN}_{m}^{i}}{\mathrm{FN}_{m}^{\mathrm{max}}}\right), & \text{otherwise.} \end{cases}$$
(9) 557

In (9),  $FP_m^i$  and  $FN_m^i$ , respectively, represent the number of FPs and FNs made by the ith individual in set  $\mathcal{A}_m$  on the training data.  $FP_m^{\max}$  and  $FN_m^{\max}$  are, respectively, the maximum possible FP and the maximum possible FN for the mth class; and  $\mathcal{A}_m^i(\mathbf{p})$  is the output from ith individual of  $\mathcal{A}_m$  for input data point  $\mathbf{p}$ . Finally,  $\mathbf{p}$  is assigned the class k, when  $\mathcal{B}_k^{\text{net}} = \frac{c}{m} \{\mathcal{B}_m^{\text{net}}\}$ . Note that  $FP_m^{\max}$  and  $FP_m^{\min}$  are determined by the training data.

The concept of net belongingness is inspired by the concept of negative voting. Negative voting has been widely used 567 in diverse applications [76]–[78]. It is more effective when 568 circumstances unfavorable to the preferences invoke stronger 569 electoral responses than the similar favorable responses, as 570 well as the behaviors of the voters are well defined [79]. In 571 our scheme, the learners for the ith class learn to vote yes 572 for the points of the ith class and no for the points which 573 do not belong to the ith class. For multiclass problems, it 574 is more likely that a binary classifier learns to say no than 575 to say yes for a much higher number of points. Therefore, 576 we found negative voting to be more suitable in this context. 577 However, we have used a weighted negative voting scheme. 578 The accuracies for the responses yes and no of the ith binary 579 classifier of mth class are, respectively,  $(1.0 - FP_m^i/FP_m^{max})$  580 and  $(1.0 - FN_m^i/FN_m^{max})$ . These values have been used as corresponding weights for the responses yes and no of the ith 582 binary classifier of the mth class. We have used the positive 583

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TABLE I PARAMETER SETTINGS FOR THE PROPOSED METHOD

Parameter	Value
Set of functions $(\mathcal{F})$	$\overline{\{+,-, imes,\div\}}$
Range of initial values of constants $(C)$	[0, 2]
Maximum depth of tree during initialization	6
Maximum allowable depth of tree	10
Maximum archive size $(N_{max})$	50
Minimum archive size $(N_{min})$	30
Initial Probability of feature nodes $(p_{var})$	0.8
Probability of crossover $(p_c)$	0.8
Probability of crossover for terminal nodes $(p_t^c)$	0.2
Probability of mutation for constants $(p_c^m)$	0.3
Probability of mutation for function nodes $(p_f^m)$	0.1
Function evaluations for each binary classifier	400000

TABLE II SUMMARY OF MICROARRAY DATA SETS

	Data Set	Features (F)	Samples $(S)$	Classes (C)	$\frac{\overline{\left(\frac{F}{S}\right)}}{}$
1	Colon	2000	62	2	32.26
2	TOX-171	5748	171	4	33.61
3	Leukemia 1	7129	34	2	209.68
4	Leukemia 2	7129	38	2	187.61
5	CLL-SUB-111	11340	111	3	102.16
6	GCM	16063	144	14	111.55
7	SMK-CAN-187	19993	187	2	106.91
8	GLA-BRA-180	49151	180	4	273.06

and the negative signs to indicate acceptance and rejection of 585 the data point for the mth class, respectively.

#### IV. EXPERIMENTATION

#### 587 A. Experimental Settings

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We have repeated tenfold cross validation of the proposed 589 method for ten times. Table I shows the parameter settings 590 that we have used for this purpose. The training data is 591 Z-score normalized. Furthermore, based on the means and the 592 standard deviations of the features of the training data, the 593 test data was Z-score normalized. Note that except  $N_{\text{max}}$  and  $N_{\min}$ , all parameters are standard parameters used in any GP simulations, while  $N_{\text{max}}$  and  $N_{\text{min}}$  are needed for archive main-596 tenance. Although all the parameters can be chosen using a 597 cross validation mechanism, because of huge computational 598 overhead, we could not do that. Based on a few experi-599 ments we selected these parameters. These choices are not 600 optimal. However, since the same set of values are used for widely different types of data sets, it demonstrates the effec-602 tiveness of the proposed scheme. The proposed method has 603 been implemented in Java with the help of jMetal [80], [81]. We have used eight microarray and eleven text data sets which are summarized in Tables II and III, respectively.

#### 606 B. Importance of FS and Rule Size Reduction

To demonstrate the importance of the proposed FS and rule 607 size reduction scheme, we have compared our method with GP without FS and no restriction to equation size. To do that, we have made the following changes in the proposed method.

- 1) No explicit FS as described in Section III-C is done.
- 2) There are only two objectives, FP and FN.

TABLE III SUMMARY OF TEXT DATA SETS

	Data Set	Features	Samples	Classes	(F)
	Data Set	(F)	(S)	(C)	$(\overline{s})$
1	oh0.wc	3182	1003	10	3.17
2	oh10.wc	3238	1050	10	3.08
3	tr12.wc	5804	313	8	18.54
4	tr23.wc	5832	204	6	28.59
5	tr11.wc	6429	414	9	15.53
6	tr21.wc	7902	336	6	23.52
7	wap.wc	8460	1560	20	5.42
8	ohscal.wc	11465	11162	10	1.03
9	la2s.wc	12432	3075	6	4.04
10	la1s.wc	13195	3204	6	4.12
11	new3s.wc	26832	9558	44	2.81

All other parts of the algorithm and the parameter values 613 remain unchanged. Similar to the proposed scheme, we have 614 also executed tenfold cross validation for ten times for all the 615 data sets. Along with results (mean values of the correspond- 616 ing ten runs) obtained using the proposed method, the results 617 obtained using this scheme for microarray and for text data 618 sets are, respectively, summarized in Tables IV and V. From 619 these two tables, we observe the following.

- 1) In all cases, the test accuracy is much higher for the pro- 621 posed method. Especially, for GCM having 14 classes, 622 the difference between the test accuracies are remarkably 623
- 2) The tree size increases significantly when the third 625 objective, i.e., the restriction on rule size, is not used.
- 3) For most of the data sets the proposed method selects 627 smaller number of distinct features per tree as well as 628 for per classifier.

These observations clearly demonstrate the importance of 630 the FS as well as constraining the rule size. Since our FS 631 scheme discards features with poor relevance and uses features 632 with good discriminating power yet avoiding use of redundant 633 features, it not only makes the discovery of useful rules eas- 634 ier but also implicitly constrains the rule length. Thus, FS 635 plays a very important role having two positive impacts: it 636 makes identification of useful rules easier and it promotes the 637 minimization of the third objective.

#### C. Comparing With Other Methods

To compare the performance of the proposed method 640 we have used the experimental results reported in [82] (see 641 [82, Tables IV-VII]). Song et al. [82] used four different 642 types of classification algorithms: 1) probability-based naive 643 Bayes (NB); 2) tree based C4.5; 3) instance-based lazy learning algorithm IB1; and 4) rule-based RIPPER both before and 645 after FS. Along with the full feature set, they have used six 646 FS algorithms in their experiment.

- 1) FAST [82].
- 2) FCBF [83], [84].
- 3) CFS [85].
- 4) ReliefF [86].
- 5) Consist [87].
- 6) FOCUS-SF [88].

TABLE IV
EXPERIMENTAL RESULTS ON MICROARRAY DATA SETS (MEAN VALUES OF TEN RUNS OF TENFOLD CROSS VALIDATION)

Data Set	%TA <sup>a</sup>		]	$FS^b$		$TS^c$		$(F/T)^d$		$\%\mathrm{F}^e$		$(\%F/T)^f$	
Data Set	$PM^g$	$\mathrm{W}^h_{\mathrm{F\&R}}$	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	
Colon	85.12 (2.07)	71.93 (4.12)	195.0	182.5	6.76	123.60	3.11	8.56	9.75	9.13	0.16	0.43	
TOX-171	81.07 (3.42)	58.52 (4.57)	407.6	540.9	8.83	148.44	3.53	11.97	7.09	9.41	0.06	0.21	
Leukemia1	93.50 (2.85)	74.08 (6.42)	188.6	276.6	3.01	76.09	2.00	6.52	2.65	3.88	0.03	0.09	
Leukemia2	91.58 (3.67)	77.33 (6.84)	147.8	229.0	3.50	74.16	2.02	5.72	2.07	3.21	0.03	0.08	
CLL-SUB-111	80.52 (2.60)	54.51 (3.51)	335.3	465.3	7.29	134.28	3.20	10.75	2.96	4.10	0.03	0.09	
GCM	69.35 (1.96)	33.97 (2.60)	854.3	1086.0	4.70	105.42	1.91	6.22	5.32	6.76	0.01	0.04	
SMK-CAN-187	68.68 (1.18)	62.12 (2.30)	319.9	435.8	22.23	135.88	6.41	15.33	1.60	2.18	0.03	0.08	
GLA-BRA-180	68.22(2.25)	58.89 (2.75)	784.4	569.9	11.30	150.81	4.33	11.40	1.60	1.16	0.01	0.02	

<sup>a</sup>Test Accuracy (standard deviation is provided within parenthesis), <sup>b</sup>Number of Features Selected per Classifier, <sup>c</sup>Tree Size, <sup>d</sup>Number of Features per Tree, <sup>e</sup>Percentage of Features Selected, <sup>f</sup>Percentage of Features Selected per Tree, <sup>g</sup>Proposed Method, <sup>h</sup>GP without FS and Rule Size Reduction

 ${\it TABLE~V}\\ {\it Experimental~Results~on~Text~Data~Sets~(Mean~Values~of~Ten~Runs~of~Tenfold~Cross~Validation)}$ 

Data Set	%Т	$A^a$	F	$FS^b$	Т	$S^c$	(F/	$(T)^d$	%	$\%\mathrm{F}^e$		$(\%F/T)^f$	
Data Set	$-$ PM $^g$	$\mathrm{W}^h_{\mathrm{F\&R}}$	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	
oh0.wc	87.75 (0.51)	70.53 (1.17)	484.1	2080.7	17.06	145.38	6.46	25.90	15.21	65.39	0.20	0.81	
oh10.wc	81.06 (0.61)	66.11 (1.52)	439.6	2166.8	24.11	140.67	7.12	26.03	13.58	66.92	0.22	0.80	
tr12.wc	87.86 (1.50)	60.55 (2.36)	603.7	1697.3	8.67	123.91	4.17	17.22	10.40	29.24	0.07	0.30	
tr23.wc	93.95 (1.19)	64.90 (2.14)	396.5	1154.2	6.10	117.15	3.09	14.81	6.80	19.79	0.05	0.25	
tr11.wc	86.08 (0.72)	64.63 (2.56)	631.6	1785.8	8.82	128.57	4.03	17.03	9.82	27.78	0.06	0.26	
tr21.wc	89.64 (1.14)	71.46 (2.62)	362.0	1219.2	9.51	114.51	4.17	15.00	4.58	15.43	0.05	0.19	
wap.wc	79.60 (0.60)	58.96 (1.64)	1199.8	4377.5	17.38	125.53	6.07	21.02	14.18	51.74	0.07	0.25	
ohscal.wc	73.45 (0.23)	62.59 (1.21)	232.9	3853.8	63.48	111.52	7.78	24.87	2.03	33.61	0.07	0.22	
la2s.wc	83.95 (0.62)	67.32 (0.99)	354.6	2369.1	53.17	133.76	11.41	28.65	2.85	19.06	0.09	0.23	
la1s.wc	83.06 (0.36)	65.62 (1.05)	380.6	2372.0	56.40	133.21	12.30	28.35	2.88	17.98	0.09	0.21	
new3s.wc	81.32 (0.27)	58.96 (1.64)	1674.2	4377.5	33.93	125.53	7.10	21.02	6.24	16.31	0.03	0.08	

<sup>a</sup>Test Accuracy (standard deviation is provided within parenthesis), <sup>b</sup>Number of Features Selected per Classifier, <sup>c</sup>Tree Size, <sup>d</sup>Number of Features per Tree, <sup>e</sup>Percentage of Features Selected, <sup>f</sup>Percentage of Features Selected per Tree, <sup>g</sup>Proposed Method, <sup>h</sup>GP without FS and Rule Size Reduction

Use of all features can be viewed as the seventh FS algofine rithm. To make this paper comprehensive, we are not disfine cussing the experimental settings used in [82]. Note that for accuracies for few data sets for few pairs of FS schemes are for not available in [82].

1) Results With Microarray Data Sets: Table IV presents 660 the results of the proposed method on microarray data sets. We have already stated that for each classifier, Song et al. [82] used seven FS schemes (six FS method as well as the set of all features). For each FS method five repetitions of the ten-664 fold cross validation experiment were done in [82]. And then, 665 for each FS method, the average accuracy over the five rep-666 etitions is reported. We compare this average accuracy with 667 the average accuracy that we have obtained by our method 668 over the ten repetitions of the tenfold cross validation experiments. In particular, we count the number of cases (each case 670 refers to one FS scheme) in which our algorithm outperforms. 671 Note that, for some combination of data set and classifier, the 672 total number of cases is less than seven as for those combi-673 nations some results are not available. Table VI reports these 674 counts. To elaborate Table VI, consider the entry correspond-675 ing to column IB1 and row CLL-SUB-111. For the data set 676 CLL-SUB-111, in [82, Table VI], Song et al. reported the per-677 formance of the algorithm IB1 for six different FS algorithms. 678 Our algorithm is found to perform better than five of the six 679 FS algorithms and hence the entry for row CLL-SUB-111 and 680 column IB1 is 5/6. Note that, for this data set, Song et al. [82] 681 did not report performance of IB1 using all features. All but 682 the entries in the last column of Table VI are generated in

TABLE VI COMPARISON WITH NB, C4.5, IB1, AND RIPPER ON MICROARRAY DATA SETS

Data Set	NB	C4.5	IB1	RIPPER	Total
Colon	4/7	2/7	4/7	6/7	16/28
TOX-171	4/7	7/7	3/7	7/7	21/28
Leukemia1	2/7	2/7	2/7	2/7	8/28
Leukemia2	5/7	6/7	6/7	5/7	22/28
CLL-SUB-111	4/7	6/7	5/6	4/7	19/27
GCM	4/7	7/7	6/7	7/7	24/28
SMK-CAN-187	2/6	2/6	2/6	2/6	8/24
GLA-BRA-180	3/6	5/6	1/6	5/6	14/24
Total	28/54	37/54	29/53	38/54	132/215

the same manner. The last column of Table VI, which reports 683 the row total, reveals that our method performs the best for 684 61.40% (132 out of 215) test cases.

If we compute the percentage of features selected by the ensembles, it may not be very small for some data sets, like 687 Colon. But, if we consider the number of features selected per 688 binary classifier (tree), we find that this number is quite small, 689 e.g., the maximum value is 0.16% for Colon. We assume that 690 binary classifiers (binary trees) having less than twenty nodes are concise enough. We need to remember that we are talking 692 about raw rules (equations) directly obtained from GP which 693 are most likely affected by bloating. Simplification of these 694 rules may lead to reduction in their sizes. Based on this, in 695 all but one data set we could find easy to analyze rules. For 696 SMK-CAN-187 the extracted rules are more complex possibly 697 because of complex structure of the data.

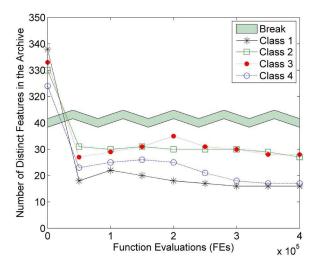


Fig. 1. Showing the number of distinct features present in the archive with respect to function evaluations for GLA-BRA-180 data set.

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In Table S-I (see supplementary materials), we present the best rules (or binary classifiers or GPs) we found for each class of each microarray data set. These GPs have the highest train-702 ing accuracy among the GPs obtained from the first fold of the 703 first ten fold cross validation. If there are more than one rule 704 having the same maximum training accuracy, the rule with the smallest length has been reported. The features in the equations are indexed starting from "0." From Table S-I, we can 707 observe that for several classes the proposed method could find substantially small rules. Noticeably, for four, six, eight, and 709 three classes, the proposed method could find the best binary 710 classifier having only 1–4 distinct variables, respectively. So, 711 21 out of 33 (i.e., 63.64%) cases, we could find considerably 712 small (and hence easy to interpret) rules. For some classes, 713 the rules having the highest training accuracy were not very 714 comprehensible because the length of the rule was not very <sub>715</sub> small. If we think that  $(2.0 \times x_i)$  is more easy to understand 716 than  $(x_i + x_i)$ , though both equations have the same size, we observe that for 21 out of 33 (i.e., 63.64%) cases the proposed 718 method could find rules having highest accuracy, which are 719 not at all affected by bloating and are comprehensible without 720 simplification.

To investigate how the number of distinct features changes 722 in the archive, we have executed our algorithm with 400 000 function evaluations using the entire GLA-BRA-180 data set. 724 In Fig. 1, we have plotted the number of distinct features 725 after initial and after each 12.5% of maximum function eval-726 uations. For all four classes of GLA-BRA-180 data set, the 727 number of distinct features in the archive initially falls dras-728 tically depicting the impact of FS. After some generations, it 729 becomes almost constant. Moreover, the number of final dis-730 tinct features for each class is quite small. This indeed reveals a desirable behavior of the our scheme.

To show how the individual binary classifiers' accuracies 733 change with function evolutions, we have plotted each individuals' FPs and FNs for all four classes of GLA-BRA-180 735 data set in Figs. S-1 and S-2 (see supplementary materials). For 736 this part of the experiment also, we have used the entire data

TABLE VII COMPARISON WITH NB, C4.5, IB1, AND RIPPER ON TEXT DATA SETS

Data Set	NB	C4.5	IB1	RIPPER	Total
oh0.wc	7/7	7/7	7/7	6/6	27/27
oh10.wc	7/7	7/7	7/7	6/6	27/27
tr12.wc	7/7	7/7	7/7	7/7	28/28
tr23.wc	7/7	5/7	7/7	4/7	23/28
tr11.wc	7/7	7/7	7/7	6/6	27/27
tr21.wc	6/7	6/7	6/7	3/6	21/27
wap.wc	7/7	6/6	6/6	6/6	25/25
ohscal.wc	4/4	4/4	4/4	4/4	16/16
la2s.wc	6/6	5/5	5/5	5/5	21/21
la1s.wc	6/6	5/5	5/5	5/5	21/21
new3s.wc	3/3	3/3	3/3	3/3	12/12
Total	67/68	62/65	64/65	55/61	248/259

set for training. From the figures, it is observed that with the 737 increase in number of evolutions, the average accuracy of the 738 solutions tends to increase. However, for class four, some solu-739 tions having lower level of accuracies (having higher FPs and 740 FNs) are there even after 400 000 function evaluations. This is 741 because, even after such high number of function evaluations, 742 the algorithm was still searching for more concise solutions, 743 and could find some trees of comparatively smaller size.

2) Results With Text Data Sets: Similar to Table VI with 745 microarray data sets, we present the same result (number of 746 test cases for which our algorithm provides the best results 747 for each classifier and data set pair) with text data sets in 748 Table VII. Table VII reveals that for text data sets the proposed 749 scheme performs the best for 95.75% (248 out of 259) cases. 750

If we consider the same criteria that binary classifiers (trees) 751 having less than twenty nodes are concise enough, then our 752 method could not find interpretable rules for 5 (oh10.wc, 753 ohoscal.wc, la2s.wc, la1s.wc, and new3s.wc) out of the 11 754 text data sets. The number of selected features is not at all 755 small for most of the text data sets. Some reasons behind 756 this may be that the number of classes is high for the text 757 data sets and the existence of more complex class structure, 758 which is defined by the keywords and relation of keywords to 759 the imposed classes is usually not as straightforward as genes 760 have to cancers. However, the percentage of features selected 761 per binary classifiers (trees) is quite small. Noticeably, the 762 accuracy obtained for new3s.wc (having 44 classes), is much 763 higher than that of the other methods (for accuracies of other 764 methods, see [82]). We can also observe that for data sets having more than or equal to ten classes, our methods performs 766 comparatively better than other methods.

## D. Statistical Significance Testing

To compare the proposed method with existing FS and clas-769 sification methods, we consider four classification and six 770 FS methods as well as with the full feature set. Thus we 771 compare our algorithm with 28 FS and classification algo-772 rithm pairs. We have performed Wilcoxon signed ranks test 773 to show that the performance of the proposed algorithm is 774 significantly different over 28 pairs of FS and classification 775 algorithm. For this, we have considered both the microarray 776 and the text data sets together and have used the average test 7777

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TABLE VIII WILCOXON SIGNED RANKS TEST (ONE-TAILED) FOR PAIRWISE Comparisons with the Proposed Method at  $\alpha=0.05$ 

	NID	01.5	TD 1	DIDDED
	NB	C4.5	IB1	RIPPER
FAST	A	R	R	R
FCBF	R	R	R	R
CFS	R	R	R	R
ReliefF	R	R	R	R
Consist	R	R	R	R
FOCUS-SF	R	R	R	R
Full Set	R	R	R	R

A:  $H_0$  Accepted, R:  $H_0$  Rejected.

778 accuracies achieved with different algorithms on these data 779 sets. Moreover, we have removed the cases for which accu-780 racies are not known (see [82, Tables IV-VII]). Table VIII shows that out of the 28 cases, only in one case the null hypothesis  $H_0$  was accepted. Here the null hypothesis is that 783 there is no significant difference in performance between our 784 algorithm and a comparing algorithm. We have also used 785 Friedman test [89], [90] to check if all the 29 (28 existing 786 and our proposed) algorithms perform similarly over seven 787 data sets: Colon, TOX-171, Leukemia1, Leukemia2, GCM, 788 tr12.wc, and tr23.wc (see [82, Tables IV-VII], some accu-789 racies for other data sets are not available). The obtained Friedman statistics is 60.13, which is significant at  $\alpha = 0.001$ , <sub>791</sub> as the corresponding statistic  $\chi^2$  with 28 degrees of freedom 792 is 56.90. Thus, Friedman test suggests existence of significant 793 difference among the algorithms.

#### V. CONCLUSION

In this paper, we have used a MOGP, called ASMiGP, to 796 evolve diverse sets of binary classifiers to solve multiclass clas-797 sification problems. Simultaneous FS and rule extraction are erformed during the genetic evolution. An important objecye of this paper is to find simple classification rules that may human understandable, which in the given context translates to rules with simple operations and short length. The 801 proposed method is found to achieve its goal.

Ensembles perform better when weighted voting is used, the 804 members of the ensembles are diverse enough, and the classifiers are accurate [21]. Here, we have created c sets of diverse 806 ensembles. Unlike other ensemble-based method, here each 807 ensemble represents diverse classifiers for just one class. The 808 number of features used by the ensembles is high with respect 809 to the number of features selected per (binary classifier) tree. 810 This suggests that the binary classifiers are diverse enough. In  $^{811}$  our algorithm, we evolve c distinct species in parallel, which 812 try to learn distinct patterns and no interspecies gene exchange ever allowed. This property makes each species different 814 from the other species and the system becomes less vulner-815 able, especially when each species has successfully learnt its 816 designated patterns.

Our method has been tested on nineteen (eight microar-818 ray and eleven text) data sets. The experimental results 819 show that we could find easy-to-understand rules for overall 820 63.2% (87.5% for microarray and 54.5% for text) data sets. 821 We compared our method with four classification methods in conjunction with seven FS methods including use of 822 the all-feature set. For 80.17% (61.40% for microarray and 823 95.75% for text) cases our method outperforms others. The 824 improvement in performance is shown statistically significant 825 compared to the others.

The overall performance of the proposed method is better 827 on text data sets compared to that of microarray data sets. Two 828 important differences between these two groups of data sets are 829 that: 1) microarray data sets have comparatively large feature- 830 to-sample ratios and may not have enough number of points 831 in each class for MOGP to learn the structure of the data sets 832 and 2) the text data sets have comparatively large number of 833 classes as well as instances. Our limited experiments suggest 834 that when there are enough points in each class so that each 835 species can successfully learn its target pattern, the proposed 836 method works better. We found that for text data our method 837 performs noticeably better than the other methods particularly 838 when number of classes is high (ten or more than that).

We have shown that our method is very effective when the 840 dimension of the data sets are as high as 49 151. But in all our 841 data sets, number of samples were not very big. If we apply 842 the proposed method on a data set with a really large num- 843 ber samples, it may require a significant amount of time. The 844 method may also take a substantial amount of time when the 845 number of classes is high and we have limited parallel process- 846 ing capability. With the today's high performance computing 847 technologies, however, these are not really crucial shortcom- 848 ings. Yet, we have not applied it to truly big data. This paper 849 can be adapted to deal with big data, especially using Hadoop. 850

Our future research interest is to use MOGP to classify 851 multiclass text data, where each text may belong to more than 852 one category (class) and to use net belongingness as a fuzzy 853 membership of the documents to the corresponding category. 854 We also intend to modify the proposed learning method to 855 stepwise learning, so that we can use it for big text data.

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## **AUTHOR QUERIES**

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# A Multiobjective Genetic Programming-Based Ensemble for Simultaneous Feature Selection and Classification

Kaustuv Nag and Nikhil R. Pal, Fellow, IEEE

Abstract—We present an integrated algorithm for simultane-2 ous feature selection (FS) and designing of diverse classifiers 3 using a steady state multiobiective genetic programming (GP). 4 which minimizes three objectives: 1) false positives (FPs); 2) false 5 negatives (FNs); and 3) the number of leaf nodes in the tree. 6 Our method divides a c-class problem into c binary classifica- $_{7}$  tion problems. It evolves c sets of genetic programs to create c 8 ensembles. During mutation operation, our method exploits the 9 fitness as well as unfitness of features, which dynamically change 10 with generations with a view to using a set of highly relevant 11 features with low redundancy. The classifiers of ith class deter-12 mine the net belongingness of an unknown data point to the ith 13 class using a weighted voting scheme, which makes use of the 14 FP and FN mistakes made on the training data. We test our 15 method on eight microarray and 11 text data sets with diverse 16 number of classes (from 2 to 44), large number of features 17 (from 2000 to 49151), and high feature-to-sample ratio (from 18 1.03 to 273.1). We compare our method with a bi-objective GP 19 scheme that does not use any FS and rule size reduction strat-20 egy. It depicts the effectiveness of the proposed FS and rule size 21 reduction schemes. Furthermore, we compare our method with 22 four classification methods in conjunction with six features selec-23 tion algorithms and full feature set. Our scheme performs the 24 best for 380 out of 474 combinations of data sets, algorithm and 25 FS method.

26 Index Terms—Classification, ensemble, feature selection (FS), 27 genetic programming (GP).

#### I. INTRODUCTION

LASSIFICATION is one of the most important and frequently encountered problems in data mining and machine learning. A wide range of real world problems of different domains can be restated as classification problems. This includes diagnosis from microarray data, text categorization, medical diagnosis, software quality assurance, and many more. The objective of classification is to take an input vector  $\mathbf{x} = (x_1, \dots, x_d)^T$  and to assign it to one of the K classes  $C_k$ ,

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where k = 1, ..., K. A model, called classifier, is used to solve this problem. The classifier encodes a set of criteria. Bepending upon some features of the data point, these criteria assign the data point to a particular class [1]. Sometimes, ensembles of weak classifiers are used to obtain better classification accuracy. High dimensionality, high feature-to-sample ratio, and redundant and/or noisy features are some common sources of difficulties associated with classification.

Feature selection (FS) is a process to select a small but useful subset of features from the set of available features which
is adequate for solving the problem in an efficient manner.
Some available features may be redundant, not useful, and may
cause confusion during the learning phase. These unwanted
features needlessly increase the size and complexity of the feature space. It increases the computation cost for learning, and
may sometimes be responsible for finding suboptimal solutions of the problem. This makes FS techniques important for
the analysis of high dimensional data sets, especially when
feature-to-sample ratio is extremely high.

The microarray technology has made it possible to diagnose different types of cancers directly using the microarray data sets. One of the main difficulties we face to do this is the high feature-to-sample ratio of microarray data sets, which makes FS an important step. Finding keywords as well as contexts from text data is essential to detect (without human intervention) the context of web pages, emails, or questions/answers, etc. A large set of distinct words in large texts (high number of features) and many categories of texts (high number of classes) are the two complicated challenges that we face in this task.

Genetic programming (GP) [2]–[5] is a biological-evolution inspired methodology where each solution is a program or an equation that evolves with one or more objective functions to perform specific tasks. References [6]–[12] used GP to design classifiers or to generate rules for binary classification problems. Some researchers have also attempted to solve multiclass problems [13]–[17]. GP has also been used for simultaneous FS and classification [18]. Liu and Xu [19] vused GP to create ensembles of classifiers (genetic programs). They have used these ensembles to classify microarray data sets. Though GP is a powerful tool, it has a drawback: without special care each genetic program (equation) becomes huge. As an effect, they do not learn the patterns in the training data. Rather, memorizes them. It also makes genetic programs to be difficult to comprehend. Besides, though ensembles can

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<sub>82</sub> perform better than individual classifiers [20], to obtain better 83 performance, each ensemble should be diverse and each mem-84 ber of the ensemble should be accurate [20]-[22]. Without 85 special care, due to lack of explicit diversity preservation 86 mechanism, the solutions of single objective GP may lose

The objective of this paper is to find an embedded method-89 ology of simultaneous FS and classification employing GP as a 90 tool. Some of the novel contributions of our schemes are as fol-91 lows. We have introduced a new multiobjective GP (MOGP), 92 called archive-based steady state micro GP (ASMiGP). It 93 is enriched by several new operators. The mating selec-94 tion judicially uses Roulette wheel selection, instead of two 95 tire multiobjective selection scheme (where domination is 96 preferred over diversity). The crossover is new and uses male-97 female differentiation so that the off-spring is more likely to be 98 close to the female parent in the genotypic space. The mutation 99 is restrictive and performs less exploration in the hypothesis 100 space. Thus, it reduces disruption. For feature nodes, instead of fitness, mutation uses unfitness to select the mutation point. 102 Altering the fitness and unfitness of the features in different 103 stages of learning, we change the objective of searching in the 104 corresponding stages. We use ASMiGP to learn c diverse sets 105 of classifiers (equations) minimizing three objectives: 1) false 106 positive (FP); 2) false negative (FN); and 3) number of leaf 107 nodes of a tree to restrict the rule size. Throughout the learning 108 process, implicit FS is performed using MOGP, whereas sev-109 eral filter-based approaches are used in different stages of the 110 procedure. In this way, we obtain concise rules that involve only simple arithmetic operations. A weighted negative vot-112 ing is then used among the rules of each ensemble. These 113 weights are determined on the basis of the performance of 114 the binary classifiers on the training data set. A new measure of weighted negative voting, called net belongingness, is also 116 introduced.

The proposed method has been tested on eight multiclass 117 118 microarray data sets having large number of features, varying 119 from 2000 to 49 151, and high feature-to-sample ratio, vary-120 ing from 32.26 to 273.06. It has also been tested on eleven high dimensional (varying from 3182 to 26832) text data sets, where the number of classes (categories) vary from 6 to 44. 123 Experimental results reveal that our method can generate 124 ensembles of classifiers with concise rules that can do a good 125 job of classification with a small subset of features.

#### II. BACKGROUND AND RELATED WORKS

This section provides a background to GP, GP-based online 128 FS and classification, ensembles, voting schemes, and concise 129 rule finding. This section also includes some related works on 130 these topics.

#### 131 A. Concise Introduction to GP

GP [2]–[5] is an approach to find programs that can solve 133 a given problem. GP uses Darwinian principle of "survival of 134 the fittest." It evolves the programs using biologically inspired 135 genetic operations like reproduction, crossover, and mutation 136 in the search space to find such programs which would be able to solve the given problem [15], [23], [24]. The overall search 137 process of traditional single objective GP is quite similar to 138 traditional population-based genetic algorithm. The main dif- 139 ference among them is in the representation of solutions. The 140 usual steps of traditional single objective GP can be found 141 in [2], [15], and [24].

There exist several ways to encode a program. Probably, the 143 most popular one is to use a tree structure [25]-[27] which 144 we use. In tree-based GP, a program is represented by a 145 tree where the internal nodes are from a set of functions  $\mathcal{F}$ , 146 and the leaf nodes are from a set of terminals  $\mathcal{T}$ . The sub- 147 trees of a function node are the arguments of that function. 148 The sets  ${\mathcal F}$  and  ${\mathcal T}$  must satisfy the closure and sufficiency 149 properties [2], [15]. To satisfy the closure property,  $\mathcal{F}$  must 150 be well defined and closed for any combination of probable 151 arguments that it may encounter [15]. Again, to satisfy the 152 sufficiency property,  $\mathcal F$  and  $\mathcal T$  must be able to represent any 153 possible valid solution of the problem.

## B. FS: Why Embedded?

FS methods are generally divided into two main groups: 156 1) filter method and 2) wrapper method [28]. A filter method 157 does not use any feedback from the classifier or any mining 158 algorithm. It relies on the general characteristics of data. On 159 the contrary, to measure the goodness of features, a wrapper 160 method uses a predetermined classifier or mining algorithm, 161 which will finally use the selected features. Consequently, a 162 wrapper method exploits interactions among the subset of fea- 163 tures on which it is tested. But, to find an optimal set of 164 features, a wrapper method needs to measure performances 165 on all possible subsets of features. This becomes infeasible 166 for high dimensional data sets. To overcome this problem, 167 wrapper methods typically use a heuristic-based forward or 168 backward selection mechanism [28], which does not evaluate 169 all possible subsets. So, in this paper, we consider embed- 170 ded methods, where FS and designing of the classification 171 system are done together. Embedded methods do not need 172 to evaluate all possible subsets. Moreover, they can account 173 for interaction between features and the classifier that is used 174 to solve the problem [29]. Usually, embedded methods attain 175 comparable accuracy to wrapper methods as well as compara- 176 ble efficiency to filter methods. Though for every classification 177 tool it may not be easy to define such an integrated mecha- 178 nism, several attempts of FS using embedded methods have 179 already been made. These attempts include using single objec- 180 tive GP [18], neural networks [30], [31], and support vector 181 machines [32].

## C. GP in Classification and FS

Many researchers have used GP as a tool for classifi- 184 cation and FS. Some literature on this topic can be found 185 in [1] and [33]. It has been used in both filter [34]-[37] 186 and wrapper [38]-[41] approaches. GP has also been 187 used for extracting decision trees [42]–[47]. Among these 188 in [45] and [46], MOGP has been used. GP has also been 189 adopted for learning rule-based systems [7]-[9], [48]-[51]. 190 classification [6], [7], [10]-[12], [48] binary

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192 multiclass [8], [9], [13]–[17], [49]–[51] classification prob-193 lems have been addressed by GP-based (rule-based) 194 systems. have Even, researchers applied GP-based 195 (rule-based) system for binary classification of imbal-196 anced data [52], [53]. Discriminant functions (DFs)-based 197 GP for online FS and classification has been adopted 198 in [18] to solve multiclass problems. It is noteworthy 199 that GP has also been used in feature extraction for edge 200 detection [54].

Since, in this paper, we have used MOGP for learning DFs, 202 we discuss some relevant GP-based systems. In DFs-based GP, 203 each program is a mathematical equation, where the variables 204 are features of the data. Usually every program is associated 205 with a class. For every input data point, the program converts 206 it to a single output value. If this output value is more than 207 a predefined threshold (usually zero), the point belongs to the 208 class to which the program is associated with. Thus, a sin-209 gle equation is enough for binary classification problems. For 210 c-class problems, there are two common ways. The first and 211 more frequently used approach is to consider a c-class problem 212 as c binary classification problems [1]. Thus, c number of DFs 213 are used to discriminate c classes. The second and less popular <sup>214</sup> approach is to use a single DF with (c-1) threshold values to create c intervals. Each of these intervals is then assigned to a 216 particular class. For both categories, a common practice is to 217 evolve a population where each individual encodes either one 218 (for binary classification problems having single threshold, or 219 for multiclass problems having multiple thresholds) or multi-220 ple DFs each of which uses a single threshold. Such encoding schemes have been used in [15] and [18]. In another practice, 222 each solution encodes multiple DFs having a single threshold. The final output value in this case may be obtained using a (weighted) voting scheme among the output values of each 225 function of the same individual. An example of this scheme can be found in [19].

In the recent years, researchers have made some notable 227 attempts to solve classification problems using MOGP. Wang et al. [55] proposed a MOGP to obtain a group of nondominated classifiers, with which the maximum receiver operating characteristic convex hull (ROCCH) can be obtained. To achieve this, they have adopted four different multiobjec-233 tive frameworks into GP. For further improvement of each individual GPs performance, they have defined two local search strategies that have been especially designed for classification problems. The experimental results in [55] have 237 demonstrated the efficacy of the proposed memetic scheme in 238 their MOGP framework. Another convex hull-based MOGP, 239 called CH-MOGP, can be found in [56]. Wang et al. [56] 240 showed the differences between the conventional multiobjec-241 tive optimization problem and ROCCH maximization problem. Wang et al. introduced a convex hull-based sorting without 243 redundancy and a new selection procedure which are suitable 244 for ROCCH maximization problem. Again, Bhowan et al. [22] 245 proposed a MOGP-based approach that is especially designed 246 for unbalanced data sets. This approach [22] evolves diverse 247 and accurate ensembles of GP classifiers with good per-248 formance on both the majority and the minority classes. 249 The individual members of the evolved ensembles, that are composed of nondominated solutions, vote on class 250 membership.

#### D. GP, Bloating, and Concise Rules

During evolution of GP, variable length genomes gradually 253 start to increase its length without significant improvement in 254 fitness. This incident, called bloating [57], is a well known 255 phenomenon in GP. Bloating causes genetic programs: 1) to 256 keep reducible genome structures and 2) to memorize training 257 data points, rather than recognizing patterns hidden in them. 258 To find rules which are to some extent human interpretable and 259 can be analyzed, each of the genetic programs must be concise. 260 A plausible way to achieve this target is to control bloat- 261 ing. A popular way to handle bloating is to take into account 262 the program size [2], [58]-[61]. Some other methods include 263 spatially-structured populations [62], [63], island-based mod- 264 els to introduce spatial structure to the population [62], [63], 265 intron deletion [64], and dynamic population sizing [65], [66]. 266 Song et al. [67] attempted to understand the GP evolved solu- 267 tions; while Luna et al. [68] attempted to find comprehensible 268 rules in subgroup discovery.

## E. Ensemble Classifier

In classification, the basic task is to search through a 271 hypothesis space to find a suitable hypothesis that will 272 be able to classify the data points in a better way. An 273 ensemble combines multiple hypotheses to form a better 274 one [19], [21], [22], [53], [69], [70]. Empirically, an ensem- 275 ble performs better when each of the classifiers is highly 276 accurate (strong learner) and the members of the ensemble are 277 significantly diverse. The explanation behind the better perfor- 278 mance of ensemble classifiers than a single classifier has been 279 described in [20]. Normally, to decide the class label of a data 280 point, the member classifiers of an ensemble use (weighted) 281 voting. Ensembles are often used in bio-informatics [71].

#### III. PROPOSED WORK

#### A. Representation of Classifiers or Solutions

In this paper, we evolve c-populations of genetic programs. 285 Each individual of these populations is a binary classifier. Each 286 binary classifier is represented by a single tree. When a data 287 point is passed through an individual of the ith population, 288 if the output value is positive, the individual says that the 289 passed data point belongs to the ith class; otherwise it says that 290 the point does not belong to that class. The internal (nonleaf) 291 nodes of these trees are functions  $\mathcal{F}$ . The terminal nodes must 292 be either a feature or a constant from the set C. We have 293 imposed some constraint on the minimum size (architecture) 294 of the trees. In each tree there must be at least one function 295 node and two terminal nodes (with at least one feature node). 296 Though, a single feature (terminal) node might be enough to 297 determine the class label, this would rarely happen in practice. 298 The above restrictions make the trees more useful without any 299 loss of generalization capability. Again, after generation of any 300 tree throughout the learning phase (using mutation, crossover, 301 or random initialization), the largest subtree consisting of only 302

303 constants as its leaf nodes is replaced by a constant leaf node 304 having the equivalent constant value.

#### 305 B. MOGP for Learning

Larger genetic programs may memorize the training patterns 306 which, in turn, may increase the training accuracy and reduce 308 the understandability of the rules. Therefore, we aim to find smaller but accurate classifiers. Again, when c is high enough,  $_{310}$  even a balanced c-class data set may get converted to c number of highly imbalanced bi-classification data sets. Instead of 312 minimization of classification error, simultaneous minimiza-313 tion of FP and FN would be more appropriate in this regard. Suppose a classifier makes some mistakes  $m=m_p+m_n$  on a given training data set, where  $m_p$  and  $m_n$  are, respectively, the 316 number of FPs and FNs. Consider two classifiers, each making  $_{317}$  the same number of mistakes m on a given data set. Let for the 318 first classifier  $m_p = m_n$  and for the second classifier  $m_p \gg m_n$ or  $m_p \ll m_n$ . If the cost of an FP is the same as that of a FN, we would prefer the first classifier. Consequently, minimization of both FP and FN would be a better strategy than minimiza-322 tion of the total number of misclassification, particularly for 323 imbalanced data sets. Thus, we have three objectives, i.e., minimizations of: 1) FP; 2) FN; and 3) rule size. Moreover, when different classes are overlapped, minimization of FP is usually in conflict with the minimization of FN and vice versa. Multiobjective optimization is more suitable when we need to optimize more than one conflicting objective. Therefore, dur-329 ing the learning of each binary classifier, we minimize three 330 objectives using an MOGP: 1) FP; 2) FN; and 3) number of 331 leaf nodes in the tree. The third objective is used to reduce 332 the size of the tree which enhances the understandability and 333 reduces the pattern memorization capability. The algorithm, proposed in this paper, is called ASMiGP, which is presented 335 in Algorithm 1.

In an evolutionary search, it is desired to have as many generations as possible and steady state nature of an algorithm maximizes the number of generations when the number of function evaluations is fixed [72]. Due to maximization of generations, a steady state evolutionary search is more exploitative to enhance the searching in a region which is more likely to have or closer to the Pareto front and avoiding exploration in regions that are less likely to improve the solutions. It causes faster convergence. In other words, independent of the fitness evaluation process, steady state selection is more performant than discrete generational selection [73]. Therefore, we have used a steady state algorithm instead of a generational one.

#### 348 C. FS

In this paper, we have used the embedded model of FS. Explicit FS is performed during population initialization and mutation. Implicit FS is performed during crossover. Filtering is also performed at three different stages of the learning process; in particular, at the beginning and after 50% and after 55% of evaluations as described next in this subsection.

To facilitate the FS, following [74], we define an index that assesses the discriminating ability of a feature. Consider a two-class problem. Note that for a multiclass problem, the

#### **Algorithm 1:** ASMiGP

20 return first front of Fronts.

```
1 Initialize population using ramped-half-and-half method.
2 Initialize the archive solutions using initial solutions.
  while Evaluations^{Current} \leq Evaluations^{Maximum} do
       repeat
5
           operator = Select crossover or mutation.
           if operator = crossover then
6
              Select male and female parents (mating
              selection).
              Perform crossover.
8
9
           end
           else
10
              Select an individual (mating selection).
              Mutate the individual.
12
          end
       until the infix equation of off-spring is distinct from
       infix equation of any individual of the archive
       Evaluate the new off-spring.
15
       Evaluations^{Current} = Evaluations^{Current} + 1
16
       Update the archive using new offspring
17
       (multi-objective environmental selection).
18 end
  \mathcal{F}ronts = Perform fast-non-dominated-sort.
```

one-versus-all case can also be viewed as a two-class prob- 358 lem. Let there be  $n_p$  number of training points and the class 359 label for the *j*th data point be +1 if it belongs to class 1 and -1 360 if it belongs to class 2. Let the value of the fth feature for the 361 ith data point be  $f_i$ ;  $i = 1, ..., n_p$ . If the fth feature is a good 362 discriminatory feature then for all data points from class 1, 363 it should have high values and for all points from class 2, it 364 should have low values or vice-versa. Hence for a good dis- 365 criminatory feature, we can define an ideal feature vector with 366 values 1, if the data point is from class 1 and 0 otherwise; or 367 the feature value is 0, if it is from class 1, otherwise, it is 0. 368 Let  $S_f$  be the vector containing the ideal feature values for feature f and  $s_{fi}$  be the ideal feature value of the fth feature for  $_{370}$ the *i*th sample. Note that, there could other important features 371 that are not linearly related to the class structure. We are not 372 considering them in this preliminary filtering step. As in [74], 373 we compute the Pearson's correlation (or any other measure of 374 similarity) between f and s as a measure of feature relevance 375

$$C_f = \sum_{j=1}^{n_p} (s_{ji} - \bar{s}) (f_j - \bar{f}) / \sqrt{\sum_{j=1}^{n_p} (s_{ji} - \bar{s})^2 \sum_{j=1}^{n_p} (f_j - \bar{f})^2}.$$
 376

A higher value of  $|C_f|$  indicates a stronger discriminative power of feature f. For a multiclass problem, using the oneversus-all strategy, for the ith binary classification problem (class i versus the rest), the correlation for the fth feature is denoted by  $C_f^i$ .

Now, we describe the FS procedure. Let the set of all features be  $\mathcal{F}_{all}$ . We intend to incorporate only those features trom  $\mathcal{F}_{all}$  which are more likely to help the classifiers to 385

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386 decide the class label. We assign different fitness and unfit-387 ness measures to the features during the learning phase. To 388 remove a feature node from any tree (during mutation), we 389 select it using Roulette wheel selection on the unfitness vales of the features which are present in that tree. Similarly, when a new feature is inserted in the tree, it is selected using oulette wheel selection on the fitness values. During the first 50% evaluations, the fitness and unfitness features are defined as

$$F_{\text{fitness}}^{0\%,i}(f,i) = \begin{cases} \left(\frac{C_f^i}{C_{\text{max}}^i}\right)^2, & \text{if } \frac{\left|C_f^i\right|}{C_{\text{max}}^i} > 0.3 \\ 0, & \text{otherwise} \end{cases}$$
 (2)

$$F_{\text{unfitness}}^{0\%,i}(f,i) = 1.0 - F_{\text{fitness}}^{0\%,i} \tag{3}$$

 $_{^{397}}$  where  $C^i_{\max}=\max_{f\in\mathcal{F}_{\mathrm{all}}}|C^i_f|.$  Equation (2) sets the fitness of  $_{^{398}}$  very poor (poor with respect to its discriminating power) to 399 zero to eliminate their impact during the initial evolution. Let  $\mathcal{F}_{\text{eval}=0\%,i} \subseteq \mathcal{F}_{\text{all}}$  be the features with nonzero fitness values. 401 Basically, at this stage we are using a filter on the feature set 402  $\mathcal{F}_{all}$  to obtain a smaller feature set.

After completion of 50% evaluations for each population, 404 we find the features used in that population. Let the feature set be  $\mathcal{F}_{\text{eval}=50\%,i}$ . Then we make the fitness of all features in  $\mathcal{F}_{all} - \mathcal{F}_{eval=50\%,i}$  to zero. This is done with the assumption 407 that after 50% evaluations useful features have been used by 408 the collection of decision trees. Now, the fitness and unfitness 409 values of all features in  $\mathcal{F}_{\text{eval}=50\%,i}$  are modified according 410 to (4) and (5), respectively

$$F_{\text{fitness}}^{50\%,i}(f,i) = \begin{cases} \frac{|C_f^i|}{\sum_{\substack{f \neq g \\ g \in \mathcal{F}_{50\%,i}}} |\rho_{fg}|}, & \text{if } f \in \mathcal{F}_{\text{eval}=50\%,i} \\ 0, & \text{otherwise} \end{cases}$$

$$F_{\text{unfitness}}^{50\%,i}(f,i) = e^{-\frac{F_{\text{fitness}}^{50\%,i}\{F_{\text{fitness}}^{50\%,i}\} - \min_{f}\{F_{\text{fitness}}^{50\%,i}\} - \min_{f}\{F_{\text{fitness}}^{50\%,i}\} }$$
(5)

$$F_{\text{unfitness}}^{50\%,i}(f,i) = e^{-\frac{F_{\text{fitness}}^{50\%,i}(f,i) - \min_{f} \left\{F_{\text{fitness}}^{50\%,i}\right\} - \min_{f} \left\{F_{\text{fitness}}^{50\%,i}\right\}}$$
(5)

413 where  $\rho_{fg}$  is the Pearson's correlation between fth and gth features. Here, we try to select features with higher relevance but reducing the redundancy in the set of selected features. The fitness, defined in (4), increases when the feature is highly 417 correlated with class label. Similarly, it reduces when it is more 418 correlated with other existent features. This is done to achieve maximum relevance minimum redundancy.

After 75% function evaluations, again we take another 420 snapshot of the population. Let the existent features for the population be  $\mathcal{F}_{\text{eval}=75\%,i} \subseteq \mathcal{F}_{\text{eval}=50\%,i}$ . Then, the fitness and unfitness values of the features in  $\mathcal{F}_{\text{eval}=75\%,i}$  are defined 424 in (6) and (7), respectively

$$F_{\text{fitness}}^{75\%,i}(f,i) = \begin{cases} F_{\text{fitness}}^{0\%}(f,i), & \text{if } f \in \mathcal{F}_{\text{eval}=75\%,i} \\ 0, & \text{otherwise} \end{cases}$$
 (6)

$$F_{\text{unfitness}}^{75\%,i}(f,i) = 1.0 - F_{\text{fitness}}^{75\%,i}(f,i).$$
 (7)

#### D. Population and Archive Initialization

We initialize each population using ramped-half-and-half 428 method. While constructing the random trees, selection of ter- 429 minal nodes has been made with a probability  $p_{\text{var}}$ . To insert a 430 terminal node in a tree, a random number  $r_n$  is drawn in [0, 1]. 431 If  $r_n < p_{\text{var}}$  then a feature node is added, otherwise a constant node is added. The function nodes are chosen from the 433 set  $\mathcal{F}$ , with equal probability of inclusion for all functions. The 434 feature nodes are selected using Roulette wheel selection on 435 fitness  $F_{\text{fitness}}^{0\%}$ , defined in (2).

To initialize the archive from the initial population, we have 437 used the multiobjective archive initialization scheme present 438 in [72] and [75]. It requires two parameters: 1) maximum 439 archive size  $(N_{\text{max}})$  and 2) minimum archive size  $(N_{\text{min}})$ .

#### E. Selection of Crossover or Mutation

Since ASMiGP is a steady state MOGP, in each generation 442 we generate only one offspring. We use either crossover or 443 mutation to do that. A random number  $r_c$  is drawn in [0, 1]. 444 if  $r_c < p_c$  then crossover operator is selected otherwise the 445 mutation operator is selected for that generation.

## F. Mating Selection

ASMiGP uses crossover with male and female differenti- 448 ation which needs one male and female parent. We perform 449 Roulette wheel selection using classification accuracy of the 450 binary classifiers as fitness to select the female parent. Then 451 the male parent is selected randomly from the remaining 452 archive. The only condition to be satisfied is that the male 453 and female parents must be distinct. For mutation, we need 454 only one individual and it is selected in the same way as done 455 for the female parent in case of crossover operator.

A choice of mating selection could have been the use 457 of some bi-level selection operator, where Pareto dominance 458 is preferred over diversity. In that case, solutions along the 459 whole Pareto optimal solution set with good diversity would 460 have been selected as the primary (female) parents. Note that, 461 we have used crossover with male-female differentiation that 462 tries to generate an off-spring near the primary parent in the 463 hypothesis space. Consequently, this might cause generation of 464 Pareto optimal binary classifiers along the whole Pareto opti- 465 mal solution set. Though they are Pareto optimal, these binary 466 classifiers may have poor accuracies. This is because of the 467 implicit imbalance nature of the binary classification problems 468 (due to conversion from multiclass classification problems) 469 and different classifier sizes. An ensemble classifier, however, 470 performs better when individual members of the ensemble 471 are more accurate. Therefore, we use classification accuracy- 472 based mating selection. It guides the search to generate more 473 accurate binary classifiers.

### G. Crossover

In this paper, we have used crossover operation with male 476 and female differentiation. We want the off-spring to be near 477 the female (acceptor) parent in the hypothesis space. The 478 male (donor) parent is used to make the off-spring diverse 479

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 $^{480}$  from its mother. To do this, two random points (nodes) are  $^{481}$  selected from each of the parents. The probabilities of selection of terminal nodes and function nodes as a crossover point  $^{482}$  (node) are, respectively,  $p_t^c$  and  $(1-p_t^c)$ . Then, the subtree  $^{484}$  rooted at the selected node of the mother tree is replaced with  $^{485}$  a similarly selected subtree from the father tree. If the off- $^{486}$  spring is identical to any of its parents, the whole procedure  $^{487}$  is repeated (before evaluation/learning of the off-spring).

#### 488 H. Mutation

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In most of the GP-based systems, for mutation a subtree rooted at a randomly selected node is replaced by a new randomly generated subtree. Though this kind of mutation explores more in the hypothesis space, it may be too disruptive in nature. Therefore, we intend to use less exploration by keeping the tree structure unaltered. During mutation we perform the following operations on a tree.

- 1) Each constant of the tree is replaced by another random constant with probability  $p_c^m$ .
- 2) Each function node of the tree is replaced by anther random function node with probability  $p_f^m$ .
- Only one feature node of the tree is replaced by another feature node.

For feature nodes, to select the mutation point Roulette wheel selection is performed on the unfitness of the features which are present in the tree. Similarly, to insert a new feature at the mutation point, we select a feature using Roulette wheel selection based on the fitness values (probability proportional to fitness) of the features.

This restricted mutation scheme ensures that the tree struc-509 ture of an equation remains the same. It also ensures that the 510 variables in an equation do not change drastically—changing 511 more than one variable would shift the solution (equation) in 512 the hypothesis space by a larger amount.

#### 513 I. Environmental Selection

ASMiGP uses the archive truncation strategy used 515 in [72] and [75]. This multiobjective archive truncation strat-516 egy uses Pareto-based fitness function, i.e., fitness is Pareto 517 dominance rank. This scheme maintains an archive (ensemble) 518 which has an adaptive and dynamic size. It does not allow the archive to fall below a minimum size ensuring diversity in the 520 genotypic space. Moreover, the environmental selection dimin-521 ishes the exploration in areas of objective space that are less 522 likely to yield improved solutions [72], ensuring diversity in 523 phenotypic space. Furthermore, we have made the following 524 difference in the environmental selection. ASMiGP ensures 525 that the infix expression of every off-spring (after mutation or 526 crossover) is distinct from every member of the archive. To 527 achieve this, before evaluating the offspring, ASMiGP converts it to its infix expression and then compares the expression with that of each individual of the archive. Only if the expression is unique, the off-spring is evaluated and added to the archive. Otherwise it is discarded and a new off-spring is gen-532 erated. Another noticeable difference is that here the number of objectives is three. Note that the diversity maintenance in each 534 ensemble both in phenotypic space and in genotypic space finds a diverse set of trees (bi-classifiers). Trees, being diverse, 595 enhance the performance of the corresponding ensemble. In 596 this context, it is worth mentioning that the archive, along 597 with the archive truncation strategy, helps to realize a good 598 Pareto front by explicitly maintaining diversity among the fit 699 (according to rank) solutions. However, the archive alone is not 540 sufficient to evolve a good Pareto front along all the objectives. 541

#### J. Decision Making

To determine the class label, we find the net belongingness 543 of a point to each class. The net belongingness lies in [0, 1]. 544 A higher value indicates more net belongingness to that class. 545 A data point is assigned to that class for which it has the 546 highest net belongingness. 547

After the learning, we obtain a set of c archives,  $\mathcal{A} = {}^{548}\{\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_c\}; \ \forall i, 1 \leq |\mathcal{A}_i| \leq N_{\text{max}}, \ \text{where } c \ \text{is the num-} \ \text{ber of classes, and } \mathcal{A}_i \ \text{is the set of all binary classifiers for the } \ \text{550} \ \text{ith class.}$  To determine the net belongingness of a data point  $\mathbf{p}$  551 to class m,  $\mathcal{B}_m^{\text{net}}(\mathbf{p})$ , it is passed through all genetic programs 552 of set  $\mathcal{A}_m$ . The net belongingness,  $\mathcal{B}_m^{\text{net}}(\mathbf{p})$ , of the point  $\mathbf{p}$  for 553 class m is computed using

$$\mathcal{B}_{m}^{\text{net}}(\mathbf{p}) = \frac{1}{2} \left( \frac{1}{|\mathcal{A}_{m}|} \sum_{i=1}^{|\mathcal{A}_{m}|} \mathcal{B}_{m}^{i}(\mathbf{p}) + 1.0 \right)$$
(8) 555

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where  $\mathcal{B}_{m}^{i}$  is defined as

$$\mathcal{B}_{m}^{i}(\mathbf{p}) = \begin{cases} +\left(1.0 - \frac{\mathrm{FP}_{m}^{i}}{\mathrm{FP}_{m}^{\mathrm{max}}}\right), & \text{if } \mathcal{A}_{m}^{i}(\mathbf{p}) > 0\\ -\left(1.0 - \frac{\mathrm{FN}_{m}^{i}}{\mathrm{FN}_{m}^{\mathrm{max}}}\right), & \text{otherwise.} \end{cases}$$
(9) 557

In (9),  $FP_m^i$  and  $FN_m^i$ , respectively, represent the number of FPs and FNs made by the ith individual in set  $\mathcal{A}_m$  on the training data.  $FP_m^{\max}$  and  $FN_m^{\max}$  are, respectively, the maximum possible FP and the maximum possible FN for the mth class; and  $\mathcal{A}_m^i(\mathbf{p})$  is the output from ith individual of  $\mathcal{A}_m$  for input data point  $\mathbf{p}$ . Finally,  $\mathbf{p}$  is assigned the class k, when  $\mathcal{B}_k^{\text{net}} = \frac{c}{m} \{\mathcal{B}_m^{\text{net}}\}$ . Note that  $FP_m^{\max}$  and  $FP_m^{\min}$  are determined by the training data.

The concept of net belongingness is inspired by the concept of negative voting. Negative voting has been widely used 567 in diverse applications [76]–[78]. It is more effective when 568 circumstances unfavorable to the preferences invoke stronger 569 electoral responses than the similar favorable responses, as 570 well as the behaviors of the voters are well defined [79]. In 571 our scheme, the learners for the ith class learn to vote yes 572 for the points of the ith class and no for the points which 573 do not belong to the ith class. For multiclass problems, it 574 is more likely that a binary classifier learns to say no than 575 to say yes for a much higher number of points. Therefore, 576 we found negative voting to be more suitable in this context. 577 However, we have used a weighted negative voting scheme. 578 The accuracies for the responses yes and no of the ith binary 579 classifier of mth class are, respectively,  $(1.0 - FP_m^i/FP_m^{max})$  580 and  $(1.0 - FN_m^i/FN_m^{max})$ . These values have been used as corresponding weights for the responses yes and no of the ith 582 binary classifier of the mth class. We have used the positive 583

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TABLE I PARAMETER SETTINGS FOR THE PROPOSED METHOD

Parameter	Value
Set of functions $(\mathcal{F})$	$\overline{\{+,-, imes,\div\}}$
Range of initial values of constants $(C)$	[0, 2]
Maximum depth of tree during initialization	6
Maximum allowable depth of tree	10
Maximum archive size $(N_{max})$	50
Minimum archive size $(N_{min})$	30
Initial Probability of feature nodes $(p_{var})$	0.8
Probability of crossover $(p_c)$	0.8
Probability of crossover for terminal nodes $(p_t^c)$	0.2
Probability of mutation for constants $(p_c^m)$	0.3
Probability of mutation for function nodes $(p_f^m)$	0.1
Function evaluations for each binary classifier	400000

TABLE II SUMMARY OF MICROARRAY DATA SETS

	Data Set	Features (F)	Samples $(S)$	Classes (C)	$\left(\frac{F}{S}\right)$
1	Colon	2000	62	2	32.26
2	TOX-171	5748	171	4	33.61
3	Leukemia 1	7129	34	2	209.68
4	Leukemia 2	7129	38	2	187.61
5	CLL-SUB-111	11340	111	3	102.16
6	GCM	16063	144	14	111.55
7	SMK-CAN-187	19993	187	2	106.91
_8	GLA-BRA-180	49151	180	4	273.06

and the negative signs to indicate acceptance and rejection of 585 the data point for the mth class, respectively.

#### IV. EXPERIMENTATION

#### 587 A. Experimental Settings

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We have repeated tenfold cross validation of the proposed 589 method for ten times. Table I shows the parameter settings 590 that we have used for this purpose. The training data is 591 Z-score normalized. Furthermore, based on the means and the 592 standard deviations of the features of the training data, the 593 test data was Z-score normalized. Note that except  $N_{\text{max}}$  and  $N_{\min}$ , all parameters are standard parameters used in any GP simulations, while  $N_{\text{max}}$  and  $N_{\text{min}}$  are needed for archive main-596 tenance. Although all the parameters can be chosen using a 597 cross validation mechanism, because of huge computational 598 overhead, we could not do that. Based on a few experi-599 ments we selected these parameters. These choices are not 600 optimal. However, since the same set of values are used for widely different types of data sets, it demonstrates the effec-602 tiveness of the proposed scheme. The proposed method has 603 been implemented in Java with the help of jMetal [80], [81]. We have used eight microarray and eleven text data sets which are summarized in Tables II and III, respectively.

#### 606 B. Importance of FS and Rule Size Reduction

To demonstrate the importance of the proposed FS and rule 607 size reduction scheme, we have compared our method with GP without FS and no restriction to equation size. To do that, we have made the following changes in the proposed method.

- 1) No explicit FS as described in Section III-C is done.
- 2) There are only two objectives, FP and FN.

TABLE III SUMMARY OF TEXT DATA SETS

	Data Set	Features (F)	Samples (S)	Classes (C)	$\left(\frac{F}{S}\right)$
	oh0.wc	3182	1003	10	3.17
2	oh10.wc	3238	1050	10	3.08
3	tr12.wc	5804	313	8	18.54
4	tr23.wc	5832	204	6	28.59
5	tr11.wc	6429	414	9	15.53
6	tr21.wc	7902	336	6	23.52
7	wap.wc	8460	1560	20	5.42
8	ohscal.wc	11465	11162	10	1.03
9	la2s.wc	12432	3075	6	4.04
10	la1s.wc	13195	3204	6	4.12
11	new3s.wc	26832	9558	44	2.81

All other parts of the algorithm and the parameter values 613 remain unchanged. Similar to the proposed scheme, we have 614 also executed tenfold cross validation for ten times for all the 615 data sets. Along with results (mean values of the correspond- 616 ing ten runs) obtained using the proposed method, the results 617 obtained using this scheme for microarray and for text data 618 sets are, respectively, summarized in Tables IV and V. From 619 these two tables, we observe the following.

- 1) In all cases, the test accuracy is much higher for the pro- 621 posed method. Especially, for GCM having 14 classes, 622 the difference between the test accuracies are remarkably 623
- 2) The tree size increases significantly when the third 625 objective, i.e., the restriction on rule size, is not used.
- 3) For most of the data sets the proposed method selects 627 smaller number of distinct features per tree as well as 628 for per classifier.

These observations clearly demonstrate the importance of 630 the FS as well as constraining the rule size. Since our FS 631 scheme discards features with poor relevance and uses features 632 with good discriminating power yet avoiding use of redundant 633 features, it not only makes the discovery of useful rules eas- 634 ier but also implicitly constrains the rule length. Thus, FS 635 plays a very important role having two positive impacts: it 636 makes identification of useful rules easier and it promotes the 637 minimization of the third objective.

#### C. Comparing With Other Methods

To compare the performance of the proposed method 640 we have used the experimental results reported in [82] (see 641 [82, Tables IV-VII]). Song et al. [82] used four different 642 types of classification algorithms: 1) probability-based naive 643 Bayes (NB); 2) tree based C4.5; 3) instance-based lazy learning algorithm IB1; and 4) rule-based RIPPER both before and 645 after FS. Along with the full feature set, they have used six 646 FS algorithms in their experiment.

- 1) FAST [82].
- 2) FCBF [83], [84].
- 3) CFS [85].
- 4) ReliefF [86].
- 6) FOCUS-SF [88].

5) Consist [87].

TABLE IV
EXPERIMENTAL RESULTS ON MICROARRAY DATA SETS (MEAN VALUES OF TEN RUNS OF TENFOLD CROSS VALIDATION)

Data Set	$\%\mathrm{TA}^a$		]	$FS^b$		$TS^c$		$(F/T)^d$		$% \mathrm{F}^{e}$		$(\%F/T)^f$	
Data Sci	$PM^g$	$\mathrm{W}^h_{\mathrm{F\&R}}$	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	
Colon	85.12 (2.07)	71.93 (4.12)	195.0	182.5	6.76	123.60	3.11	8.56	9.75	9.13	0.16	0.43	
TOX-171	81.07 (3.42)	58.52 (4.57)	407.6	540.9	8.83	148.44	3.53	11.97	7.09	9.41	0.06	0.21	
Leukemia1	93.50 (2.85)	74.08 (6.42)	188.6	276.6	3.01	76.09	2.00	6.52	2.65	3.88	0.03	0.09	
Leukemia2	91.58 (3.67)	77.33 (6.84)	147.8	229.0	3.50	74.16	2.02	5.72	2.07	3.21	0.03	0.08	
CLL-SUB-111	80.52 (2.60)	54.51 (3.51)	335.3	465.3	7.29	134.28	3.20	10.75	2.96	4.10	0.03	0.09	
GCM	69.35 (1.96)	33.97 (2.60)	854.3	1086.0	4.70	105.42	1.91	6.22	5.32	6.76	0.01	0.04	
SMK-CAN-187	68.68 (1.18)	62.12 (2.30)	319.9	435.8	22.23	135.88	6.41	15.33	1.60	2.18	0.03	0.08	
GLA-BRA-180	68.22 (2.25)	58.89 (2.75)	784.4	569.9	11.30	150.81	4.33	11.40	1.60	1.16	0.01	0.02	

<sup>a</sup>Test Accuracy (standard deviation is provided within parenthesis), <sup>b</sup>Number of Features Selected per Classifier, <sup>c</sup>Tree Size, <sup>d</sup>Number of Features per Tree, <sup>e</sup>Percentage of Features Selected, <sup>f</sup>Percentage of Features Selected per Tree, <sup>g</sup>Proposed Method, <sup>h</sup>GP without FS and Rule Size Reduction

 ${\it TABLE~V}\\ {\it Experimental~Results~on~Text~Data~Sets~(Mean~Values~of~Ten~Runs~of~Tenfold~Cross~Validation)}$ 

Data Set	$\% \mathrm{TA}^a$		$FS^b$		Т	$TS^c$		$(F/T)^d$		%	$\%\mathrm{F}^e$		$(\%F/T)^f$	
Data Set	$-$ PM $^g$	$\mathrm{W}^h_{\mathrm{F\&R}}$	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>		PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	PM	W <sub>F&amp;R</sub>	
oh0.wc	87.75 (0.51)	70.53 (1.17)	484.1	2080.7	17.06	145.38	457	6.46	25.90	15.21	65.39	0.20	0.81	
oh10.wc	81.06 (0.61)	66.11 (1.52)	439.6	2166.8	24.11	140.67		7.12	26.03	13.58	66.92	0.22	0.80	
tr12.wc	87.86 (1.50)	60.55 (2.36)	603.7	1697.3	8.67	123.91		4.17	17.22	10.40	29.24	0.07	0.30	
tr23.wc	93.95 (1.19)	64.90 (2.14)	396.5	1154.2	6.10	117.15		3.09	14.81	6.80	19.79	0.05	0.25	
tr11.wc	86.08 (0.72)	64.63 (2.56)	631.6	1785.8	8.82	128.57		4.03	17.03	9.82	27.78	0.06	0.26	
tr21.wc	89.64 (1.14)	71.46 (2.62)	362.0	1219.2	9.51	114.51		4.17	15.00	4.58	15.43	0.05	0.19	
wap.wc	79.60 (0.60)	58.96 (1.64)	1199.8	4377.5	17.38	125.53		6.07	21.02	14.18	51.74	0.07	0.25	
ohscal.wc	73.45 (0.23)	62.59 (1.21)	232.9	3853.8	63,48	111.52		7.78	24.87	2.03	33.61	0.07	0.22	
la2s.wc	83.95 (0.62)	67.32 (0.99)	354.6	2369.1	53.17	133.76		11.41	28.65	2.85	19.06	0.09	0.23	
la1s.wc	83.06 (0.36)	65.62 (1.05)	380.6	2372.0	56.40	133.21		12.30	28.35	2.88	17.98	0.09	0.21	
new3s.wc	81.32 (0.27)	58.96 (1.64)	1674.2	4377.5	33.93	125.53		7.10	21.02	6.24	16.31	0.03	0.08	

<sup>a</sup>Test Accuracy (standard deviation is provided within parenthesis), <sup>b</sup>Number of Features Selected per Classifier, <sup>c</sup>Tree Size, <sup>d</sup>Number of Features per Tree, <sup>e</sup>Percentage of Features Selected, <sup>f</sup>Percentage of Features Selected per Tree, <sup>g</sup>Proposed Method, <sup>h</sup>GP without FS and Rule Size Reduction

Use of all features can be viewed as the seventh FS algofinithm. To make this paper comprehensive, we are not disfinithm. To make this paper comprehensive, we are not disfinithm course for the settings used in [82]. Note that for accuracies for few data sets for few pairs of FS schemes are for not available in [82].

1) Results With Microarray Data Sets: Table IV presents 660 the results of the proposed method on microarray data sets. We have already stated that for each classifier, Song et al. [82] 662 used seven FS schemes (six FS method as well as the set of 663 all features). For each FS method five repetitions of the ten-664 fold cross validation experiment were done in [82]. And then, 665 for each FS method, the average accuracy over the five rep-666 etitions is reported. We compare this average accuracy with 667 the average accuracy that we have obtained by our method 668 over the ten repetitions of the tenfold cross validation experiments. In particular, we count the number of cases (each case 670 refers to one FS scheme) in which our algorithm outperforms. 671 Note that, for some combination of data set and classifier, the 672 total number of cases is less than seven as for those combi-673 nations some results are not available. Table VI reports these 674 counts. To elaborate Table VI, consider the entry correspond-675 ing to column IB1 and row CLL-SUB-111. For the data set 676 CLL-SUB-111, in [82, Table VI], Song et al. reported the per-677 formance of the algorithm IB1 for six different FS algorithms. 678 Our algorithm is found to perform better than five of the six 679 FS algorithms and hence the entry for row CLL-SUB-111 and 680 column IB1 is 5/6. Note that, for this data set, Song et al. [82] 681 did not report performance of IB1 using all features. All but 682 the entries in the last column of Table VI are generated in

TABLE VI COMPARISON WITH NB, C4.5, IB1, AND RIPPER ON MICROARRAY DATA SETS

Data Set	NB	C4.5	IB1	RIPPER	Total
Colon	4/7	2/7	4/7	6/7	16/28
TOX-171	4/7	7/7	3/7	7/7	21/28
Leukemia1	2/7	2/7	2/7	2/7	8/28
Leukemia2	5/7	6/7	6/7	5/7	22/28
CLL-SUB-111	4/7	6/7	5/6	4/7	19/27
GCM	4/7	7/7	6/7	7/7	24/28
SMK-CAN-187	2/6	2/6	2/6	2/6	8/24
GLA-BRA-180	3/6	5/6	1/6	5/6	14/24
Total	28/54	37/54	29/53	38/54	132/215

the same manner. The last column of Table VI, which reports 683 the row total, reveals that our method performs the best for 684 61.40% (132 out of 215) test cases.

If we compute the percentage of features selected by the ensembles, it may not be very small for some data sets, like 687 Colon. But, if we consider the number of features selected per 688 binary classifier (tree), we find that this number is quite small, 689 e.g., the maximum value is 0.16% for Colon. We assume that 690 binary classifiers (binary trees) having less than twenty nodes are concise enough. We need to remember that we are talking 692 about raw rules (equations) directly obtained from GP which 693 are most likely affected by bloating. Simplification of these 694 rules may lead to reduction in their sizes. Based on this, in 695 all but one data set we could find easy to analyze rules. For 696 SMK-CAN-187 the extracted rules are more complex possibly 697 because of complex structure of the data.

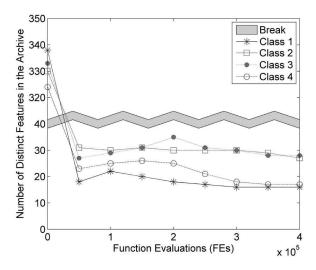


Fig. 1. Showing the number of distinct features present in the archive with respect to function evaluations for GLA-BRA-180 data set.

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In Table S-I (see supplementary materials), we present the best rules (or binary classifiers or GPs) we found for each class of each microarray data set. These GPs have the highest train-702 ing accuracy among the GPs obtained from the first fold of the 703 first ten fold cross validation. If there are more than one rule 704 having the same maximum training accuracy, the rule with the smallest length has been reported. The features in the equations are indexed starting from "0." From Table S-I, we can 707 observe that for several classes the proposed method could find substantially small rules. Noticeably, for four, six, eight, and 709 three classes, the proposed method could find the best binary 710 classifier having only 1–4 distinct variables, respectively. So, 711 21 out of 33 (i.e., 63.64%) cases, we could find considerably 712 small (and hence easy to interpret) rules. For some classes, 713 the rules having the highest training accuracy were not very 714 comprehensible because the length of the rule was not very <sub>715</sub> small. If we think that  $(2.0 \times x_i)$  is more easy to understand 716 than  $(x_i + x_i)$ , though both equations have the same size, we observe that for 21 out of 33 (i.e., 63.64%) cases the proposed 718 method could find rules having highest accuracy, which are 719 not at all affected by bloating and are comprehensible without 720 simplification.

To investigate how the number of distinct features changes 722 in the archive, we have executed our algorithm with 400 000 function evaluations using the entire GLA-BRA-180 data set. 724 In Fig. 1, we have plotted the number of distinct features 725 after initial and after each 12.5% of maximum function eval-726 uations. For all four classes of GLA-BRA-180 data set, the 727 number of distinct features in the archive initially falls dras-728 tically depicting the impact of FS. After some generations, it 729 becomes almost constant. Moreover, the number of final dis-730 tinct features for each class is quite small. This indeed reveals a desirable behavior of the our scheme.

To show how the individual binary classifiers' accuracies 733 change with function evolutions, we have plotted each individuals' FPs and FNs for all four classes of GLA-BRA-180 735 data set in Figs. S-1 and S-2 (see supplementary materials). For 736 this part of the experiment also, we have used the entire data

TABLE VII COMPARISON WITH NB, C4.5, IB1, AND RIPPER ON TEXT DATA SETS

Data Set	NB	C4.5	IB1	RIPPER	Total
oh0.wc	7/7	7/7	7/7	6/6	27/27
oh10.wc	7/7	7/7	7/7	6/6	27/27
tr12.wc	7/7	7/7	7/7	7/7	28/28
tr23.wc	7/7	5/7	7/7	4/7	23/28
tr11.wc	7/7	7/7	7/7	6/6	27/27
tr21.wc	6/7	6/7	6/7	3/6	21/27
wap.wc	7/7	6/6	6/6	6/6	25/25
ohscal.wc	4/4	4/4	4/4	4/4	16/16
la2s.wc	6/6	5/5	5/5	5/5	21/21
la1s.wc	6/6	5/5	5/5	5/5	21/21
new3s.wc	3/3	3/3	3/3	3/3	12/12
Total	67/68	62/65	64/65	55/61	248/259

set for training. From the figures, it is observed that with the 737 increase in number of evolutions, the average accuracy of the 738 solutions tends to increase. However, for class four, some solu-739 tions having lower level of accuracies (having higher FPs and 740 FNs) are there even after 400 000 function evaluations. This is 741 because, even after such high number of function evaluations, 742 the algorithm was still searching for more concise solutions, 743 and could find some trees of comparatively smaller size.

2) Results With Text Data Sets: Similar to Table VI with 745 microarray data sets, we present the same result (number of 746 test cases for which our algorithm provides the best results 747 for each classifier and data set pair) with text data sets in 748 Table VII. Table VII reveals that for text data sets the proposed 749 scheme performs the best for 95.75% (248 out of 259) cases. 750

If we consider the same criteria that binary classifiers (trees) 751 having less than twenty nodes are concise enough, then our 752 method could not find interpretable rules for 5 (oh10.wc, 753 ohoscal.wc, la2s.wc, la1s.wc, and new3s.wc) out of the 11 754 text data sets. The number of selected features is not at all 755 small for most of the text data sets. Some reasons behind 756 this may be that the number of classes is high for the text 757 data sets and the existence of more complex class structure, 758 which is defined by the keywords and relation of keywords to 759 the imposed classes is usually not as straightforward as genes 760 have to cancers. However, the percentage of features selected 761 per binary classifiers (trees) is quite small. Noticeably, the 762 accuracy obtained for new3s.wc (having 44 classes), is much 763 higher than that of the other methods (for accuracies of other 764 methods, see [82]). We can also observe that for data sets having more than or equal to ten classes, our methods performs 766 comparatively better than other methods.

## D. Statistical Significance Testing

To compare the proposed method with existing FS and clas-769 sification methods, we consider four classification and six 770 FS methods as well as with the full feature set. Thus we 771 compare our algorithm with 28 FS and classification algo-772 rithm pairs. We have performed Wilcoxon signed ranks test 773 to show that the performance of the proposed algorithm is 774 significantly different over 28 pairs of FS and classification 775 algorithm. For this, we have considered both the microarray 776 and the text data sets together and have used the average test 7777

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TABLE VIII WILCOXON SIGNED RANKS TEST (ONE-TAILED) FOR PAIRWISE Comparisons with the Proposed Method at  $\alpha=0.05$ 

	NB	C4.5	IB1	RIPPER
FAST	A	R	R	R
FCBF	R	R	R	R
CFS	R	R	R	R
ReliefF	R	R	R	R
Consist	R	R	R	R
FOCUS-SF	R	R	R	R
Full Set	R	R	R	R

A:  $H_0$  Accepted, R:  $H_0$  Rejected.

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778 accuracies achieved with different algorithms on these data 779 sets. Moreover, we have removed the cases for which accu-780 racies are not known (see [82, Tables IV-VII]). Table VIII shows that out of the 28 cases, only in one case the null hypothesis  $H_0$  was accepted. Here the null hypothesis is that 783 there is no significant difference in performance between our 784 algorithm and a comparing algorithm. We have also used 785 Friedman test [89], [90] to check if all the 29 (28 existing 786 and our proposed) algorithms perform similarly over seven 787 data sets: Colon, TOX-171, Leukemia1, Leukemia2, GCM, 788 tr12.wc, and tr23.wc (see [82, Tables IV-VII], some accu-789 racies for other data sets are not available). The obtained Friedman statistics is 60.13, which is significant at  $\alpha = 0.001$ , <sub>791</sub> as the corresponding statistic  $\chi^2$  with 28 degrees of freedom 792 is 56.90. Thus, Friedman test suggests existence of significant 793 difference among the algorithms.

#### V. CONCLUSION

In this paper, we have used a MOGP, called ASMiGP, to 796 evolve diverse sets of binary classifiers to solve multiclass clas-797 sification problems. Simultaneous FS and rule extraction are erformed during the genetic evolution. An important objecye of this paper is to find simple classification rules that may human understandable, which in the given context translates to rules with simple operations and short length. The proposed method is found to achieve its goal.

Ensembles perform better when weighted voting is used, the 804 members of the ensembles are diverse enough, and the classifiers are accurate [21]. Here, we have created c sets of diverse 806 ensembles. Unlike other ensemble-based method, here each 807 ensemble represents diverse classifiers for just one class. The 808 number of features used by the ensembles is high with respect 809 to the number of features selected per (binary classifier) tree. 810 This suggests that the binary classifiers are diverse enough. In  $^{811}$  our algorithm, we evolve c distinct species in parallel, which 812 try to learn distinct patterns and no interspecies gene exchange ever allowed. This property makes each species different 814 from the other species and the system becomes less vulner-815 able, especially when each species has successfully learnt its 816 designated patterns.

Our method has been tested on nineteen (eight microar-818 ray and eleven text) data sets. The experimental results 819 show that we could find easy-to-understand rules for overall 820 63.2% (87.5% for microarray and 54.5% for text) data sets. 821 We compared our method with four classification methods in conjunction with seven FS methods including use of 822 the all-feature set. For 80.17% (61.40% for microarray and 823 95.75% for text) cases our method outperforms others. The 824 improvement in performance is shown statistically significant 825 compared to the others.

The overall performance of the proposed method is better 827 on text data sets compared to that of microarray data sets. Two 828 important differences between these two groups of data sets are 829 that: 1) microarray data sets have comparatively large feature- 830 to-sample ratios and may not have enough number of points 831 in each class for MOGP to learn the structure of the data sets 832 and 2) the text data sets have comparatively large number of 833 classes as well as instances. Our limited experiments suggest 834 that when there are enough points in each class so that each 835 species can successfully learn its target pattern, the proposed 836 method works better. We found that for text data our method 837 performs noticeably better than the other methods particularly 838 when number of classes is high (ten or more than that).

We have shown that our method is very effective when the 840 dimension of the data sets are as high as 49 151. But in all our 841 data sets, number of samples were not very big. If we apply 842 the proposed method on a data set with a really large num- 843 ber samples, it may require a significant amount of time. The 844 method may also take a substantial amount of time when the 845 number of classes is high and we have limited parallel process- 846 ing capability. With the today's high performance computing 847 technologies, however, these are not really crucial shortcom- 848 ings. Yet, we have not applied it to truly big data. This paper 849 can be adapted to deal with big data, especially using Hadoop. 850

Our future research interest is to use MOGP to classify 851 multiclass text data, where each text may belong to more than 852 one category (class) and to use net belongingness as a fuzzy 853 membership of the documents to the corresponding category. 854 We also intend to modify the proposed learning method to 855 stepwise learning, so that we can use it for big text data.

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## **AUTHOR QUERIES**

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