QFC: a parallel software tool for feature construction, based on Grammatical Evolution

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Abstract

This paper presents and analyzes a programming tool that implements a method for classification and function regression problems. This method builds new features from existing ones with the assistance of a hybrid algorithm that makes use of artificial neural networks and Grammatical Evolution. The implemented software exploits modern multi-core computing units for faster execution. The method has been applied to a variety of classification and function regression problems and an extensive comparison with other methods of computational intelligence is made.

1 Introduction

Many problems from various research areas can be considered as classification or regression problems, such as problems from physics [1, 2, 3, 4], chemistry [5, 6, 7], economics [8, 9], pollution [10, 11, 12], medicine [13, 14] etc. These problems are usually tackled by learning models such as Artificial Neural Networks [15, 16], Radial Basis Function (RBF) networks [17, 18], Support Vector Machines (SVM) [19], etc. A review of the methods used in classification can be found in the work of Kotsiantis et al [20].

Learning data is usually divided into two parts: training data and test data. Learning models adjust their parameters, taking the training data as input and are evaluated on the test data. The number of learning model parameters directly depends on the dimension of the input problem (number of features) and this means that for large problems, large amounts of memory are required to store and manage the learning models. In addition, as the number of parameters of the computational models grows, a longer time is required to adjust the parameters. Also, as the dimension of the data grows, more samples (patterns) are required in order to achieve high learning rates. A discussion on how the dimensionality of the input problems affects the effectiveness of neural networks is presented in [21]. A common approach to reduce the dimension of the input data is the Principal Component Analysis (PCA) technique [22, 23, 24] or the Minimum redundancy feature selection (MRMR) technique [25, 26]. Also, Wang

et al [27] proposed an auto-encoder based dimensionality reduction method for large datasets. An overview of dimensionality reduction techniques can be found in the work of Ayesha et al [28].

The current article describes the method and the software associated with a feature construction method based on Grammatical Evolution [29], which is an evolutionary process that can create programs in any programming language. This process has been used in a variety of cases, such as automatic composition of music [30], construction of neural networks [31, 32], automatic constant creation [33], evolution of video games [34], energy demand estimation [35] etc. The described method constructs subsets of features from the original ones using nonlinear combinations of them. The method is graphically illustrated in Figure 1. Initially, the method was described in [36] and it has been utilized in a variety of cases, such as Spam Identification [37], Fetal heart classification [38], epileptic oscillations in clinical intracranial electroencephalograms [39], classification of EEG signals [40] etc.

The proposed software has been implemented in ANSI C++ utilizing the freely available library of QT from https://www.qt.io. The user should supply the training and test data of the underlying problem as well as the desired number of features that will be created. The evaluation of the constructed features can be made using a variety of machine learning models and the user can easily extend the software to add more learning models. Also, the software has a variety of command line options to control the parameters of the learning models or to manage the output of the method. Finally, since the process of Grammatical Evolution can require a lot of execution time, parallel computation is included in the proposed software through the OpenMP programming library [41].

The rest of this article is organized as follows: in section 2 the proposed method is analyzed, in section 3 the proposed software is outlined in detail, in section 4 a variety of experiments are conducted and presented and finally in section 5 some conclusions and future guidelines are discussed.

2 Methods

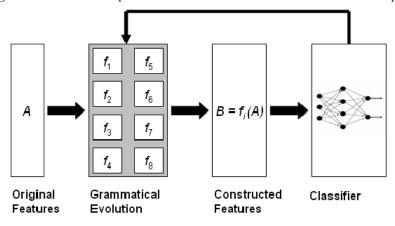
The proposed technique is divided into two phases: in the first phase, new features are constructed from the old ones using Grammatical Evolution and in the second phase these new features modify the control set and a machine learning model is applied to the new control set.

2.1 Grammatical Evolution

Grammatical evolution is a biologically inspired procedure that can create artificial programs in any language. In Grammatical evolution the chromosomes enclose production rules from a BNF (Backus–Naur form) grammar[42]. These grammars usually described as a set G = (N, T, S, P), where

 \bullet N is the set of non-terminal symbols.

Figure 1: Schematic representation of the feature construction technique.



- \bullet T is the set of terminal symbols.
- \bullet S is a non-terminal symbol defined as the start symbol of the grammar.
- P is a set of production rules in the form $A \to a$ or $A \to aB$, $A,B \in N, \ a \in T$.

In order for Grammatical Evolution to work, the original grammar is expanded by enumerating all production rules. For example, consider the modified grammar of Figure 2. The symbols that are in <> are considered as non-terminal symbols. The numbers in parentheses are the production sequence numbers for each non-terminal symbol. The constant N is the original number of features for the input data. In Grammatical Evolution, the chromosomes are expressed as vectors of integers. Every element of each chromosome denotes a production rule from the provided BNF grammar. The algorithm starts from the start symbol of the grammar and gradually produces some program string, by replacing non - terminal symbols with the right hand of the selected production rule. The selection of the rule has two steps:

- Take the next element from the chromosome and denote it as V.
- Select the next production rule according to the the scheme Rule = V mod R, where R is the number of production rules for the current non terminal symbol.

For example, consider the chromosome chromosome x = [9, 8, 6, 4, 16, 10, 17, 23, 8, 14] and N = 3. The steps of mapping this chromosome to the valid expression $f(x) = x_2 + \cos(x_3)$ are illustrated in Table 1.

Figure 2: BNF grammar of the proposed method.

```
S::=<expr>
            (0)
<expr> ::= (<expr> <op> <expr>) (0)
          | <func> ( <expr> )
                               (1)
          <terminal>
                               (2)
<op> ::=
                  (0)
                  (1)
                  (2)
                  (3)
          | /
<func> ::= sin (0)
          | cos (1)
          exp
                (2)
          log
                (3)
<terminal>::=<xlist>
                                 (0)
          |<digitlist>.<digitlist> (1)
<xlist>::=x1
              (0)
          | x2 (1)
          . . . . . . . . .
          | xN (N)
<digitlist>::=<digit>
                                    (0)
           <digit><digit>
                                    (1)
          (2)
<digit> ::= 0 (0)
          1 (1)
          2 (2)
          3 (3)
          4 (4)
          5 (5)
          6 (6)
          7 (7)
          8 (8)
          9 (9)
```

Table 1: Steps to produce a valid expression from the BNF grammar.

String	Chromosome	Operation	
<expr></expr>	9,8,6,4,16,10,17,23,8,14	$9 \mod 3 = 0$	
(< expr > < op > < expr >)	8,6,4,16,10,17,23,8,14	$8 \mod 3 = 2$	
(< terminal > < op > < expr >)	6,4,16,10,17,23,8,14	$6 \mod 2 = 0$	
(<xlist $><$ op $><$ expr $>)$	4,16,10,17,23,8,14	$4 \mod 3 = 1$	
(x2 < op > < expr >)	16,10,17,23,8,14	$16 \mod 4 = 0$	
$(\mathrm{x}2+<\!\mathrm{expr}>)$	10,17,23,8,14	$10 \mod 3 = 1$	
$(\mathrm{x2} + <\mathrm{func}>(<\mathrm{expr}>))$	17,23,8,14	$17 \mod 4 = 1$	
$(\mathrm{x2} + \mathrm{cos}(< \mathrm{expr}>))$	23,8,14	$23 \mod 2 = 1$	
$(\mathrm{x2}\!+\!\mathrm{cos}(<\!\mathrm{terminal}>))$	8,14	$8 \mod 2 = 0$	
$(\mathrm{x}2\!+\!\cos(<\!\mathrm{xlist}>))$	14	$14 \mod 3 = 2$	
$(x2+\cos(x3))$			

2.2 The feature construction procedure

The following procedure is executed in order to produce N_f features from the original ones for a given chromosome X:

- 1. **Split** X into N_f parts.
- 2. For $i = 1..N_f$ denote each part as x_i .
- 3. For every part x_i construct a feature FT_i using the grammar given in 2

Every feature FT_i is considered as a mapping function, that transforms the original features to a new one. For example the feature

$$FT_1 = x_1^2 + \sin((x_2))$$

is a non-linear function that maps the original feature (x_1, x_2) into FT₁. Let $(x_1, x_2) = (2, 1)$. The mapping procedure will create the value $4 + \sin(1)$.

2.3 The feature construction step

The method has the following steps:

- 1. Initialization step.
 - (a) **Read** the train data. The train data contains M patterns as pairs (x_i, t_i) , i = 1..M where t_i is the actual output for pattern x_i .
 - (b) **Set** N_G , the maximum number of generations.
 - (c) **Set** N_C , the number of chromosomes.
 - (d) **Set** p_S , the selection rate.
 - (e) Set N_f , the desired number of features.

- (f) Set p_M , the mutation rate.
- (g) **Initialize** the chromosomes of the population. Every element of each chromosome is initialized randomly in the range [0,255].
- (h) **Set** iter=1

2. Genetic step

- (a) **For** $i = 1, ..., N_q$ **do**
 - i. Create using the procedure of subsection 2.2 a set of N_f for the corresponding chromosome g_i .
 - ii. **Transform** the original train data to the new train data using the previously created features. Denote the new train set as $(x_{q_i,j},t_i)$, j=1,..M
 - iii. Apply a learning model C (such as RBF) to the new data and calculate the fitness f_i as

$$f_i = \sum_{j=1}^{M} (C(x_{g_i,j}) - t_j)^2$$
 (1)

- iv. **Apply** the selection procedure. During selection, the chromosomes are classified according to their fitness. The best $(1-p_s) \times N_C$ chromosomes are transferred without changes to the next generation of the population. The rest will be replaced by chromosomes that will be produced at the crossover.
- v. Apply the crossover procedure. During this process, $p_s \times N_c$ chromosomes will be created. Firstly, for every pair of produced offsprings, two distinct chromosomes (parents) are selected from the current population using tournament selection: First, a subset of K>1 randomly selected chromosomes is created and the chromosome with the best fitness value is selected as parent. For every pair (z, w) of parents, two new offsprings \tilde{z} and \tilde{w} are created through one point crossover as graphically shown in Figure 3.
- vi. **Apply** the mutation procedure. For every element of each chromosome, select a random number $r \in [0, 1]$ and alter the corresponding chromosome if $r \leq p_m$.
- (b) EndFor
- 3. **Set** iter=iter+1
- 4. If iter $\leq N_G$ goto Genetic Step, else terminate and obtain g^* as the best chromosome in the population.

9 12 11 100 300 400 9 12 11 100 40 30
10 11 9 50 40 30 10 11 9 50 300 400

Parents Children

Figure 3: Example of one - point crossover.

2.4 The feature evaluation step

During the feature evaluation step, the following steps are executed:

- 1. **Denote** as $T = (x_i, y_i)$, i = 1, ..., K the original test set.
- 2. **Obtain** the best chromosome g^* of the feature construction step.
- 3. Construct N_f features for g^* using the procedure of subsection 2.2.
- 4. **Transform** T into $T' = (x_{g^*,i}, y_i)$, i = 1, ..., K using the previously constructed features.
- 5. **Apply** a learning model such as RBF or a neural network to T' and obtain the test error.

3 The software

3.1 Installation procedure

The software is entirely written in ANSI C++ using the freely available QT programming library. The library can be downloaded from https://www.qt.io As expected, the software can be installed on the majority of operating systems, even on mobile devices (Android, Ios etc). The program is freely available from https://github.com/itsoulos/QFc and the user should issue the following commands under most UNIX systems to compile the project:

- 1. Download QFc-master.zip from the above url
- 2. gunzip QFc-master.zip
- 3. cd QFc

Figure 4: Example of input file for regression/classification.

- 4. qmake.
- 5. make

The final outcome of the previous steps is a command line program called qfc.

3.2 Data format

Classification and regression problems should be formatted in files according to the format shown in Figure 4. The integer number D denotes the number of features of the dataset and M represents the number of patterns. In every subsequent line of the file there should be the input pattern and the final column is the real output (category) for the corresponding pattern.

3.3 The program qfc

The program qfc has a variety of command line options. All options are in form --key=value, where key is the name of the option and value is the actual option value. The main options of the program are:

- 1. —trainFile=filename, where filename is the full path to data containing the input train set. The file must be in the format of Figure 4.
- 2. ——testFile=filename, where filename is the full path to data containing the input test set. The format of this file should be the same as the train data. The user should at least provide the train and test set in order to execute the program.
- 3. ——features=n, set as the n the number of features that will be constructed by the method. The default value is 1.
- 4. —randomSeed=r, set as r the random seed generator. The default value for this parameter is 1 and the drand48() random generator of c++ language was used.
- 5. ——featureCreateModel=model, the string parameter model sets the name of the used feature construction model. The default value is "rbf" and accepted values are:

- (a) **copy**. With this value, no feature construction is done and the original data set is used for training by the model specified by the option ——featureEvaluateModel.
- (b) **rbf**. This value is used to utilize a Radial Basis Function neural network for the evaluation of the constructed features.
- (c) neural. This value is used to use a neural network for the evaluation of the constructed features.
- (d) knn. A simple K-nearest neighbor (KNN) method is used [43].
- (e) **osamaRbf**. A simple RBF implementation as downloaded from https://github.com/osama-afifi/RBF-Radial-Basis-Function-Network.
- 6. ——featureEvaluateModel=model, the string parameter model sets the name of the used model for the evaluation of the constructed features. The default value is "neural" but other accepted values are: rbf, knn, osamaRbf, nnc. The value nnc refers to the Neural Network Construction model as proposed by Tsoulos et al [44].
- 7. ——threads=t, the number of OpenMP threads used. The default value is 1.
- 8. ——neural_trainingMethod=m. This is the option that defines the method used for neural network training. The default value for m is "bfgs" and accepted values are
 - (a) **bfgs**. This value sets as a training method a BFGS variant of Powell [45].
 - (b) **lbfgs**. This value sets as a training method the limited memory BFGS [46, 47].
 - (c) **genetic**. With this value, a simple genetic algorithm [48, 49] is used to train the neural network.
- 9. —neural_weights=n, the weights used in neural networks. The default value is 1.
- 10. —knn_weights=n, the weights (neighbors) used in the knn model. The default value is 1.
- 11. --rbf weights=n, the weights used in the rbf model.
- 12. —ge_chromosomes=n, the number of chromosomes in the Grammatical Evolution procedure. The default value is 500.
- 13. —ge_maxGenerations=n, the maximum number of generations for the Grammatical Evolution procedure. The default value is 200.
- 14. —ge_selectionRate=f, the selection rate used in the Grammatical Evolution procedure. The default value is 0.10 (10%).

- 15. —ge_mutationRate=f, the mutation rate used in the Grammatical Evolution procedure. The default value is 0.05 (5%).
- 16. --ge_length=n, the length of chromosomes in the Grammatical Evolution procedure. The default value is $40 \times d$, where d is the number of features that will be created.
- 17. —genetic_chromosomes=n, the number of chromosomes used in the genetic algorithm for neural network training. The default value is 500.
- 18. ——genetic_maxGenerations=n, the maximum number of generations for the genetic algorithm used for neural network training. The default value is 200.
- 19. —genetic_selectionRate=f, the selection rate used in the genetic algorithm of neural network training. The default value is 0.1 (10%).
- 20. —genetic_mutationRate=f, the mutation rate used in the genetic algorithm of neural network training. The default value is 0.05 (5%).
- 21. —bfgs_iterations=n, the maximum number of iterations for the BFGS method. The default value is 2001.
- 22. ——export_train_file=f. The value f specifies the file where the training set will be exported after new features are constructed. The new file will have the same format and the same number of templates as the original, but the dimension will be changed to the one defined with the parameter—features.
- 23. —export_test_file=f, The value f specifies the file where the test set will be exported after new features are constructed. The new file will have the same format and the same number of templates as the original, but the dimension will be changed to the one defined with the parameter —features.
- 24. —export_cpp_file=f, where f is the output of the constructed features in the C++ programming language. As an example, consider the file outlined in Figure 5. The function fcMap() is a function with two array arguments:
 - (a) the argument inx denotes an input pattern with the original dimension. For the case of BL dataset the original dimension is 7.
 - (b) the argument outx stands for the features created by the algorithm. In this case, outx[0] is the first feature and outx[1] is the second feature.
- 25. —help, prints a help screen and terminates the program.

Figure 5: An example output file for the BL dataset.

3.4 Example run

As an example run consider the wdbc dataset located in the *examples* folder of the distribution. The following command:

will produce the following output

```
Teration: 1 Best Fitness: -52.1562
Best program: 1 Iteration: 2 Best Fitness: -52.1562
Best program: 2 Best Fitness: -52.1562
Best program: 3 Best Fitness: -52.1562
Best program: 4 Iteration: 3 Best Fitness: -51.8369
Best program: 5 Best program: 6 Iteration: 4 Best program: 7 Iteration: 4 Best program: 7 Iteration: 4 Best program: 7 Iteration: 5 Best program: 7 Iteration: 5 Best program: 7 Iteration: 5 Best Fitness: -51.7176
Best program: 7 Iteration: 5 Best Fitness: -51.5149
Best program: 7 Iteration: 7 I
```

4 Experiments

A series of experiments were performed in order to evaluate the reliability and accuracy of the proposed methodology. In these experiments, the accuracy of the proposed methodology against other techniques, the running time of the experiments, and the sensitivity of the experimental results to various critical parameters, such as the number of features or the maximum number of generations of the genetic algorithm, were measured. All the experiments were conducted 30 times with different seeds for the random number generator each time and averages were taken. All the experiments were conducted on an AMD Ryzen 5950X equipped with 128GB of RAM. The operating system used was OpenSUSE Linux and all the programs were compiled using the GNU C++ compiler. In all the experiments, the parameter ——featureCreateModel had

the value rbf, since it is the fastest model that could be used and has high learning rates. For classification problems, the average classification error on the test set is shown and, for regression datasets the average mean squared error on the test set is displayed. In all cases, 10 fold cross validation was used and the number of parameters for neural networks and for rbf networks was set to 10. The evaluation of the features constructed by Grammatical Evolution was made using the Function Parser library [50].

4.1 Experimental datasets

The validity of the method was tested on a series of well known datasets from the relevant literature. The main repositories for the testing was:

- The UCI Machine Learning Repository http://www.ics.uci.edu/~mlearn/ MLRepository.html
- 2. The Keel repository https://sci2s.ugr.es/keel/
- 3. The Statlib repository ftp://lib.stat.cmu.edu/datasets/index.html

The classification datasets are:

- 1. **Australian** dataset [51], the dataset is related to credit card applications.
- 2. Alcohol dataset, a dataset about Alcohol consumption [52].
- 3. Balance dataset [53], which is used to predict psychological states.
- 4. **Cleveland** dataset, a dataset used to detect heart disease used in various papers[54, 55].
- 5. **Dermatology** dataset [56], which is used for differential diagnosis of erythemato-squamous diseases.
- 6. **Glass** dataset. This dataset contains glass component analysis for glass pieces that belong to 6 classes.
- 7. **Hayes Roth** dataset [57]. This dataset contains **5** numeric-valued attributes and 132 patterns.
- 8. Heart dataset [58], used to detect heart disease.
- 9. **HouseVotes** dataset [59], which is about votes in the U.S. House of Representatives Congressmen.
- 10. **Liverdisorder** dataset [60], used for detect liver disorders in peoples using blood analysis.
- 11. **Ionosphere** dataset, a meteorological dataset used in various research papers [61, 62].

- 12. **Mammographic** dataset [63]. This dataset be used to identify the severity (benign or malignant) of a mammographic mass lesion from BI-RADS attributes and the patient's age. It contains 830 patterns of 5 features each.
- 13. **PageBlocks** dataset. The dataset contains blocks of the page layout of a document that has been detected by a segmentation process. It has 5473 patterns with 10 features each.
- 14. **Parkinsons** dataset,[64] which is created using a range of biomedical voice measurements from 31 people, 23 with Parkinson's disease (PD). The dataset has 22 features.
- 15. **Pima** dataset [65], used to detect the presence of diabetes.
- 16. PopFailures dataset [66], used in meteorology.
- 17. **Regions2** dataset. It is created from liver biopsy images of patients with hepatitis C [67]. From each region in the acquired images, 18 shape-based and color-based features were extracted, while it was also annotated form medical experts. The resulting dataset includes 600 samples belonging into 6 classes.
- 18. Saheart dataset [68], used to detect heart disease.
- 19. **Segment** dataset [69]. This database contains patterns from a database of 7 outdoor images (classes).
- 20. **Sonar** dataset [70]. The task here is to discriminate between sonar signals bounced off a metal cylinder and those bounced off a roughly cylindrical rock.
- 21. **Spiral** dataset, which is an artificial dataset with two classes. The features in the first class are constructed as:: $x_1 = 0.5t\cos(0.08t)$, $x_2 = 0.5t\cos(0.08t + \frac{\pi}{2})$ and for the second class the used equations are : $x_1 = 0.5t\cos(0.08t + \pi)$, $x_2 = 0.5t\cos(0.08t + \frac{3\pi}{2})$
- 22. Wine: dataset, which is related to chemical analysis of wines [71, 72].
- 23. Wdbc dataset [73], which contains data for breast tumors.
- 24. Eeg dataset. As an real word example, consider an EEG dataset described in [74, 75] is used here. The dataset consists of five sets (denoted as Z, O, N, F and S) each containing 100 single-channel EEG segments each having 23.6 sec duration. Sets Z and O have been taken from surface EEG recordings of five healthy volunteers with eye open and closed, respectively. Signals in two sets have been measured in seizure-free intervals from five patients in the epileptogenic zone (F) and from the hippocampal formation of the opposite hemisphere of the brain (N). Set S contains seizure activity, selected from all recording sites exhibiting ictal activity. Sets Z and O have

- been recorded extracranially, whereas sets N, F and S have been recorded intracranially.
- 25. **Zoo** dataset [76], where the task is classify animals in seven predefined classes.

The regression datasets used are the following:

- 1. **Abalone** dataset [77]. This data set can be used to obtain a model to predict the age of abalone from physical measurements.
- 2. Airfoil dataset, which is used by the NASA for a series of aerodynamic and acoustic tests [78].
- 3. Baseball dataset, a dataset to predict the salary of baseball players.
- 4. **BK** dataset, used to estimate the points scored per minute in a basketball game.
- 5. **BL** dataset, which is related with the affects of machine adjustments on the time to count bolts.
- 6. Concrete dataset. This dataset is taken from civil engineering [79].
- 7. **Dee** dataset, used to predict the daily average price of the electricity energy in Spain.
- 8. **Diabetes** dataset, a medical dataset.
- 9. **FA** dataset, which contains percentage of body fat and ten body circumference measurements. The goal is to fit body fat to the other measurements.
- 10. **Housing** dataset. This dataset was taken from the StatLib library and it is described in [80].
- 11. **MB** dataset. This dataset is available from Smoothing Methods in Statistics [81] and it includes 61 patterns.
- MORTGAGE dataset, which contains the Economic data information of USA.
- 13. NT dataset [82], which is related to the body temperature measurements.
- 14. **PY** dataset [83], used to learn Quantitative Structure Activity Relationships (QSARs).
- 15. **Quake** dataset, used to estimate the strength of a earthquake.
- 16. Treasure dataset, which contains Economic data information of USA from 01/04/1980 to 02/04/2000 on a weekly basis.
- 17. Wankara dataset, which contains weather information.

4.2 Experimental results

The experimental results for the classification datasets are listed in Table 2 and for regression datasets in Table 3. The number of features constructed by the Grammatical Evolution was set to 2. In both tables, an additional row was added at the end showing the average classification or regression error for all datasets and it is denoted by the name AVERAGE. The columns of both tables have the following meaning:

- 1. The column RBF stands for the results from an RBF network with 10 parameters.
- 2. The column MLP stands for the results of a neural network trained by a genetic algorithm. The number of weights was set to 10.
- 3. The column FCRBF represents the results of the proposed method, when an RBF network was used as the evaluation model.
- 4. The column FCMLP represents the results of the proposed method, when a neural network trained by a genetic algorithm was used as the evaluation model.
- 5. The column FCNNC stands for the results of the proposed method, when the neural network construction model (nnc) was utilized as the evaluation model

From the experimental results and especially from the average errors, we can see that the proposed method significantly outperforms the other computational methods. In the case of data classification, there is a gain of the order of 30% and in the case of regression data the gain from the application of the proposed technique exceeds 50%. Also, among the three cases of models used to evaluate the constructed features (FCRBF, FCMLP, FCNNC), there does not seem to be any clear superiority of any of the three. However, we would say that the nnc method slightly outperforms the simple genetic algorithm.

In addition, one more experiment was done in order to establish the impact of the number of features on the accuracy of the proposed method. In this case, the rbf (FCRBF) network was used as the feature evaluator, and the number of generated features was in the interval [1..4]. The average classification error and the average regression error for all datasets are shown in Table 4. From the experimental results, the robustness of the proposed methodology is clearly visible, as 1 or 2 features seem to be enough to achieve high learning rates for the experimental data used.

Furthermore, one more experiment was conducted to determine the effect of the maximum number of generations on the accuracy of the proposed method. Again, as an evaluator model the RBF was used. The number of generations was varied from 50 to 400 and the average classification error and average regression error for all datasets were measured. The results for this experiment are presented in Table 5. Once again, the dynamics of the proposed method appear as a few generations are enough to achieve high learning rates.

Table 2: Experimental results between the method and other techniques for the classification datasets.

DATASET	RBF	MLP	FCRBF	FCMLP	FCNNC
ALCOHOL	49.19%	47.49%	35.56%	26.57%	28.58%
AUSTRALIAN	34.89%	32.21%	15.37%	14.31%	14.24%
BALANCE	33.42%	8.97%	14.39%	1.42%	1.52%
DERMATOLOGY	62.34%	30.58%	22.42%	15.06%	15.42%
GLASS	50.16%	60.25%	49.81%	55.94%	52.62%
HAYES ROTH	64.36%	56.18%	34.59%	29.58%	30.67%
HEART	31.20%	28.34%	18.61%	15.67%	17.21%
HOUSEVOTES	5.99%	6.62%	7.15%	5.22%	3.96%
IONOSPHERE	16.22%	15.14%	9.83%	9.48%	9.92%
LIVERDISORDER	30.84%	31.11%	30.77%	31.98%	30.24%
MAMMOGRAPHIC	21.38%	19.88%	16.68%	17.92%	16.75%
PAGEBLOCKS	10.09%	8.06%	9.24%	5.58%	5.85%
PARKINSONS	17.41%	18.05%	8.48%	10.82%	12.53%
PIMA	25.75%	32.19%	24.07%	30.02%	25.01%
POPFAILURES	7.04%	5.94%	4.94%	4.94%	4.43%
REGIONS2	37.49%	29.39%	25.49%	27.52%	24.40%
SAHEART	32.19%	34.86%	29.10%	27.91%	27.17%
SEGMENT	59.69%	57.72%	39.35%	49.52%	46.14%
SONAR	27.85%	26.97%	24.35%	25.38%	23.68%
SPIRAL	44.87%	45.77%	34.34%	45.53%	42.69%
TAE	60.07%	56.22%	50.95%	56.87%	55.67%
WDBC	7.27%	8.56%	3.39%	4.36%	4.51%
WINE	31.41%	19.20%	7.61%	11.08%	11.61%
Z_F_S	13.16%	10.73%	5.48%	6.72%	6.63%
ZO_NF_S	9.02%	8.41%	4.08%	4.25%	4.34%
ZONF_S	4.03%	2.60%	1.89%	4.62%	3.18%
Z_O_N_F_S	48.71%	65.45%	39.29%	40.93%	41.19%
ZOO	21.77%	16.67%	26.07%	13.30%	10.33%
AVERAGE	31.89%	28.80%	22.11%	22.02%	21.22%

Table 3: Experiments for regression datasets.

DATASET	RBF	MLP	FCRBF	FCMLP	FCNNC
ABALONE	7.32	7.17	4.46	4.18	4.39
AIRFOIL	0.05	0.003	0.002	0.001	0.001
BASEBALL	78.89	103.60	48.04	52.50	51.40
BK	0.02	0.03	0.02	0.02	0.02
BL	0.01	5.74	0.04	0.001	0.01
CONCRETE	0.01	0.01	0.006	0.004	0.005
DEE	0.17	1.01	0.18	0.40	0.38
DIABETES	0.49	19.86	1.49	0.58	0.61
HOUSING	57.68	43.26	12.78	28.47	17.47
FA	0.01	1.95	0.01	0.02	0.01
MB	1.91	3.39	0.48	0.12	0.06
MORTGAGE	1.45	2.41	0.66	1.37	0.22
NT	8.15	0.05	0.25	0.007	0.02
PY	0.02	105.41	0.17	0.03	0.03
QUAKE	0.07	0.04	0.06	0.02	0.04
TREASURY	2.02	2.93	0.29	1.41	0.11
WANKARA	0.001	0.012	0.0004	0.0002	0.0002
AVERAGE	9.31	17.46	4.06	5.24	4.4

Table 4: Average errors regarding the number of features.

FEATURES	AVERAGE CLASS	AVERAGE REGRESSION
1	23.02%	4.73
2	22.11%	4.06
3	21.03%	4.23
4	22.16%	4.28

Table 5: Average error depending on the number of generations.

GENERATIONS	AVERAGE CLASS	AVERAGE REGRESSION
50	22.38%	5.61
200	22.11%	4.06
400	21.46%	4.21

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5 Conclusions

A feature construction method and its accompanying software were analyzed in this paper. The software is developed in ANSI C++ and is freely available on the internet. The proposed method constructs new features for classification or regression data in a fully automatic manner and these features are evaluated by machine learning models. The user can choose between several learning models and can customize the course of the technique through a series of command line parameters. From the extensive execution of experiments and the comparison with other learning methods, the superiority of the proposed technique and its ability to achieve high learning rates even with a limited number of constructed features or a maximum number of iterations emerge. These results combined with the ability of the method to run on multiple threads through the OpenMP library make it ideal for learning large sets of data in a satisfactory execution time.

The method can be extended in several ways, such as:

- 1. Incorporation of advanced stopping rules.
- 2. Usage of more advanced learning models such as SVM.
- 3. Addition of more input formats such as the ARFF format or CSV format.
- 4. Incorporation of the MPI library [84] for large network of computers.

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Compliance with Ethical Standards

All authors declare that they have no conflict of interest.

References

- [1] E.M. Metodiev, B. Nachman, J. Thaler, Classification without labels: learning from mixed samples in high energy physics. J. High Energ. Phys. 2017, article number 174, 2017.
- [2] P. Baldi, K. Cranmer, T. Faucett et al, Parameterized neural networks for high-energy physics, Eur. Phys. J. C 76, 2016.

- [3] J. J. Valdas and G. Bonham-Carter, Time dependent neural network models for detecting changes of state in complex processes: Applications in earth sciences and astronomy, Neural Networks 19, pp. 196-207, 2006
- [4] G. Carleo, M. Troyer, Solving the quantum many-body problem with artificial neural networks, Science **355**, pp. 602-606, 2017.
- [5] C. Güler, G. D. Thyne, J. E. McCray, K.A. Turner, Evaluation of graphical and multivariate statistical methods for classification of water chemistry data, Hydrogeology Journal 10, pp. 455-474, 2002
- [6] E. Byvatov ,U. Fechner ,J. Sadowski , G. Schneider, Comparison of Support Vector Machine and Artificial Neural Network Systems for Drug/Nondrug Classification, J. Chem. Inf. Comput. Sci. 43, pp 1882–1889, 2003.
- [7] Kunwar P. Singh, Ankita Basant, Amrita Malik, Gunja Jain, Artificial neural network modeling of the river water quality—A case study, Ecological Modelling 220, pp. 888-895, 2009.
- [8] I. Kaastra, M. Boyd, Designing a neural network for forecasting financial and economic time series, Neurocomputing 10, pp. 215-236, 1996.
- [9] Moshe Leshno, Yishay Spector, Neural network prediction analysis: The bankruptcy case, Neurocomputing 10, pp. 125-147, 1996.
- [10] A. Astel, S. Tsakovski, V, Simeonov et al., Multivariate classification and modeling in surface water pollution estimation. Anal Bioanal Chem **390**, pp. 1283–1292, 2008.
- [11] A. Azid, H. Juahir, M.E. Toriman et al., Prediction of the Level of Air Pollution Using Principal Component Analysis and Artificial Neural Network Techniques: a Case Study in Malaysia, Water Air Soil Pollut 225, pp. 2063, 2014.
- [12] H. Maleki, A. Sorooshian, G. Goudarzi et al., Air pollution prediction by using an artificial neural network model, Clean Techn Environ Policy 21, pp. 1341–1352, 2019.
- [13] Igor I. Baskin, David Winkler and Igor V. Tetko, A renaissance of neural networks in drug discovery, Expert Opinion on Drug Discovery 11, pp. 785-795, 2016.
- [14] Ronadl Bartzatt, Prediction of Novel Anti-Ebola Virus Compounds Utilizing Artificial Neural Network (ANN), Chemistry Faculty Publications 49, pp. 16-34, 2018.
- [15] C. Bishop, Neural Networks for Pattern Recognition, Oxford University Press, 1995.
- [16] G. Cybenko, Approximation by superpositions of a sigmoidal function, Mathematics of Control Signals and Systems 2, pp. 303-314, 1989.

- [17] J. Park and I. W. Sandberg, Universal Approximation Using Radial-Basis-Function Networks, Neural Computation 3, pp. 246-257, 1991.
- [18] H. Yu, T. Xie, S. Paszczynski, B. M. Wilamowski, Advantages of Radial Basis Function Networks for Dynamic System Design, in IEEE Transactions on Industrial Electronics 58, pp. 5438-5450, 2011.
- [19] I. Steinwart, A. Christmann, Support Vector Machines, Information Science and Statistics, Springer, 2008.
- [20] S.B. Kotsiantis, I.D. Zaharakis, P.E. Pintelas, Machine learning: a review of classification and combining techniques, Artif Intell Rev **26**, pp. 159–190, 2006.
- [21] Verleysen M., Francois D., Simon G., Wertz V., On the effects of dimensionality on data analysis with neural networks. In: Mira J., Álvarez J.R. (eds) Artificial Neural Nets Problem Solving Methods. IWANN 2003. Lecture Notes in Computer Science, vol 2687. Springer, Berlin, Heidelberg. 2003.
- [22] Burcu Erkmen, Tülay Yıldırım, Improving classification performance of sonar targets by applying general regression neural network with PCA, Expert Systems with Applications 35, pp. 472-475, 2008.
- [23] Jing Zhou, Aihuang Guo, Branko Celler, Steven Su, Fault detection and identification spanning multiple processes by integrating PCA with neural network, Applied Soft Computing 14, pp. 4-11, 2014.
- [24] Ravi Kumar G., Nagamani K., Anjan Babu G., A Framework of Dimensionality Reduction Utilizing PCA for Neural Network Prediction. In: Borah S., Emilia Balas V., Polkowski Z. (eds) Advances in Data Science and Management. Lecture Notes on Data Engineering and Communications Technologies, vol 37. Springer, Singapore. 2020
- [25] Hanchuan Peng, Fuhui Long, and Chris Ding, Feature selection based on mutual information: criteria of max-dependency, max-relevance, and min-redundancy, IEEE Transactions on Pattern Analysis and Machine Intelligence 27, pp.1226-1238, 2005.
- [26] Chris Ding, and Hanchuan Peng, Minimum redundancy feature selection from microarray gene expression data, Journal of Bioinformatics and Computational Biology 3, pp.185-205, 2005
- [27] Y. Wang, H. Yao, S. Zhao, Auto-encoder based dimensionality reduction, Neurocomputing 184, pp. 232-242, 2016.
- [28] S. Ayesha, M. Kashif Hanif, R. Talib, Information Fusion 59, pp. 44-58, 2020.

- [29] M. O'Neill, C. Ryan, Grammatical evolution, IEEE Trans. Evol. Comput. 5,pp. 349–358, 2001.
- [30] A.O. Puente, R. S. Alfonso, M. A. Moreno, Automatic composition of music by means of grammatical evolution, In: APL '02: Proceedings of the 2002 conference on APL: array processing languages: lore, problems, and applications July 2002 Pages 148–155.
- [31] Lídio Mauro Limade Campo, R. Célio Limã Oliveira, Mauro Roisenberg, Optimization of neural networks through grammatical evolution and a genetic algorithm, Expert Systems with Applications **56**, pp. 368-384, 2016.
- [32] K. Soltanian, A. Ebnenasir, M. Afsharchi, Modular Grammatical Evolution for the Generation of Artificial Neural Networks, Evolutionary Computation 30, pp 291–327, 2022.
- [33] I. Dempsey, M.O' Neill, A. Brabazon, Constant creation in grammatical evolution, International Journal of Innovative Computing and Applications 1, pp 23–38, 2007.
- [34] E. Galván-López, J.M. Swafford, M. O'Neill, A. Brabazon, Evolving a Ms. PacMan Controller Using Grammatical Evolution. In: , et al. Applications of Evolutionary Computation. EvoApplications 2010. Lecture Notes in Computer Science, vol 6024. Springer, Berlin, Heidelberg, 2010.
- [35] D. Martínez-Rodríguez, J. M. Colmenar, J. I. Hidalgo, R.J. Villanueva Micó, S. Salcedo-Sanz, Particle swarm grammatical evolution for energy demand estimation, Energy Science and Engineering 8, pp. 1068-1079, 2020.
- [36] Dimitris Gavrilis, Ioannis G. Tsoulos, Evangelos Dermatas, Selecting and constructing features using grammatical evolution, Pattern Recognition Letters 29,pp. 1358-1365, 2008.
- [37] Dimitris Gavrilis, Ioannis G. Tsoulos, Evangelos Dermatas, Neural Recognition and Genetic Features Selection for Robust Detection of E-Mail Spam, Advances in Artificial Intelligence Volume 3955 of the series Lecture Notes in Computer Science pp 498-501, 2006.
- [38] George Georgoulas, Dimitris Gavrilis, Ioannis G. Tsoulos, Chrysostomos Stylios, João Bernardes, Peter P. Groumpos, Novel approach for fetal heart rate classification introducing grammatical evolution, Biomedical Signal Processing and Control 2,pp. 69-79, 2007
- [39] Otis Smart, Ioannis G. Tsoulos, Dimitris Gavrilis, George Georgoulas, Grammatical evolution for features of epileptic oscillations in clinical intracranial electroencephalograms, Expert Systems with Applications 38, pp. 9991-9999, 2011

- [40] A. T. Tzallas, I. Tsoulos, M. G. Tsipouras, N. Giannakeas, I. Androuli-dakis and E. Zaitseva, Classification of EEG signals using feature creation produced by grammatical evolution, In: 24th Telecommunications Forum (TELFOR), pp. 1-4, 2016.
- [41] L. Dagum, R. Menon, OpenMP: an industry standard API for shared-memory programming, IEEE Computational Science and Engineering 5, pp. 46-55, 1998.
- [42] J. W. Backus. The Syntax and Semantics of the Proposed International Algebraic Language of the Zurich ACM-GAMM Conference. Proceedings of the International Conference on Information Processing, UNESCO, 1959, pp.125-132
- [43] E. Fix, J.L. Hodges, Joseph, Discriminatory Analysis. Nonparametric Discrimination: Consistency Properties, USAF School of Aviation Medicine, Randolph Field, Texas, 1951.
- [44] I. Tsoulos, D. Gavrilis, E. Glavas, Neural network construction and training using grammatical evolution, Neurocomputing **72**, pp. 269-277, 2008.
- [45] M.J.D Powell, A Tolerant Algorithm for Linearly Constrained Optimization Calculations, Mathematical Programming 45, pp. 547-566, 1989.
- [46] R. H. Byrd, P. Lu, J. Nocedal, C. Zhu, A limited memory algorithm for bound constrained optimization, SIAM J. Scientific Computing 16, pp. 1190-1208, 1995.
- [47] R. Byrd, J. Nocedal, R. Schnabel Representations of Quasi-Newton Matrices and their use in Limited Memory Methods', Mathematical Programming 63, pp. 129-156, 1994.
- [48] Z. Michaelewicz, Genetic Algorithms + Data Structures = Evolution Programs. Springer Verlag, Berlin, 1996.
- [49] P. Kaelo, M.M. Ali, Integrated crossover rules in real coded genetic algorithms, European Journal of Operational Research 176, pp. 60-76, 2007.
- [50] J. Nieminen and J. Yliluoma, "Function Parser for C++, v2.7", available from http://warp.povusers.org/FunctionParser/
- [51] J.R. Quinlan, Simplifying Decision Trees. International Journal of Man-Machine Studies 27, pp. 221-234, 1987.
- [52] K.D. Tzimourta, I. Tsoulos, Ioannis T. Bilero, A.T. Tzallas, M.G. Tsipouras, N. Giannakeas, Direct Assessment of Alcohol Consumption in Mental State Using Brain Computer Interfaces and Grammatical Evolution, Inventions 3, pp. 1-12, 2018.
- [53] T. Shultz, D. Mareschal, W. Schmidt, Modeling Cognitive Development on Balance Scale Phenomena, Machine Learning 16, pp. 59-88, 1994.

- [54] Z.H. Zhou, Y. Jiang, NeC4.5: neural ensemble based C4.5," in IEEE Transactions on Knowledge and Data Engineering 16, pp. 770-773, 2004.
- [55] R. Setiono, W.K. Leow, FERNN: An Algorithm for Fast Extraction of Rules from Neural Networks, Applied Intelligence 12, pp. 15-25, 2000.
- [56] G. Demiroz, H.A. Govenir, N. Ilter, Learning Differential Diagnosis of Eryhemato-Squamous Diseases using Voting Feature Intervals, Artificial Intelligence in Medicine. 13, pp. 147–165, 1998.
- [57] B. Hayes-Roth, B., F. Hayes-Roth. Concept learning and the recognition and classification of exemplars. Journal of Verbal Learning and Verbal Behavior 16, pp. 321-338, 1977.
- [58] I. Kononenko, E. Šimec, M. Robnik-Šikonja, Overcoming the Myopia of Inductive Learning Algorithms with RELIEFF, Applied Intelligence 7, pp. 39–55, 1997.
- [59] R.M. French, N. Chater, Using noise to compute error surfaces in connectionist networks: a novel means of reducing catastrophic forgetting, Neural Comput. 14, pp. 1755-1769, 2002.
- [60] J. Garcke, M. Griebel, Classification with sparse grids using simplicial basis functions, Intell. Data Anal. 6, pp. 483-502, 2002.
- [61] J.G. Dy, C.E. Brodley, Feature Selection for Unsupervised Learning, The Journal of Machine Learning Research 5, pp 845–889, 2004.
- [62] S. J. Perantonis, V. Virvilis, Input Feature Extraction for Multilayered Perceptrons Using Supervised Principal Component Analysis, Neural Processing Letters 10, pp 243–252, 1999.
- [63] M. Elter, R. Schulz-Wendtland, T. Wittenberg, The prediction of breast cancer biopsy outcomes using two CAD approaches that both emphasize an intelligible decision process, Med Phys. **34**, pp. 4164-72, 2007.
- [64] M.A. Little, P.E. McSharry, E.J. Hunter, Lorraine O. Ramig (2008), Suitability of dysphonia measurements for telemonitoring of Parkinson's disease, IEEE Transactions on Biomedical Engineering 56, pp. 1015-1022, 2009.
- [65] J.W. Smith, J.E. Everhart, W.C. Dickson, W.C. Knowler, R.S. Johannes, Using the ADAP learning algorithm to forecast the onset of diabetes mellitus, In: Proceedings of the Symposium on Computer Applications and Medical Care IEEE Computer Society Press, pp.261-265, 1988.
- [66] D.D. Lucas, R. Klein, J. Tannahill, D. Ivanova, S. Brandon, D. Domyancic, Y. Zhang, Failure analysis of parameter-induced simulation crashes in climate models, Geoscientific Model Development 6, pp. 1157-1171, 2013.

- [67] N. Giannakeas, M.G. Tsipouras, A.T. Tzallas, K. Kyriakidi, Z.E. Tsianou, P. Manousou, A. Hall, E.C. Karvounis, V. Tsianos, E. Tsianos, A clustering based method for collagen proportional area extraction in liver biopsy images (2015) Proceedings of the Annual International Conference of the IEEE Engineering in Medicine and Biology Society, EMBS, 2015-November, art. no. 7319047, pp. 3097-3100.
- [68] T. Hastie, R. Tibshirani, Non-parametric logistic and proportional odds regression, JRSS-C (Applied Statistics) **36**, pp. 260–276, 1987.
- [69] M. Dash, H. Liu, P. Scheuermann, K. L. Tan, Fast hierarchical clustering and its validation, Data & Knowledge Engineering 44, pp 109–138, 2003.
- [70] R.P. Gorman, T.J. Sejnowski, Analysis of Hidden Units in a Layered Network Trained to Classify Sonar Targets, Neural Networks 1, pp. 75-89, 1988.
- [71] M. Raymer, T.E. Doom, L.A. Kuhn, W.F. Punch, Knowledge discovery in medical and biological datasets using a hybrid Bayes classifier/evolutionary algorithm. IEEE transactions on systems, man, and cybernetics. Part B, Cybernetics: a publication of the IEEE Systems, Man, and Cybernetics Society, 33, pp. 802-813, 2003.
- [72] P. Zhong, M. Fukushima, Regularized nonsmooth Newton method for multi-class support vector machines, Optimization Methods and Software 22, pp. 225-236, 2007.
- [73] W.H. Wolberg, O.L. Mangasarian, Multisurface method of pattern separation for medical diagnosis applied to breast cytology, Proc Natl Acad Sci U S A. 87, pp. 9193–9196, 1990.
- [74] R. G. Andrzejak, K. Lehnertz, F.Mormann, C. Rieke, P. David, and C. E. Elger, "Indications of nonlinear deterministic and finite-dimensional structures in time series of brain electrical activity: dependence on recording region and brain state," Physical Review E, vol. 64, no. 6, Article ID 061907, 8 pages, 2001.
- [75] A. T. Tzallas, M. G. Tsipouras, and D. I. Fotiadis, "Automatic Seizure Detection Based on Time-Frequency Analysis and Artificial Neural Networks," Computational Intelligence and Neuroscience, vol. 2007, Article ID 80510, 13 pages, 2007. doi:10.1155/2007/80510
- [76] M. Koivisto, K. Sood, Exact Bayesian Structure Discovery in Bayesian Networks, The Journal of Machine Learning Research 5, pp. 549–573, 2004.
- [77] W. J Nash, T.L. Sellers, S.R. Talbot, A.J. Cawthor, W.B. Ford, The Population Biology of Abalone (_Haliotis_ species) in Tasmania. I. Blacklip Abalone (_H. rubra_) from the North Coast and Islands of Bass Strait, Sea Fisheries Division, Technical Report No. 48 (ISSN 1034-3288), 1994.

- [78] T.F. Brooks, D.S. Pope, A.M. Marcolini, Airfoil self-noise and prediction. Technical report, NASA RP-1218, July 1989.
- [79] I.Cheng Yeh, Modeling of strength of high performance concrete using artificial neural networks, Cement and Concrete Research. 28, pp. 1797-1808, 1998.
- [80] D. Harrison and D.L. Rubinfeld, Hedonic prices and the demand for clean ai, J. Environ. Economics & Management 5, pp. 81-102, 1978.
- [81] J.S. Simonoff, Smooting Methods in Statistics, Springer Verlag, 1996.
- [82] P.A. Mackowiak, S.S. Wasserman, M.M. Levine, A critical appraisal of 98.6 degrees f, the upper limit of the normal body temperature, and other legacies of Carl Reinhold August Wunderlich. J. Amer. Med. Assoc. 268, pp. 1578–1580, 1992.
- [83] R.D. King, S. Muggleton, R. Lewis, M.J.E. Sternberg, Proc. Nat. Acad. Sci. USA 89, pp. 11322–11326, 1992.
- [84] Richard L. Graham, Timothy S. Woodall, Jeffrey M. Squyres, Open MPI: A Flexible High Performance MPI, Parallel Processing and Applied Mathematics Volume 3911 of the series Lecture Notes in Computer Science, pp 228-239, 2006.