A Regression-like Classification System for Geometric Semantic Genetic Programming

Illya Bakurov[1], Mauro Castelli[1], Francesco Fontanella[2] and Leonardo Vanneschi[1]
[1]*NOVA Information Management School (NOVA IMS), Universidade Nova de Lisboa, Campus de Campolide, 1070-312, Lisbon, Portugal*
[2]*Department of Electrical Engineering and Information, Universitá degli Studi di Cassino e del Lazio Meridionale, 03043, Cassino, Italy*

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Abstract: Geometric Semantic Genetic Programming (GSGP) is a recent variant of Genetic Programming, that is gaining popularity thanks to its ability to induce a unimodal error surface for any supervised learning problem. Nevertheless, so far GSGP has been applied to the real world basically only on regression problems. This paper represents an attempt to apply GSGP to real world classification problems. Taking inspiration from Perceptron neural networks, we represent class labels as numbers and we use an activation function to constraint the output of the solutions in a given range of possible values. In this way, the classification problem is turned into a regression one, and traditional GSGP can be used. In this work, we focus on binary classification; logistic constraining outputs in [0,1] is used as an activation function and the class labels are transformed into 0 and 1. The use of the logistic activation function helps to improve the generalization ability of the system. The presented results are encouraging: our regression-based classification system was able to obtain results that are better than, or comparable to, the ones of a set of competitor machine learning methods, on a rather rich set of real-life test problems.

1 INTRODUCTION

Geometric Semantic Genetic Programming (GSGP) (Moraglio et al., 2012) is a recent development of Genetic Programming (GP) (Koza, 1992). GSGP uses particular genetic operators, called Geometric Semantic Operators (GSOs) and it has gained noteworthy popularity among researchers in the last few years. This popularity is probably because GSOs can induce a unimodal error surface (i.e., with no locally optimal solutions) for any supervised learning problem. This property bestows a remarkable optimization power on GSGP. Furthermore, in several references (see for instance (Castelli et al., 2015a)), it was shown that, in some particular circumstances, GSOs are also able to limit overfitting. Thanks to these important properties, and also to a very efficient implementation presented in (Castelli et al., 2015a), GSGP was successful in several different real-life applications in recent years (a rather complete summary of the applications is reported in (Vanneschi et al., 2014)).

However, looking at the different applications that have been developed with GSGP, it is possible to notice a clear trend: those applications are mainly regression and forecasting problems. In other words, almost no relevant results showing successful applications of GSGP on classification problems were presented. This does not happen by chance: even though in the contribution that originally introduced GSGP (Moraglio et al., 2012) a version of GSOs for classification was presented, that version of the operators is not very easy to use. More specifically, those operators assume that GSGP is evolving individuals that are classification rules. Even though systems evolving rules, like decision trees, using GP have been presented so far, this is not the most typical use of GP. GP individuals are, typically, mathematical functions of the inputs, returning as output numbers. As such, GP is naturally more prone to be used for regression than for classification.

In this paper, we intend to fill this gap, proposing a GSGP-based approach for classification for the first time, where individuals are numeric expressions, as is usual in GP. The approach is straightforward and inspired by the output layer of Artificial Neural Networks (ANNs), where an activation function is applied to the output. Similarly to ANNs, a logistic ac-

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tivation is applied to the output of a GSGP individual, and compared to the target of a binary classification, appropriately transformed into binary values (with 0 representing one class label, and 1 representing the other). It is worth noticing that, since the problem is "de facto" transformed into a regression and the logistic function is increasing monotonically, the property of GSOs of inducing a unimodal error surface is maintained. Despite its simplicity, we think that, if successful, this idea may have a significant impact, paving the way for new GSGP contributions for real-life classification problems.

The paper is organized as follows: in Section 2, we describe GSGP; Section 3 presents our idea of a regression-like classification system based on GSGP; Section 4.3 contains our experimental study. More specifically, in the first part of this section, we present experiments aimed at tuning two important system parameters, while in the second part we present an experimental comparison of the proposed approach with Support Vector Machines, one of the most popular and powerful classification algorithms. The comparison is made on 10 complex real-life datasets. Finally, Section 5 concludes the work, and presents ideas for future investigation.

2 GEOMETRIC SEMANTIC GENETIC PROGRAMMING

Let $\mathbf{X} = \{\overrightarrow{x_1}, \overrightarrow{x_2}, ..., \overrightarrow{x_n}\}$ be the set of input data (training instances, observations or fitness cases) of a symbolic regression problem, and $\overrightarrow{t} = [t_1, t_2, ..., t_n]$ the vector of the respective expected output or target values (in other words, for each $i = 1, 2, ..., n$, t_i is the expected output corresponding to input $\overrightarrow{x_i}$). A GP individual (or program) P can be seen as a function that, for each input vector $\overrightarrow{x_i}$ returns the scalar value $P(\overrightarrow{x_i})$. Following (Moraglio et al., 2012), we call *semantics* of P the vector $\overrightarrow{sP} = [P(\overrightarrow{x_1}), P(\overrightarrow{x_2}), ..., P(\overrightarrow{x_n})]$. This vector can be represented as a point in an n-dimensional space, that we call *semantic space*. Remark that the target vector $\overrightarrow{t}$ itself is a point in the semantic space.

As explained above, GSGP is a variant of GP where the traditional crossover and mutation are replaced by new operators called Geometric Semantic Operators (GSOs). The objective of GSOs is to define modifications on the syntax of GP individuals that have a precise effect on their semantics. More in particular, as schematically shown in Figure 1, GSOs are:

- Geometric Semantic Crossover. This operator generates only one offspring, whose semantics stands in the line joining the semantics of the two parents in the semantic space.
- Geometric Semantic Mutation. With this operator, by mutating an individual i, we obtain another individual j such that the semantics of j stands inside a ball of a given predetermined radius, centered in the semantics of i.

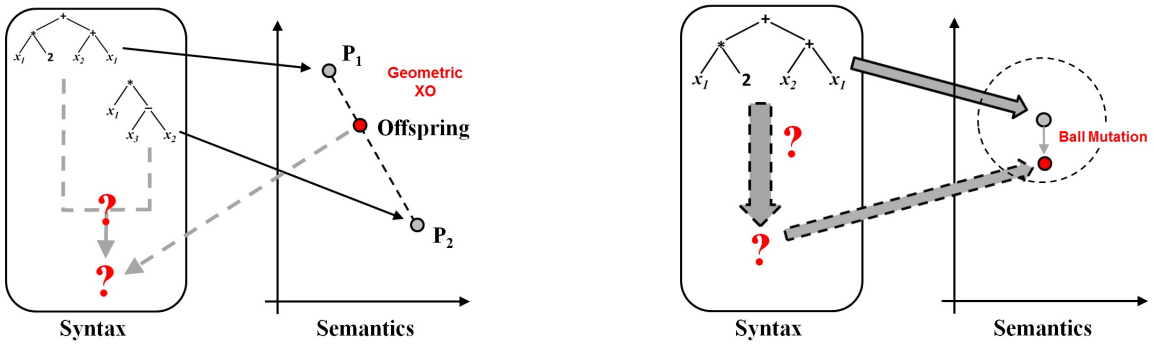
One of the reasons why GSOs became so popular in the GP community (Castelli et al., 2015d; Castelli et al., 2013; Castelli et al., 2015c; Ruberto et al., 2014; Castelli et al., 2015e; Castelli et al., 2016b; Castelli et al., 2015b; Vanneschi et al., 2017; Bakurov et al., 2018; Bartashevich et al., 2018) is related to the fact that GSOs induce an unimodal error surface (on training data) for any supervised learning problem, where fitness is calculated using an error measure between outputs and targets. In other words, using GSOs the error surface on training data is guaranteed to not have any locally optimal solution. This property holds, for instance, for any regression or classification problem, independently of how big and how complex data are (Vanneschi et al., 2014; Castelli et al., 2016a). The definitions of the GSOs are, as given in (Moraglio et al., 2012), respectively:

Geometric Semantic Crossover (GSC). Given two parent functions $T_1, T_2 : \mathbb{R}^n \rightarrow \mathbb{R}$, the geometric semantic crossover returns the real function $T_{XO} = (T_1 \cdot T_R) + ((1 - T_R) \cdot T_2)$, where T_R is a random real function whose output values range in the interval $[0, 1]$.

Geometric Semantic Mutation (GSM). Given a parent function $T : \mathbb{R}^n \rightarrow \mathbb{R}$, the geometric semantic mutation with mutation step ms returns the real function $T_M = T + ms \cdot (T_{R1} - T_{R2})$, where T_{R1} and T_{R2} are random real functions.

Even though this is not in the original definition of GSM, later contributions (Castelli et al., 2015a; Castelli et al., 2014) have clearly shown that limiting the codomain of T_{R1} and T_{R2} in a predefined interval (for instace $[0, 1]$, as is done for T_R in GSC) helps improving the generalization ability of GSGP. As in several previous works (Vanneschi et al., 2014; Castelli et al., 2015a), here we constrain the outputs of T_R, T_{R1} and T_{R2} by wrapping them in a logistic function. Only the definitions of the GSOs for symbolic regression problems are given here, since they are the only ones used in this work. For the definition of GSOs for other domains, the reader is referred to (Moraglio et al., 2012). Figure 1 shows a graphical representation of the mapping between the syntactic and semantic space given by the GSOs.

Using these operators, the semantics of the offspring is completely defined by the semantics of the



(a) (b)

Figure 1: Geometric semantic crossover (plot (a)) (respectively geometric semantic mutation (plot (b))) performs a transformation on the syntax of the individual that corresponds to geometric crossover (respectively geometric mutation) on the semantic space. In this figure, the unrealistic case of a bidimensional semantic space is considered, for simplicity.

parents: the semantics of an offspring produced by GSC will lie on the segment between the semantics of both parents (geometric crossover), while GSM defines a mutation such that the semantics of the offspring lies within the ball of radius *ms* that surrounds the semantics of the parent (geometric mutation).

As reported in (Moraglio et al., 2012), the property of GSOs of inducing a unimodal error surface has a price. The price, in this case, is that GSOs always generate larger offspring than the parents, and this entails a rapid growth of the size of the individuals in the population. To counteract this problem, in (Castelli et al., 2015a) an implementation of GSOs was proposed that makes GSGP not only usable in practice, but also significantly faster than standard GP. This is possible by means of a smart representation of GP individuals, that allows us not to store their genotypes during the evolution. This is the implementation used here. Even though this implementation is efficient, it does not solve the problem of the size of the final model: the genotype of the final solution returned by GSGP can be reconstructed, but it is so large that it is practically impossible to understand. This turns GSGP into a "black-box" system, as many other popular machine learning systems are, including deep neural networks.

3 REGRESSION-LIKE CLASSIFICATION WITH GSGP

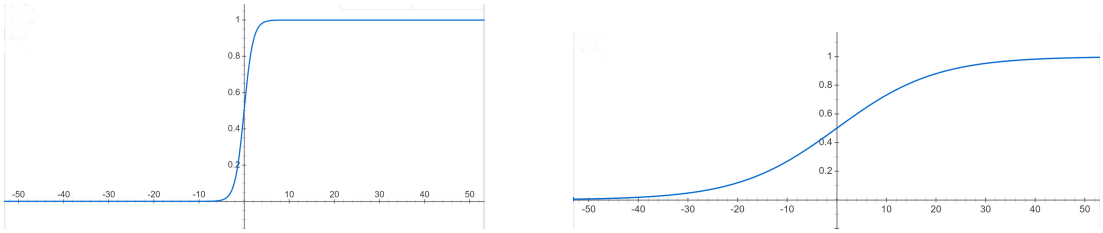
In this work, we use symbolic regression GSOs to solve binary classification problems. The used method is inspired by the functioning of the Perceptron neural network (Vanneschi and Castelli, 2019). The two class labels that characterize the problem are transformed into two numeric values. The values 0 and 1 have been used in this work. In this way, the classification problem can be imagined as a regression problem, containing only 0 and 1 as possible target values. The output of a GP individual P is given as input to an activation function, and the fitness of P is the Root Mean Square Error (RMSE) between the output of the activation function and the binary target. As customary in Perceptrons, we have used the logistic activation function:

$$L(x) = \frac{1}{1+e^{-\alpha x}} \quad (1)$$

This function has two asymptotes, respectively in 0 and 1, that are the target values we have used. Using this activation function should help us to improve the generalization ability of the system, since faithfully approximating the target values 0 and 1 entails a separation of data belonging to different classes. In other words, the evolutionary process automatically pushes towards the generation of GP individuals that return large positive values for observations labeled with 1, and large negative values for observations labeled with 0. At the same time, a good individual should not return small values for any of the observations, since those small outputs would immediately give a deteriorating contribution to the error.

This effect of data separation can be tuned by modifying constant α in Equation (1). In order to have a visual intuition of this, Figure 2 shows two different logistic functions, one with $\alpha = 1$ (plot (a)), and the other with $\alpha = 0.1$ (plot (b)).

From this figure, it is possible to see that, in order to obtain the same approximation of an output value equal to 1 (respectively 0), when $\alpha = 0.1$ the output has to be larger (respectively smaller), compared to the case $\alpha = 1$. So, for the same value of the error, data belonging to different classes are better separated for smaller values of α. On the other hand, of



(a) $\alpha = 1$ (b) $\alpha = 0.1$

Figure 2: Graphical representation of logistic functions (Equation (1)) with two different values of the α parameter. Plot (a): $\alpha = 1$; Plot (b): $\alpha = 0.1$.

course, using small values of α also has a drawback: given a prefixed value of the training error ε, finding individuals with an error equal to ε will be computationally harder for smaller values of α. All this considered, finding the appropriate value of α, representing a good compromise between generalization ability and computational cost, is a challenge and various preliminary tuning experiments have been needed, in order to obtain the value used here. Once a model optimizing the RMSE on training data has been found, it can be used for generalization on unseen data, simply using a threshold equal to zero on the output: observations with positive outputs will be predicted as belonging to one of the two classes, while the other observations will be categorized in the other class.

4 EXPERIMENTAL STUDY

4.1 Test Problems

In order to assess the effectiveness of the proposed approach, we considered ten binary classification problems, which present different characteristics in terms of the number of attributes and instances. The related datasets are publicly available on the UCI (Dua and Karra Taniskidou, 2017) and openML (Vanschoren et al., 2013) repositories. Table 1 reports, for each one of these problems, the number of input features (variables) and data instances (observations) in the respective datasets and the repository from which the data have been downloaded.

Since for each feature the range of values may vary widely, data was normalized by using the Z-normalization method: for each feature f_i, we first computed the mean μ_i and the standard deviation σ_i on the training set, then we applied the following transformation:

$$z_{ij} = \frac{x_{ij} - \mu_i}{\sigma_i}$$

where x_{ij} is the value of the i-th feature from the $j-th$ sample (both from the training or the test set) and z_{ij} is the corresponding normalized value.

Table 1: Description of the benchmark problems. For each dataset, the number of features (independent variables), the number of instances (observations) that were reported.

Dataset	#Features	#Instances	Repository
Fertility	9	100	openML
Hill	100	1212	openML
Ilpd	10	579	openML
Liver	6	345	UCI
Mammo	5	830	UCI
Musk	166	476	UCI
Qsar	41	1055	UCI
Retinopathy	19	1151	UCI
Spam	57	3037	UCI
Spect	22	266	UCI

Table 2: Parametrization used in the experiments.

Parameters	Values
Population size	500
# generations	2000
Tree initialization	Ramped Half-and-Half, maximum depth 6
Crossover rate	0.0
Mutation rate	1.0
Function set	$+, -, *$, and protected $/$
Terminal set	Input variables, random constants
tournament size	4
Elitism	Best individual always survives
# random trees	500

4.2 Experimental Settings

During the experimental study, we performed two sets of experiments. In the first set we investigated the classification performances of the proposed approach as function of α and R, which represent the steepness of the curve and width of the range for the random constants in the terminal set, respectively. In the sec-

ond set of experiments, instead, we compared the results achieved by our GSGP-based binary classification system with those of an SVM classifier.

For all the considered test problems, 30 independent runs of each studied system were executed. For each problem, the related dataset was randomly split into an equally sized and statistically independent training and test set. The RMSE (see Section 3) on the training set was used to compute the fitness of each individual, whereas the error rate on the test set[1] was used to assess the classification performance on unseen data of the best individual found at the end of each run. All the results reported in the following were computed averaging these classification results. As for the parameters, we performed some preliminary trials to set them. These parameters were used for all the experiments described below and are reported in Table 2.

4.3 Experimental Results

As mentioned in previously, we performed two sets of experiments. The first to find the best values for the parameters α and R, and the second to compare our results with those achieved by an SVM classifier. Both sets of experiments are described as follows.

In the first set of experiments, we investigated how the values ofα and R affect the classification performance of our system since both values affect the final output of the GP individuals. The former, which represents the limits of the range of the random constants $[-R,+R]$, affects the values the random constants of the terminal set can assume, thus affecting the input values given as input to the GP trees. As for α, as mentioned in Section 3, it affects the separation of samples belonging to different classes, with small α values ensuring a better separation than larger ones (see Figure 2). For this reason, we performed a factorial experiment to investigate the relationship between these two parameters. More specifically, we considered the following sets of parameters:

$S_\alpha = \{0.0001, 0.001, 0.01, 0.05, 0.1, 0.2, 0.5\}$

$S_R = \{1, 2, 5, 10, 20, 50\}$

As for the remaining parameters, we used those shown in Table 2. The plots in Figures 3 and 4 show the test error as a function of the R for the different α values tested. From the Figures it can be noted that for all the considered datasets, too low α values achieve the worse performance. In particular, the values 0.0001 and 0.001 achieve the worst performance, while for most of the datasets, the value 0.01 performs worse than the higher values. Moreover, it is worth noting that for these three values the "performance ranking", the performance differences among these values, is kept for all the datasets and for all the R values. These results prove that too low α values do not improve the "data separation" effect mentioned in Section 3. This is most probably because these values produce too flat curves (similar to straight lines with a low slope). In practice, these α values produce similar output values for a large range of input values returned by the GP individuals, thus reducing the selective pressure of the evolutionary process. It is also worth noting that the curves for these values exhibit a high variability with respect to R, even if there is no monotonic trend, that would prove that higher (lower) R values perform better. As for the remaining α values $(0.05, 0.1, 0.2, 0.5)$ from the plots, it can be noted that:

(i) in most of the cases they achieve similar results;

(ii) even when their performances are significantly different, the related curves tend to be overlapped;

(iii) on several datasets (see for example Musk in Figure 3(c) or Spam in Figure 4(c)) the value 0.5 tends to perform better than the smaller values.

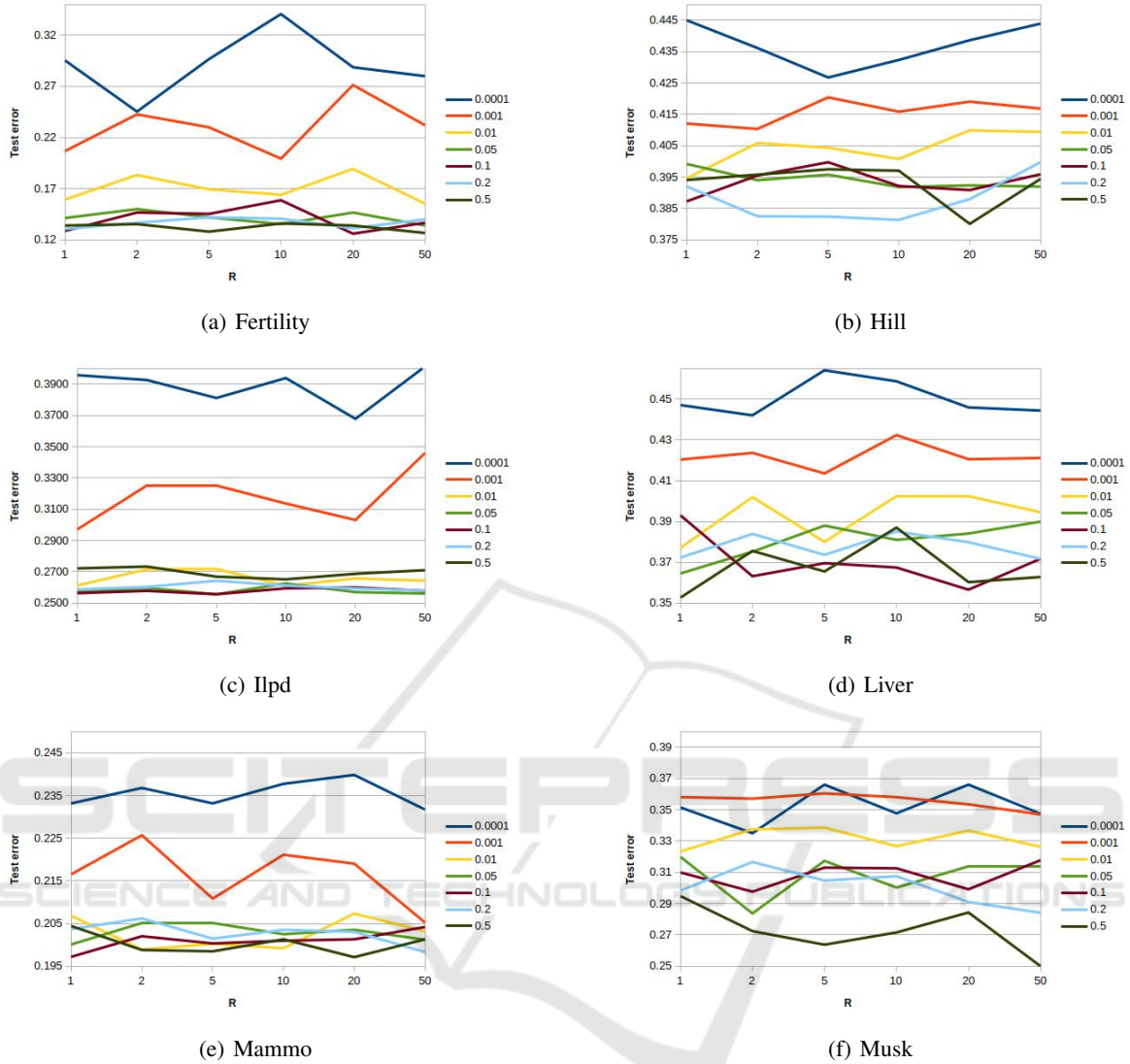
Maybe a better explanation for these results is that these α values allow better differentiation between samples belonging to different classes, with the positive (negative) ones labeled as 1 (0) and correctly classified by GP individuals yielding positive (negative) outputs. In fact, for an individual I the error for a given sample $\mathbf{x}$ is computed as

$$(L(f_I(\mathbf{x})) - l_\mathbf{x})^2 \quad (2)$$

where $f_I(\mathbf{x})$ is the function encoded by I, L the (logistic) activation function (see Equation 1) and $l_\mathbf{x}$ the label of $\mathbf{x}$ (0 or 1). Then, according to the above equation, the effect of higher α values is twofold: they allow reducing the RMSE for correct classification even when f_I returns small values and increasing the RMSE even for misclassifications characterized by small values. In practice, those higher α values better reward/penalize correctly/incorrectly classified instances.

To better explain this concept, we drew the logistic function for these values (Figure 5) and we also computed the output values of the logistic functions for these remaining α for some samples. From the table it is worth noting that for small $f(\mathbf{x})$ output values (see

[1] Given an individual GP individual I representing the function $f_I : R^n \rightarrow R$, where R^n is the feature space, the test sample $\mathbf{x}$ is labeled as belonging to the class 0 if $f(\mathbf{x}) > 0$, to the class 1 otherwise. In practice, the logistic function is only used for training the system. This because in any binary classification problem, the classifier must provide as output a class label (0 or 1), instead of a numerical value.



(a) Fertility (b) Hill

(c) Ilpd (d) Liver

(e) Mammo (f) Musk

Figure 3: Test error as a function of the limits of the range of the random constants $[-R,+R]$ for the first six datasets of Table 1.

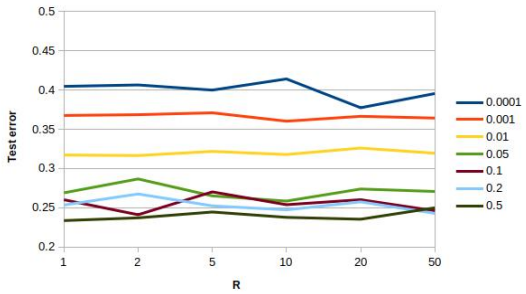
for examples the samples 1 and 3), L with $\alpha = 0.05$ returns similar values both for correctly (sample #1) and incorrectly classified (sample #3) samples, whereas with $\alpha = 0.5$ L returns quite different values for these samples. Similar considerations can be done for the other samples. For example, for the misclassified sample #8, with $f_I(\mathbf{x}) = -11.2$, L returns 0.41 with $\alpha = 0.05$, whereas it returns 0.00 with $\alpha = 0.5$.

4.4 Comparison with SVMs

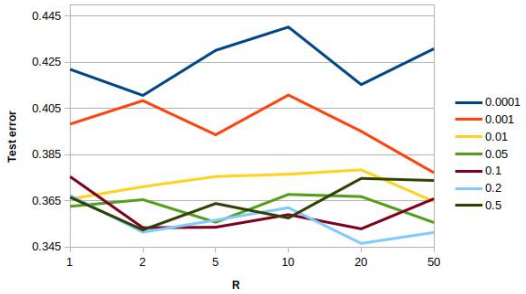
In order to test the effectiveness of the proposed approach, we compared its results with those achieved by a Support Vector Machine (SVM). Support Vector Machines (SVMs) are supervised learning meth-

Table 3: Output values of the logistic functions for some samples, where $f_I(\mathbf{x})$ is the output value of a generic GP individual I. Rows in bold represent misclassified samples.

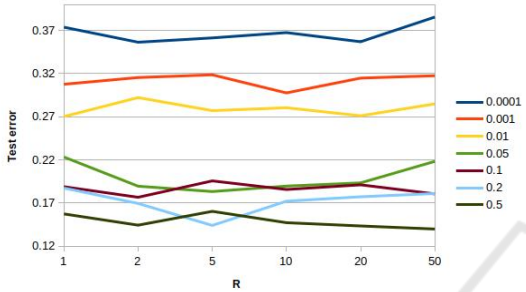
#	$l_\mathbf{x}$	$f_I(\mathbf{x})$	$(L(f_I(\mathbf{x})) - l_\mathbf{x})^2$ (Eq. (2))			
			0.05	0.1	0.2	0.5
1	0	-1.6	0.23	0.21	0.18	0.10
2	0	-16.5	0.093	0.026	0.001	6.8e-8
3	**0**	**1.2**	**0.27**	**0.28**	**0.31**	**0.42**
4	**0**	**7.2**	**0.35**	**0.45**	**0.65**	**0.95**
5	1	1.4	0.23	0.22	0.19	0.11
6	1	3.5	0.21	0.17	0.11	0.02
7	**1**	**-2**	**0.28**	**0.30**	**0.36**	**0.53**
8	**1**	**-11.2**	**0.41**	**0.57**	**0.82**	**0.99**
9	1	6.1	0.18	0.12	0.05	2.04e-3



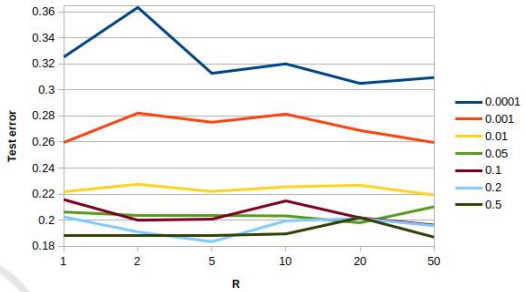
(a) Qsar



(b) Retinopathy



(c) Spam



(d) Spect

Figure 4: Test error as a function of the limits of the range of the random constants $[-R,+R]$ for the last four datasets of Table 1.

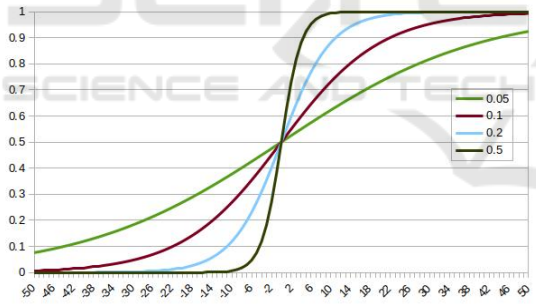


Figure 5: The logistic functions for the α values: 0.05, 0.1, 0.2 and 0.5.

ods that are based on the concept of decision planes, which linearly separates, in the feature space, objects belonging to the different classes (Cortes and Vapnik, 1995). Intuitively, given two classes to be discriminated in a given feature space, a good separation is achieved by the hyperplanes that have the largest distance to the nearest training points belonging to different classes; in general, the larger the margin, the lower the generalization error of the classifier. While the basic idea of the SVM applies to linear classifiers, they can be easily adapted to non-linear classification tasks by using the so called "kernel trick", which implies the mapping of the original features into a higher dimensional feature space. Differently from other classifier schemes, whose learning usually implies stochastic and suboptimal gradient descent procedures, e.g., NN and DT, given a training set, the SVM learning optimization problem can be solved by using quadratic programming algorithms which provide exact solutions. SVMs have shown to be effective in solving many real world applications like handwriting recognition, text categorization and image classification (Byun and Lee, 2002).

As suggested by (Lin and Lin, 2003; Keerthi and Lin, 2003), we chose the radial basis function (RBF) as kernel in our experiments:

$$K(\mathbf{x},\mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|^2}$$

where $\mathbf{x}$ and $\mathbf{y}$ are two generic samples in the feature space.

As for the implementation, we used that provided by the LIBSVM public domain software (Chang and Lin, 2011). Moreover, to perform a fair comparison with the GSGP, for each considered problem, we performed 30 runs. As mentioned before, SVMs are deterministic, i.e. for a given training set the algorithm always returns the same set of support vectors. For this reason, to get averaged results on unseen data, for each run the data was randomly shuffled and split into a training and a test set, equally sized. The results reported in the following have been averaged on the

accuracy obtained on the 30 generated test sets.

To statistically validate the comparison results, we performed the non-parametric Wilcoxon rank-sum test. The comparison results are shown in Table 4, which also shows the p-value for the Wilcoxon test. From the table it can be observed that on eight of the ten considered problems, our GSGP-based classifier outperforms the SVM, while as for the remaining two (Fertility and Mammo), the differences are not statistically significant (p-value > 0.05). Moreover, from the table it can be also noted that in most of the cases performance differences increase with the number of features. This seems to suggest that the evolutionary search process implemented by our approach is able to: (i) effectively identify the features that better discriminate samples belonging to different classes; (ii) effectively find the functions (expressions) of these features that characterize the classes of the problem at hand.

5 CONCLUSIONS AND FUTURE WORK

A new classification approach based on Geometric Semantic Genetic Programming (GSGP) was presented in this paper. Despite the simplicity of the idea, the presented results showed that this approach was able to outperform Support Vector Machines (SVMs) on 8 different complex real-life problems, returning comparable results on the remaining 2 test problems. These results encourages us to pursue the idea, and we believe that this work could pave the way to a set of applicative successes, comparable with the ones that GSGP has obtained on regression and forecasting in recent years (Vanneschi et al., 2014).

An important part of our current work is an attempt of extending the proposed approach to multi-class classification. Our objective is, if possible, to be able to solve, with success, complex multi-class classification tasks, maintaining the simplicity of the idea presented here. Furthermore, in the future, we plan to integrate the proposed approach with local search strategies and with regularization algorithms, in order to further stress, possibly at the same time, its optimization power on training data, and its generalization ability. Inheriting ideas from SVMs, like maximum separation hyperplane and kernel trick, is also a possibility that we are considering to extend the work. Last but not least, we are planning to implement a parallel and distributed version of the system, with highly heterogeneous populations. In this way, different variants of the algorithm could be executed in parallel, like different parameter settings, different representations for the solutions, different activation functions and different fitness functions, just to mention a few.

Table 4: Comparison results (accuracy, expressed in percentage) between the proposed approach and the SVM classifier. Rows in bold highlight problems with no statistical significant differences.

Dataset	SVM	GSGP	p-value
Fertility	**87.07**	**87.40**	**0.7024**
Hill	51.00	61.28	1.73e-6
Ilpd	71.16	74.44	1.90e-6
Liver	58.84	64.73	2.34e-6
Mammo	**80.23**	**80.29**	**0.7584**
Musk1	61.08	75.00	2.34e-6
Qsar	67.01	76.63	7.68e-6
Retinopathy	59.40	65.35	3.52e-6
Spam	69.86	86.01	1.73e-6
Spect	79.27	81.65	2.20e-3

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