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Article

Using optimization techniques in Grammatical Evolution

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Abstract: The Grammatical Evolution technique has been successfully applied to a wide range of problems in various scientific fields. However, in many cases, techniques that make use of Grammatical Evolution get trapped in local minima of the objective problem and fail to reach the optimal solution. One simple method to tackle such situations is the usage of hybrid techniques, where local minimization algorithms are used in conjunction with the main algorithm. However, Grammatical Evolution is an integer optimization problem and, as a consequence, techniques should be formulated that are applicable to it as well. In current work, a modified version of the Simulated Annealing algorithm is used as a local optimization procedure in Grammatical Evolution. This approach was tested on the Constructed Neural Networks and a remarkable improvement of the experimental results was shown, both in classification data and in data fitting cases.

Keywords: Grammatical Evolution; Optimization techniques; Neural networks; Evolutionary techniques; Stochastic methods.

1. Introduction

Genetic Algorithms belong to the field of evolutionary techniques [1] and were originally formulated by John Hollands and his team [2]. Genetic Algorithms are initiated by generating a series of random candidate solutions to an optimization problem. These candidate solutions are called chromosomes, and they iteratively undergo a series of operations that have their foundation in physical processes, such as selection, crossover, and mutation [3–5]. Grammatical Evolution [6] is considered as a special case of genetic algorithms, where the chromosomes are series of integer numbers. Chromosomes in the Grammatical Evolution process are rules for generating a BNF grammar [7] and can be used to create functional programs in any programming language.

Grammatical Evolution has been applied on a wide series of real - world applications, such as function approximation[8,9], credit classification [10], network security and prevention of attacks [11], monitoring of water quality [12], modeling glycemia in humans [13], automatic design of Ant algorithms [14], temperature prediction in data centers [15], solving trigonometric equations [16], composing music [17], neural network construction [18,19], producing numeric constants [20], video games [21,22], energy demand estimation[23], combinatorial optimization [24], cryptography [25], evolving of decision trees [26], automatic design of analog electronic circuits [27] etc.

The method of Grammatical Evolution has been extended by various researchers during the last years and some examples of these extensions are the Structured Grammatical Evolution [28,29], that applies an one-to-one mapping between the chromosomes and the non-terminal symbols of the grammar, the π Grammatical Evolution method [30], application of the Particle Swarm Optimization(PSO) [31] to produce programs with grammatical evolution denoted as Grammatical Swarm [32,33], the Probabilistic Grammatical Evolution [34] which introduced a new mapping mechanism for the Grammatical Evolution method, incorporation of parallel programming techniques [35,36], usage of Christiansen grammars [38] etc.

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Also, a variety of software has been developed for Grammatical Evolution, such as the GEVA [37] that proposes a GUI application for Grammatical Evolution, the gramEvol software [39] that provides a package in the R programming language, the GeLab [40] that implements a Matlab toolbox for Grammatical Evolution, the GenClass [41] software used to produce classification programs, the QFc software [42] for feature construction etc.

Although the method of Grammatical Evolution has proven to be extremely efficient, it can often get trapped in local minimum of the objective problem and its performance may not be as expected. A common method to get out of such situations is the use of local optimization techniques, which have been applied many times in combination with Genetic Algorithms [43,44]. In the case of Grammatical Evolution and due to the integral representation of the candidate solutions, local optimization techniques are not directly applicable, such as, for example, the BFGS method [45] and hence more suitable methods should be adopted. The current work utilizes a modified version of the Simulated Annealing method [46] as a local search procedure. The method of Simulated Annealing has been utilized in various cases, such as image processing [47], protein structure optimization [48], resource allocation [49], convex optimization [50], deep learning [51] etc. In this paper, the modified Simulated Annealing method was repeatedly applied to randomly chosen chromosomes of Grammatical Evolution for the problem of constructing artificial neural networks. The proposed method was tested on a wide series of classification and regression problems from the relevant literature and the results seem to be promising.

The rest of this article is divided as follows: in section 2 the Grammatical Evolution procedure is discussed and the proposed modification is outlined in detail, in section 3 the datasets used in the experiments are listed and the experimental results are presented and finally in section 4 some conclusions are presented.

2. The proposed method

This section starts with a brief description of the Grammatical Evolution process and the grammar used, then the modified Simulated Annealing method is presented, and finally the artificial neural network construction algorithm will be presented.

2.1. The Grammatical Evolution method

The chromosomes of Grammatical Evolution represent production rules of the provided BNF grammar. These grammars are usually defined as a set G = (N, T, S, P), where

- *N* is the set of non-terminal symbols.
- *T* is the set of terminal symbols.
- *S* represents that start symbol of the grammar with $S \in N$.
- *P* is the production rules of the grammar. Usually these rules are in the form $A \to a$ or $A \to aB$, $A, B \in N$, $a \in T$.

The BNF grammar is extended by using enumeration in the the production rules. The grammar shown in Figure 1 is used to construct artificial neural networks expressed in the form:

$$N(\overrightarrow{x}, \overrightarrow{w}) = \sum_{i=1}^{H} w_{(d+2)i-(d+1)} \sigma \left(\sum_{j=1}^{d} x_j w_{(d+2)i-(d+1)+j} + w_{(d+2)i} \right)$$
(1)

where H stands the number of processing units of the neural network and d is the dimension of vector \overrightarrow{x} and the vector \overrightarrow{w} defines the weight vector of the neural network. The function $\operatorname{sig}(x)$ represents the sigmoid function $\sigma(x)$ defined as:

$$\sigma(x) = \frac{1}{1 + \exp(-x)} \tag{2}$$

The notation <> is used for the non - terminal symbols of the grammar. The sequence numbers of the production rules are inside the parentheses of the extended grammar. The constant d denotes the dimension of the input data. The production of valid expressions initiates from the symbol *S* and using a series of steps, creates a program by replacing non -

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Figure 1. The used grammar in Neural Network Construction.

```
S:=<sigexpr>
                                (0)
<sigexpr>::=<Node>
                                (0)
         (1)
<Node>::=<number>*sig(<sum>+<number>) (0)
<sum>::= <number>*<xxlist>
                                (0)
         <sum>+<sum>
                                (1)
<xxlist>::= x1
               (0)
              x2 (1)
           . . . . . . . . . . . . . . .
              xd (d-1)
<number>::= (<digitlist>.<digitlist>)
                                      (0)
          (-<digitlist>.<digitlist>) (1)
<digitlist>::= <digit> (0)
          <digit>::= 0 (0)
          | 1 (1)
           9 (9)
```

terminal symbols with the right hand of the selected production rule. The Grammatical Evolution selects production rules using the following scheme:

- Get the next element V from the given chromosome.
- Select the next rule using the equation Rule = V mod NR, where NR is the number of production rules for the current non terminal symbol.

2.2. The modified Simulated Annealing algorithm

The current work utilizes a modified version of the Simulated Annealing algorithm as a local search procedure. The main steps of this procedure are shown in Algorithm 1.

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Algorithm 1 The modified version of the Simulated Annealing algorithm.

procedure $siman(x_0)$

- 1. **Set** k = 0, $T_0 > 0$, $\epsilon > 0$, $r_T > 0$, $r_T < 1$..
- 2. **Set** $N_{eps} > 0$, a positive integer indicated the number of samples drawn in every iteration.
- 3. **Set** *g* and *R*, positive integer values.
- 4. **Set** $x_b = x_0$, $f_b = f(x_b)$.
- 5. **For** $i = 1 ... N_{eps}$
 - (a) Set $y = x_k$
 - (b) **For** j = 1 ... g
 - i. **Set** $p = \text{rand}(1, \text{size}(x_0))$. The variable p indicates a randomly selected position in y.
 - ii. Set $y_p = y_p + \text{rand}(-R, R)$
 - (c) EndFor
 - (d) If $f(y) \le f(x_k)$ then $x_{k+1} = y$
 - (e) Else Set $x_{k+1} = y$ with probability $\min \left\{ 1, \exp \left(-\frac{f(y) f(x_k)}{T_k} \right) \right\}$
 - (f) **If** $f(y) < f_b$ **then** $x_b = y, f_b = f(y)$.
- 6. EndFor
- 7. **Set** $T_{k+1} = T_k r_T$
- 8. **Set** k = k + 1.
- 9. If $T_k \leq \epsilon$ terminate
- 10. **Goto** step 5.
- 11. **Return** x_h

end siman

The method accepts the chromosome x_0 as a starting point and, in each iteration, randomly generates chromosomes around it. The parameter g controls the number of changes that will be made to the chromosome and the parameter R controls the radius of these changes. The parameter T represents the temperature of the algorithm. The temperature starts at extremely high values and progressively decreases linearly. In the early stages and at high temperatures the algorithm may accept points that may have higher values of the fitness function, but as the temperature decreases, this probability also decreases.

2.3. The Neural Network Construction algorithm

The main steps of the algorithm used to construct artificial neural networks with Grammatical Evolution are listed below:

- 1. **Initialization** step.
 - (a) **Set** N_g as the maximum number of generations allowed.
 - (b) **Set** N_c as the number of chromosomes.
 - (c) **Set** p_s as the selection rate and p_m as the mutation rate.
 - (d) **Define** as L_i the number of generations that should elapse before applying the local optimization technique.
 - (e) **Define** as L_c the number of chromosomes that will participate in local search procedure.
 - (f) **Initialize** the chromosomes as vectors of random integers.
 - (g) **Set** iter=0
- 2. **Genetic** step
 - (a) **For** $i = 1, ..., N_g$ **do**

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- i. Create for every chromosome a neural network C_i using the Grammatical Evolution procedure of subsection 2.1 and the associated grammar given in Figure 1.
- ii. **Calculate** the fitness f_i on the train set of the objective problem as:

$$f_i = \sum_{j=1}^{M} \left(C_i(\overrightarrow{x}_j) - t_j \right)^2 \tag{3}$$

where the set $(\overrightarrow{x_j}, t_j)$, j = 1, ..., M is train dataset, with t_i being the actual output for the point $\overrightarrow{x_i}$.

- iii. **Perform** the selection procedure. Initially, the chromosomes are sorted according to their fitness values. The best $(1 p_s) \times N_c$ chromosomes are transferred to the next generation. The remaining chromosomes will be replaced by offsprings created during the crossover procedure.
- iv. **Perform** the crossover procedure. The crossover procedure produces $p_s \times N_c$ offsprings. For every pair of produced offsprings \tilde{z} and \tilde{w} , two offsprings (z,w) are selected using tournament selection. The new offsprings are produced using the one point crossover procedure, which is graphically shown in Figure 2.
- v. **Perform** the mutation procedure. For each element of every chromosome, a random number $r \in [0,1]$ is drawn. The corresponding element is altered if $r \leq p_m$.
- (b) EndFor

3. Local Search Step

- (a) If iters mod $L_i = 0$ Then
 - i. Create a set of randomly L_C chosen chromosomes from the genetic population. Denote this set as L_S .
 - ii. **For** every X_k **in** L_S apply the modified Simulated Annealing algorithm given in Algorithm 1: $X_k = \text{siman}(X_k)$
- 4. **set** iter=iter+1. **If** iter> N_g **goto** Evaluation step else **goto** Genetic step.
- 5. Evaluation step
 - (a) Obtain the best chromosome and create the associated neural network C^* .
 - (b) Evaluate the neural network C^* in the test set of the objective problem and report the results.

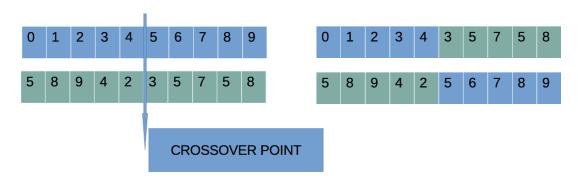


Figure 2. The one - point crossover used in Grammatical Evolution.

3. Results

The current work was applied to a wide series of datasets from different areas and the experimental results were compared with other machine learning techniques. These datasets can be downloaded freely from the following websites:

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1. The UCI dataset repository, https://archive.ics.uci.edu/ml/index.php(accessed on 20 2. The Keel repository, https://sci2s.ugr.es/keel/datasets.php(accessed on 20 March 3. The Statlib URL http://lib.stat.cmu.edu/datasets/(accessed on 20 March 2024). 3.1. Classification datasets The following series of classification datasets was used in the conducted experiments: 1. **Appendictis** a medical dataset, provided in [54]. 2. **Australian** dataset [55], which is related to credit card transactions. 3. **Balance** dataset [56], a dataset related to psychological experiments. 4. **Circular** dataset, an artificial dataset that contains 1000 examples. 5. **Cleveland** dataset, which is a medical dataset [57,58]. 6. **Dermatology** dataset [59], which is a medical dataset about dermatological deceases. 7. **Ecoli** dataset, a dataset about protein localization sites [60]. 8. Haberman dataset, related to breast cancer. 9. **Heart** dataset [61], a medical dataset about heart diseases. 10. Hayes roth dataset [62], which is a human subjects study. 11. House Votes dataset [63], related to votes in the U.S. House of Representatives Congressmen. 12. **Ionosphere** dataset, that was used in experiments related to the ionosphere [64,65]. 13. **Liverdisorder** dataset [66], a medical dataset related to liver disorders. 14. **Mammographic** dataset [67], a medical dataset related to breast cancer. 15. **Parkinsons** dataset, a medical dataset about the Parkinson's disease (PD)[68]. 16. **Pima** dataset [69], a medical dataset related to the diabetes presence. 17. **Popfailures** dataset [70], a dataset related to climate measurements. 18. **Regions2** dataset, medical dataset related to hepatitis C [71]. 19. Saheart dataset [72], a medical dataset related to heart diseases. 20. **Segment** dataset [73], an image processing dataset. 21. **Student** dataset [74], related to data collected in Portuguese schools. Transfusion dataset[75], this datasets was taken from the Blood Transfusion Service 22. Center in Hsin-Chu City in Taiwan. 23. **Wdbc** dataset [76], a medical dataset related to breast tumors. 24. Wine dataset, used to detect the origin of wines [77,78]. 25. **Eeg** datasets, a medical dataset related to EEG measurements [79]. There are 4 different cases from this dataset: Z_F_S, Z_O_N_F_S, ZO_NF_S and ZONF_S. 26. **Zoo** dataset [80], related to animal classification. 3.2. Regression datasets The following regression datasets were used in the conducted experiments: 1. **Abalone** dataset [81], a dataset related to the prediction of age of abalones. 2. Airfoil dataset, a dataset proposed by NASA [82]. 3. **Baseball** dataset, It was used to predict the income of baseball players. 4. Concrete dataset [83], which is a civil engineering dataset. 5. **Dee** dataset, related to the price of electricity. 6. **HO** dataset, downloaded from the STALIB repository. 7. **Housing** dataset, mentioned in [84]. 8. Laser dataset, which is related to laser experiments. 9. LW dataset, related to risk factors associated with low weight babies. 10. MORTGAGE dataset, a dataset related to economic measurements from USA. 11. **PL** dataset, provided from the STALIB repository. 12. **SN** dataset, provided from the STALIB repository. 13. **Treasury** dataset, a dataset related to economic measurements from USA. 14. **TZ** dataset, provided from the STALIB repository.

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3.3. Experimental results

For the execution of the experiments, code written in ANSI C++ was used and, with the help of the programming environment Optimus, that can be downloaded freely from https://github.com/itsoulos/OPTIMUS/ (accessed on 20 March 2024). The experiments were conducted 30 times using different initialization for the random seed each time. The used random generator was the function drand48() of the C programming language. The experimental results were validated using 10 - fold cross validation. The average classification error is reported for the case of classification datasets and the average regression error for the case of regression datasets. These errors are measured on the corresponding test set. The values for the experimental parameters are displayed in Table 1. The experimental results for the classification datasets are outlined in the table 2 and the results for the regression datasets are shown in the table 3. The following applies to the tables with the experimental results:

- 1. The column DATASET denotes the used dataset.
- 2. The column ADAM denotes the application of the ADAM optimization method [85] in an artificial neural network with H = 10 processing nodes.
- 3. The column NEAT stands for the usage of NEAT method (NeuroEvolution of Augmenting Topologies) [86].
- 4. The column MLP represents the results obtained by the training of an artificial neural network with H=10 processing nodes. The neural network was trained using a genetic algorithm and the BFGS local optimization method [87].
- 5. The column RBF stands for the results obtained by an RBF network with H=10 processing nodes.
- 6. The column NNC denotes the application of the original Neural Construction technique performed with the assistance of Grammatical Evolution.
- 7. The column NNC-S denotes the application of the proposed local optimization procedure in the Neural Construction technique.
- 8. The line AVERAGE denotes the average classification or regression error.

| NAME | PURPOSE | VALUE |
|------------|---------------------------------|-----------|
| N_c | Number of chromosomes | 500 |
| N_g | Number of generations | 200 |
| p_s | Selection rate | 0.10 |
| p_m | Mutation rate | 0.05 |
| 8 | Number of random changes | 10 |
| R | Range of random changes | 10 |
| ϵ | Small value used in comparisons | 10^{-5} |
| Neps | Number of random samples | 200 |
| T | Initial temperature | 108 |
| r_T | Rate of decrease in temperature | 0.8 |

Table 1. The values for the parameters used in the conducted experiments.

Table 2. Experimental results for the classification datasets. The numbers in cells represent average classification error as measured in the test set.

| DATASET | ADAM | NEAT | GENETIC | RBF | NNC | NNC-S |
|---------------|--------|--------|---------|--------|--------|--------|
| APPENDICITIS | 16.50% | 17.20% | 18.10% | 12.23% | 14.40% | 14.60% |
| AUSTRALIAN | 35.65% | 31.98% | 32.21% | 34.89% | 14.46% | 14.90% |
| BALANCE | 7.87% | 23.84% | 8.97% | 33.42% | 22.13% | 7.66% |
| CIRCULAR | 3.94% | 34.07% | 5.99% | 6.30% | 14.26% | 7.88% |
| CLEVELAND | 67.55% | 53.44% | 51.60% | 67.10% | 49.93% | 48.59% |
| DERMATOLOGY | 26.14% | 32.43% | 30.58% | 62.34% | 24.80% | 13.11% |
| ECOLI | 64.43% | 43.24% | 49.38% | 59.50% | 48.82% | 44.88% |
| HABERMAN | 29.00% | 24.04% | 28.66% | 25.10% | 28.33% | 28.73% |
| HAYES ROTH | 59.70% | 50.15% | 56.18% | 64.36% | 37.23% | 28.08% |
| HEART | 38.53% | 39.27% | 28.34% | 31.20% | 15.78% | 16.00% |
| HOUSEVOTES | 7.48% | 10.89% | 6.62% | 6.13% | 3.52% | 3.74% |
| IONOSPHERE | 16.64% | 19.67% | 15.14% | 16.22% | 11.86% | 10.03% |
| LIVERDISORDER | 41.53% | 30.67% | 31.11% | 30.84% | 32.97% | 32.82% |
| MAMMOGRAPHIC | 46.25% | 22.85% | 19.88% | 21.38% | 18.22% | 16.58% |
| PARKINSONS | 24.06% | 18.56% | 18.05% | 17.41% | 13.21% | 12.26% |
| PIMA | 34.85% | 34.51% | 32.19% | 25.78% | 28.47% | 25.26% |
| POPFAILURES | 5.18% | 7.05% | 5.94% | 7.04% | 6.83% | 5.52% |
| REGIONS2 | 29.85% | 33.23% | 29.39% | 38.29% | 25.87% | 24.47% |
| SAHEART | 34.04% | 34.51% | 34.86% | 32.19% | 30.80% | 29.52% |
| SEGMENT | 49.75% | 66.72% | 57.72% | 59.68% | 54.89% | 39.38% |
| STUDENT | 5.13% | 12.50% | 5.61% | 7.52% | 5.70% | 4.52% |
| TRANSFUSION | 25.68% | 24.87% | 25.84% | 27.36% | 25.30% | 24.33% |
| WDBC | 35.35% | 12.88% | 8.56% | 7.27% | 7.27% | 5.59% |
| WINE | 29.40% | 25.43% | 19.20% | 31.41% | 13.53% | 11.47% |
| Z_F_S | 47.81% | 38.41% | 10.73% | 13.16% | 15.30% | 7.93% |
| Z_O_N_F_S | 78.79% | 79.08% | 64.81% | 60.40% | 50.48% | 40.42% |
| ZO_NF_S | 47.43% | 43.75% | 8.41% | 9.02% | 15.22% | 6.60% |
| ZONF_S | 11.99% | 5.44% | 2.60% | 4.03% | 3.14% | 2.36% |
| ZOO | 14.13% | 20.27% | 16.67% | 21.93% | 9.10% | 7.20% |
| AVERAGE | 32.23% | 30.72% | 24.94% | 28.74% | 22.13% | 18.43% |

Table 3. Experimental results for the regression datasets. The numbers in cells stand for the average regression error as measured on the test set.

| DATASET | ADAM | NEAT | GENETIC | RBF | NNC | NNC-S |
|----------|-------|--------|---------|-------|-------|-------|
| ABALONE | 4.30 | 9.88 | 7.17 | 7.37 | 5.11 | 4.95 |
| AIRFOIL | 0.005 | 0.067 | 0.003 | 0.27 | 0.003 | 0.003 |
| BASEBALL | 77.90 | 100.39 | 103.60 | 93.02 | 59.40 | 57.30 |
| CONCRETE | 0.078 | 0.081 | 0.0099 | 0.011 | 0.008 | 0.006 |
| DEE | 0.63 | 1.512 | 1.013 | 0.17 | 0.26 | 0.23 |
| НО | 0.035 | 0.167 | 2.78 | 0.03 | 0.016 | 0.012 |
| HOUSING | 80.20 | 56.49 | 43.26 | 57.68 | 25.56 | 18.82 |
| LASER | 0.03 | 0.084 | 0.59 | 0.024 | 0.026 | 0.015 |
| LW | 0.028 | 0.17 | 1.90 | 1.14 | 0.97 | 0.038 |
| MORTGAGE | 9.24 | 14.11 | 2.41 | 1.45 | 0.29 | 0.12 |
| PL | 0.117 | 0.097 | 0.28 | 0.083 | 0.046 | 0.033 |
| SN | 0.026 | 0.174 | 2.95 | 0.90 | 0.026 | 0.024 |
| TREASURY | 11.16 | 15.52 | 2.93 | 2.02 | 0.47 | 0.18 |
| TZ | 0.07 | 0.097 | 5.38 | 4.10 | 0.06 | 0.028 |
| AVERAGE | 13.12 | 14.20 | 12.45 | 12.02 | 6.60 | 5.84 |

As it is evident, the proposed modification improves the efficiency of the proposed method in the majority of used datasets. This improvement on some datasets could be as much as an 80% percent error reduction on the test set. Figure 3 is a scatter plot that provides a detailed comparative analysis of classification error percentages for six distinct 234 machine learning and optimization algorithms: ADAM, NEAT, GENETIC, RBF, NNC, and NNC-S. Each point on the plot represents the outcome of an individual run of a model, 236 thus showcasing the range of variation in the error rates associated with these classification methods. The vertical dispersion of points for each method reflects the spread of error rates, which is critical for evaluating the reliability of each algorithm. The medians of these error rates are indicated by horizontal lines intersecting the clusters of dots, offering a snapshot of each algorithm's central tendency in performance. The asterisk-based notation 241 above the clusters denotes statistical significance levels: one asterisk (*) signifies a p-value 242 less than 0.05, two asterisks (**) denote p < 0.01, three asterisks (***) represent p < 0.001, 243 and four asterisks (****) indicate an extremely low p-value of less than 0.0001, suggesting strong evidence against the null hypothesis. Of note is the performance of the NNC-S 245 method, which not only shows a significantly lower median error rate when compared to the NNC method but also displays a notably tighter cluster of data points. This implies 247 that the NNC-S method not only tends to be more accurate on average but also provides greater consistency in its error rates across different runs, underscoring its robustness as a 249 classification tool.

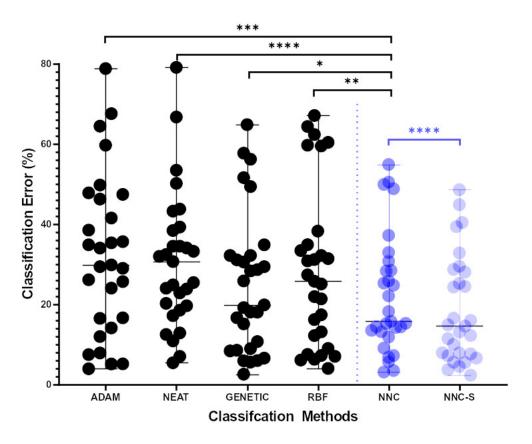


Figure 3. Scatter plot illustrating the variability and median classification error rates for six machine learning algorithms, with statistical significance denoted by asterisks. The NNC-S method demonstrates notably lower error rates, as evidenced by the high statistical significance relative to other methods, which may indicate its superior performance in classification tasks.

Building on the previous analysis of classification methods, Figure 4 extends the evaluation to regression algorithms, providing a comparative study of regression error rates for the same six methods: ADAM, NEAT, GENETIC, RBF, NNC, and NNC-S. Each

data point reflects the regression error from a specific trial, with the array of points for each method revealing the range of performance outcomes. The median error rates are again represented by horizontal lines across the clusters of dots, serving as a summary statistic that facilitates a direct comparison of the methods' central performance trends. The notation of statistical significance is consistent with the previous figure, where asterisks convey the p-value levels, identifying statistically meaningful differences in performance between the methods.

This plot reveals that the NNC-S method maintains its superior performance in the context of regression tasks, demonstrating lower median regression errors compared to the other methods. Significantly, it achieves a markedly lower median regression error than its predecessor, NNC, as indicated by the blue dots and supported by the three asterisks (***). This pattern of results underscores the broader applicability of the NNC-S method's local optimization enhancements, not only in classification accuracy but also in reducing regression errors.

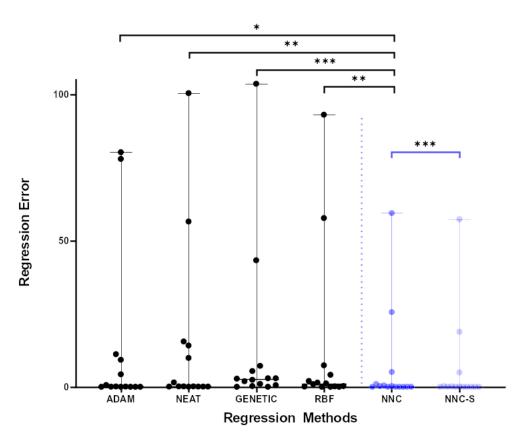


Figure 4. Scatter plot of regression error rates for various regression methods, demonstrating the distribution, median error rates, and statistical significance of differences in performance. The NNC-S method, highlighted in blue, shows statistically significant improvements in accuracy over the NNC method, underlining the efficacy of local optimization enhancements in regression tasks.

Additionally, the effectiveness and the robustness of the proposed method was evaluated by performing additional experiments with different values for the critical parameter g of the proposed Simulated Annealing variant. This parameter is used to control the number of random changes performed on any given chromosome. The experimental results in the classification datasets are shown in Table 4. Clearly, no significant variation in the performance of the proposed technique occurs when this critical parameter is varied.

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Table 4. Experiments with the parameter *g* used in the modified Simulated Annealing method.

| DATASET | NNC-S(g=2) | NNC-S($g = 5$) | NNC-S ($g = 10$) | NNC-S($g = 20$) |
|---------------|------------|-------------------------|---------------------------|--------------------------|
| APPENDICITIS | 14.90% | 15.00% | 14.60% | 14.50% |
| AUSTRALIAN | 14.59% | 14.85% | 14.90% | 15.04% |
| BALANCE | 8.53% | 7.68% | 7.66% | 7.56% |
| CIRCULAR | 10.49% | 8.81% | 7.88% | 7.50% |
| CLEVELAND | 48.41% | 48.31% | 48.59% | 48.10% |
| DERMATOLOGY | 15.09% | 13.80% | 13.11% | 13.29% |
| ECOLI | 45.30% | 45.12% | 44.88% | 44.36% |
| HABERMAN | 27.80% | 27.97% | 28.73% | 27.83% |
| HAYES ROTH | 29.85% | 28.85% | 28.08% | 29.15% |
| HEART | 16.11% | 15.04% | 16.00% | 14.78% |
| HOUSEVOTES | 3.70% | 4.22% | 3.74% | 3.70% |
| IONOSPHERE | 10.54% | 10.09% | 10.03% | 10.00% |
| LIVERDISORDER | 31.41% | 33.15% | 32.82% | 33.29% |
| MAMMOGRAPHIC | 17.16% | 17.25% | 16.58% | 16.99% |
| PARKINSONS | 12.32% | 12.89% | 12.26% | 12.11% |
| PIMA | 26.12% | 25.96% | 25.26% | 25.92% |
| POPFAILURES | 5.58% | 6.00% | 5.52% | 5.68% |
| REGIONS2 | 24.71% | 24.05% | 24.47% | 24.66% |
| SAHEART | 30.04% | 29.67% | 29.52% | 29.07% |
| SEGMENT | 46.94% | 42.37% | 39.38% | 41.19% |
| STUDENT | 4.60% | 4.73% | 4.52% | 4.48% |
| TRANSFUSION | 24.28% | 24.34% | 24.33% | 24.03% |
| WDBC | 6.23% | 6.22% | 5.59% | 5.68% |
| WINE | 12.59% | 11.30% | 11.47% | 9.24% |
| Z_F_S | 9.57% | 9.60% | 7.93% | 8.10% |
| Z_O_N_F_S | 46.04% | 43.36% | 40.42% | 41.54% |
| ZO_NF_S | 9.69% | 8.54% | 6.60% | 6.44% |
| ZONF_S | 2.58% | 2.28% | 2.36% | 2.36% |
| ZOO | 6.90% | 7.00% | 7.20% | 7.70% |
| AVERAGE | 19.38% | 18.91% | 18.43% | 18.42% |

Continuing from the previous analysis, Figure 5 presents the classification error rates for variations of the NNC-S algorithm with differing values of the parameter g. The plot aims to evaluate whether changes in the parameter g led to statistically significant differences in the algorithm's classification performance. The horizontal bars on the plot indicate the median classification error for each variation of the NNC-S method, providing a clear comparison across the different parameter values. The statistical annotations ("ns" for not significant, "**" for p < 0.01, and "***" for p < 0.001) are used to denote the statistical significance of the differences between the groups. It appears that some variations, particularly between NNC-S (g=2) and NNC-S (g=5), as well as between NNC-S (g=10) and NNC-S (g=20), do not show significant differences in performance (denoted by "ns"). In contrast, other comparisons do reveal significant differences, suggesting that certain values of g can indeed impact the classification error rates of the NNC-S algorithm.

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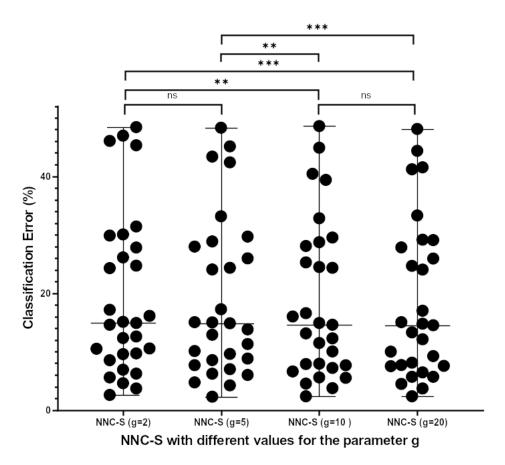


Figure 5. his figure examines the impact of varying the parameter g on the NNC-S algorithm's classification errors, revealing that while some parameter adjustments do not significantly affect performance, others result in noticeable differences, as indicated by the statistical significance annotations.

Furthermore, an additional experiment was performed by varying the parameter *R* of the proposed Simulated Annealing variant. This parameter controls the range of changes performed in any given chromosome. The results for this experiment are shown in Table 5. And this time the method appeared quite robust in its performance, without large variations in the error as measured in the test set.

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Table 5. Experiments with the parameter *R* of the modified Simulated Annealing algorithm. The parameter *g* was set to 10.

| DATASET | NNC-S(R=2) | NNC-S(R=5) | NNC-S(R = 10) | NNC-S($R = 20$) |
|---------------|------------|------------|---------------|--------------------------|
| APPENDICITIS | 14.40% | 14.90% | 14.60% | 15.20% |
| AUSTRALIAN | 14.77% | 14.78% | 14.90% | 14.70% |
| BALANCE | 7.66% | 7.74% | 7.66% | 7.66% |
| CIRCULAR | 8.39% | 8.29% | 7.88% | 7.78% |
| CLEVELAND | 49.45% | 49.28% | 48.59% | 47.11% |
| DERMATOLOGY | 14.09% | 12.54% | 13.11% | 11.34% |
| ECOLI | 44.24% | 46.30% | 44.88% | 44.48% |
| HABERMAN | 27.33% | 28.10% | 28.73% | 28.04% |
| HAYES ROTH | 29.15% | 27.92% | 28.08% | 26.46% |
| HEART | 15.67% | 15.52% | 16.00% | 15.15% |
| HOUSEVOTES | 4.00% | 3.62% | 3.74% | 4.52% |
| IONOSPHERE | 10.14% | 10.03% | 10.03% | 10.71% |
| LIVERDISORDER | 32.80% | 32.12% | 32.82% | 32.29% |
| MAMMOGRAPHIC | 17.18% | 16.78% | 16.58% | 16.62% |
| PARKINSONS | 12.68% | 12.16% | 12.26% | 11.95% |
| PIMA | 25.72% | 25.11% | 25.26% | 26.33% |
| POPFAILURES | 5.87% | 5.72% | 5.52% | 5.58% |
| REGIONS2 | 23.55% | 24.04% | 24.47% | 24.08% |
| SAHEART | 29.48% | 28.96% | 29.52% | 29.24% |
| SEGMENT | 40.32% | 40.23% | 39.38% | 40.82% |
| STUDENT | 4.18% | 4.50% | 4.52% | 4.78% |
| TRANSFUSION | 24.60% | 24.12% | 24.33% | 24.36% |
| WDBC | 6.09% | 5.68% | 5.59% | 5.46% |
| WINE | 11.00% | 10.30% | 11.47% | 9.41% |
| Z_F_S | 8.33% | 8.30% | 7.93% | 8.50% |
| Z_O_N_F_S | 41.70% | 43.42% | 40.42% | 41.44% |
| ZO_NF_S | 7.58% | 7.72% | 6.60% | 7.10% |
| ZONF_S | 2.50% | 2.54% | 2.36% | 3.00% |
| ZOO | 6.80% | 6.30% | 7.20% | 6.10% |
| AVERAGE | 18.61% | 18.52% | 18.43% | 18.28% |

4. Conclusions

In the current work, an extension of the original Grammatical Evolution has been proposed, which was applied in the Neural Construction method. In this extension, an application of a modified optimization algorithm was suggested, in order to improve the efficiency of the underlying technique. The proposed optimization algorithm was a variant of the Simulated Annealing method, that was applied on randomly selected chromosomes of the Grammatical Evolution procedure. This method was chosen because of its widespread use in many applications but because of its ability to handle integer representations, since the chromosomes in Grammatical Evolution are vectors of integers. Of course, other local optimization techniques could be incorporated, such as tabu search [88] or hill climbing [89] as feature extensions of the proposed method.

The proposed modification was applied to the Neural Network Construction method and its efficiency was measured on a wide series of classification and regression datasets from the relevant literature. Based on the experimental results, it has become clear that the proposed variant significantly improves the performance of the technique both on classification datasets and on data fitting datasets. Also, the effectiveness and the robustness of the proposed modification were measured using experiments with different values of some critical parameters of the current Simulated Annealing variant. These experiments indicated that the method does not depend heavily on the selection of any critical parameter of the Simulated Annealing variant.

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Future work may include application of the local search procedure in other Grammatical Evolution applications, such as feature construction, creation of classification rules etc. Also, the proposed process can be significantly accelerated by the use of parallel optimization techniques [90], which take advantage of modern computational structures.

Author Contributions: I.G.T., A.T. and E.K. conceived the idea and methodology and supervised the technical part regarding the software. I.G.T. conducted the experiments, employing several datasets, and provided the comparative experiments. A.T. performed the statistical analysis. E.K. and all other authors prepared the manuscript. E.K. and I.G.T. organized the research team and A.T. supervised the project. All authors have read and agreed to the published version of the manuscript.

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References

- 1. N. Yusup, A. M. Zain, S. Z. M. Hashim, Evolutionary techniques in optimizing machining parameters: Review and recent applications (2007–2011), Expert Systems with Applications 39.10, pp. 9909-9927, 2012.
- J.H. Holland, Genetic algorithms. Scientific american 267, pp. 66-73, 1992.
- 3. J. Stender, Parallel Genetic Algorithms: Theory & Applications. Edition: IOS Press, 1993.
- 4. D. Goldberg, Genetic Algorithms in Search, Optimization and Machine Learning, Addison-Wesley Publishing Company, Reading, Massachussets, 1989.
- 5. Z. Michaelewicz, Genetic Algorithms + Data Structures = Evolution Programs. Springer Verlag, Berlin, 1996.
- 6. M. O'Neill, C. Ryan, Grammatical evolution, IEEE Trans. Evol. Comput. 5,pp. 349–358, 2001.
- 7. 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.
- 8. C. Ryan, J. Collins, M. O'Neill, Grammatical evolution: Evolving programs for an arbitrary language. In: Banzhaf, W., Poli, R., Schoenauer, M., Fogarty, T.C. (eds) Genetic Programming. EuroGP 1998. Lecture Notes in Computer Science, vol 1391. Springer, Berlin, Heidelberg, 1998.
- 9. M. O'Neill, M., C. Ryan, Evolving Multi-line Compilable C Programs. In: Poli, R., Nordin, P., Langdon, W.B., Fogarty, T.C. (eds) Genetic Programming. EuroGP 1999. Lecture Notes in Computer Science, vol 1598. Springer, Berlin, Heidelberg, 1999.
- 10. A. Brabazon, M. O'Neill, Credit classification using grammatical evolution, Informatica 30.3, 2006.
- 11. S. Şen, J.A. Clark. A grammatical evolution approach to intrusion detection on mobile ad hoc networks, In: Proceedings of the second ACM conference on Wireless network security, 2009.
- 12. L. Chen, C.H. Tan, S.J. Kao, T.S. Wang, Improvement of remote monitoring on water quality in a subtropical reservoir by incorporating grammatical evolution with parallel genetic algorithms into satellite imagery, Water Research 42, pp. 296-306, 2008.
- 13. J. I. Hidalgo, J. M. Colmenar, J.L. Risco-Martin, A. Cuesta-Infante, E. Maqueda, M. Botella, J. A. Rubio, Modeling glycemia in humans by means of Grammatical Evolution, Applied Soft Computing 20, pp. 40-53, 2014.
- 14. J. Tavares, F.B. Pereira, Automatic Design of Ant Algorithms with Grammatical Evolution. In: Moraglio, A., Silva, S., Krawiec, K., Machado, P., Cotta, C. (eds) Genetic Programming. EuroGP 2012. Lecture Notes in Computer Science, vol 7244. Springer, Berlin, Heidelberg, 2012.
- 15. M. Zapater, J.L. Risco-Martín, P. Arroba, J.L. Ayala, J.M. Moya, R. Hermida, Runtime data center temperature prediction using Grammatical Evolution techniques, Applied Soft Computing 49, pp. 94-107, 2016.
- 16. C. Ryan, M. O'Neill, J.J. Collins, Grammatical evolution: Solving trigonometric identities, proceedings of Mendel. Vol. 98. 1998.
- 17. 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.
- 18. 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.
- 19. K. Soltanian, A. Ebnenasir, M. Afsharchi, Modular Grammatical Evolution for the Generation of Artificial Neural Networks, Evolutionary Computation 30, pp 291–327, 2022.
- 20. I. Dempsey, M.O' Neill, A. Brabazon, Constant creation in grammatical evolution, International Journal of Innovative Computing and Applications 1, pp 23–38, 2007.

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- 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.
- 22. N. Shaker, M. Nicolau, G. N. Yannakakis, J. Togelius, M. O'Neill, Evolving levels for Super Mario Bros using grammatical evolution, 2012 IEEE Conference on Computational Intelligence and Games (CIG), 2012, pp. 304-31.
- 23. 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.
- 24. N. R. Sabar, M. Ayob, G. Kendall, R. Qu, Grammatical Evolution Hyper-Heuristic for Combinatorial Optimization Problems, IEEE Transactions on Evolutionary Computation 17, pp. 840-861, 2013.
- 25. C. Ryan, M. Kshirsagar, G. Vaidya, G. et al. Design of a cryptographically secure pseudo random number generator with grammatical evolution. Sci Rep 12, 8602, 2022.
- 26. P.J. Pereira, P. Cortez, R. Mendes, Multi-objective Grammatical Evolution of Decision Trees for Mobile Marketing user conversion prediction, Expert Systems with Applications 168, 114287, 2021.
- 27. F. Castejón, E.J. Carmona, Automatic design of analog electronic circuits using grammatical evolution, Applied Soft Computing **62**, pp. 1003-1018, 2018.
- 28. N. Lourenço, F.B. Pereira, E, Costa, Unveiling the properties of structured grammatical evolution, Genetic Programming and Evolvable Machines 17, pp. 251-289, 2016.
- 29. N. Lourenço, F. Assunção, F.B. Pereira, E. Costa, P. Machado, Structured grammatical evolution: a dynamic approach, Handbook of grammatical evolution, pp. 137-161, 2018.
- 30. M. O'Neill, A. Brabazon, M. Nicolau, S.M. Garraghy, P. Keenan, πGrammatical Evolution. In: Deb, K. (eds) Genetic and Evolutionary Computation GECCO 2004. GECCO 2004. Lecture Notes in Computer Science, vol 3103. Springer, Berlin, Heidelberg, 2004.
- 31. Riccardo Poli, James Kennedy, Tim Blackwell, Particle swarm optimization An Overview, Swarm Intelligence 1, pp 33-57, 2007.
- 32. M. O'Neill, A. Brabazon, Grammatical swarm: The generation of programs by social programming. Natural Computing 5, pp. 443-462, 2006.
- 33. E. Ferrante, E. Duéñez-Guzmán, A.E. Turgut, T. Wenseleers, GESwarm: Grammatical evolution for the automatic synthesis of collective behaviors in swarm robotics. In Proceedings of the 15th annual conference on Genetic and evolutionary computation, pp. 17-24, 2013.
- 34. J. Mégane, N. Lourenço, P. Machado, Probabilistic Grammatical Evolution. In: Hu, T., Lourenço, N., Medvet, E. (eds) Genetic Programming. EuroGP 2021. Lecture Notes in Computer Science, vol 12691. Springer, Cham, 2021.
- 35. O. Popelka, P. Osmera, Parallel Grammatical Evolution for Circuit Optimization. In: Hornby, G.S., Sekanina, L., Haddow, P.C. (eds) Evolvable Systems: From Biology to Hardware. ICES 2008. Lecture Notes in Computer Science, vol 5216. Springer, Berlin, Heidelberg. https://doi.org/10.1007/978-3-540-85857-7_40
- 36. P. Ošmera, Two level parallel grammatical evolution, Advances in Computational Algorithms and Data Analysis pp. 509-525, 2009.
- 37. M. O'Neill, E. Hemberg, C. Gilligan, E. Bartley, J. McDermott, A. Brabazon, GEVA: grammatical evolution in Java. ACM SIGEVOlution 3, pp. 17-22, 2008.
- 38. A. Ortega, M. de la Cruz, M. Alfonseca, Christiansen Grammar Evolution: Grammatical Evolution With Semantics, IEEE Transactions on Evolutionary Computation 11, pp. 77-90, Feb. 2007.
- 39. F. Noorian, A.M. de Silva, P.H.W. Leong, gramEvol: Grammatical Evolution in R, Journal of Statistical Software 71, pp. 1–26, 2016.
- 40. M.A. Raja, C. Ryan, GELAB A Matlab Toolbox for Grammatical Evolution. In: Yin, H., Camacho, D., Novais, P., Tallón-Ballesteros, A. (eds) Intelligent Data Engineering and Automated Learning IDEAL 2018. IDEAL 2018. Lecture Notes in Computer Science(), vol 11315, 2018. Springer, Cham. https://doi.org/10.1007/978-3-030-03496-2_22
- 41. N.Anastasopoulos, I.G. Tsoulos, A. Tzallas, GenClass: A parallel tool for data classification based on Grammatical Evolution, SoftwareX 16, 100830, 2021.
- 42. I.G. Tsoulos, QFC: A Parallel Software Tool for Feature Construction, Based on Grammatical Evolution, Algorithms 15, 295, 2022.
- 43. S. Yang, S. N. Jat, Genetic Algorithms With Guided and Local Search Strategies for University Course Timetabling, IEEE Transactions on Systems, Man, and Cybernetics, Part C (Applications and Reviews) 41, pp. 93-106, 2011.
- 44. M. Sivaram, K. Batri, A.S. Mohammed, V. Porkodi, Exploiting the Local Optima in Genetic Algorithm using Tabu Search. Indian Journal of Science and Technology 12, pp. 1–13, 2019.
- 45. Y.H. Dai, Convergence Properties of the BFGS Algoritm, SIAM Journal on Optimization 13, pp. 693-701, 2002.
- 46. S. Kirkpatrick, C.D. Gelatt Jr, M.P. Vecchi, Optimization by simulated annealing, Science 220, pp. 671-680, 1983.
- 47. M.C. Robini, T. Rastello, I.E. Magnin, Simulated annealing, acceleration techniques, and image restoration, IEEE Transactions on Image processing **8.10**, pp. 1374-1387, 1999.
- 48. L. Zhang, H. Ma, W. Qian, H. Li, Protein structure optimization using improved simulated annealing algorithm on a three-dimensional AB off-lattice model. Computational Biology and Chemistry 85, 107237, 2020.
- 49. J.C.J. H. Aerts, G.B.M. Heuvelink, Using simulated annealing for resource allocation, International Journal of Geographical Information Science 16, pp. 571-587, 2002.

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481

- 50. A.T. Kalai, S. Vempala, Simulated annealing for convex optimization, Mathematics of Operations Research 31.2, pp. 253-266, 2006.
- 51. L.M. Rasdi Rere, M.I. Fanany, A. M. Arymurthy, Simulated Annealing Algorithm for Deep Learning, Procedia Computer Science 72, pp. 137-144, 2015.
- 52. M. Kelly, R. Longjohn, K. Nottingham, The UCI Machine Learning Repository. 2023. Available online: https://archive.ics.uci.edu (accessed on 18 February 2024).
- 53. J. Alcalá-Fdez, A. Fernandez, J. Luengo, J. Derrac, S. García, L. Sánchez, F. Herrera. KEEL Data-Mining Software Tool: Data Set Repository, Integration of Algorithms and Experimental Analysis Framework. Journal of Multiple-Valued Logic and Soft Computing 17, pp. 255-287, 2011.
- 54. Weiss, Sholom M. and Kulikowski, Casimir A., Computer Systems That Learn: Classification and Prediction Methods from Statistics, Neural Nets, Machine Learning, and Expert Systems, Morgan Kaufmann Publishers Inc, 1991.
- 55. J.R. Quinlan, Simplifying Decision Trees. International Journal of Man-Machine Studies 27, pp. 221-234, 1987.
- 56. T. Shultz, D. Mareschal, W. Schmidt, Modeling Cognitive Development on Balance Scale Phenomena, Machine Learning **16**, pp. 59-88, 1994.
- 57. 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.
- 58. R. Setiono , W.K. Leow, FERNN: An Algorithm for Fast Extraction of Rules from Neural Networks, Applied Intelligence 12, pp. 15-25, 2000.
- 59. 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.
- 60. P. Horton, K.Nakai, A Probabilistic Classification System for Predicting the Cellular Localization Sites of Proteins, In: Proceedings of International Conference on Intelligent Systems for Molecular Biology 4, pp. 109-15, 1996.
- 61. I. Kononenko, E. Šimec, M. Robnik-Šikonja, Overcoming the Myopia of Inductive Learning Algorithms with RELIEFF, Applied Intelligence 7, pp. 39–55, 1997
- 62. 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.
- 63. 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.
- 64. J.G. Dy , C.E. Brodley, Feature Selection for Unsupervised Learning, The Journal of Machine Learning Research 5, pp 845–889, 2004.
- 65. S. J. Perantonis, V. Virvilis, Input Feature Extraction for Multilayered Perceptrons Using Supervised Principal Component Analysis, Neural Processing Letters 10, pp 243–252, 1999.
- 66. J. Garcke, M. Griebel, Classification with sparse grids using simplicial basis functions, Intell. Data Anal. 6, pp. 483-502, 2002.
- 67. 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.
- 68. M.A. Little, P.E. McSharry, E.J. Hunter, J. Spielman, L.O. Ramig, Suitability of dysphonia measurements for telemonitoring of Parkinson's disease. IEEE Trans Biomed Eng. **56**, pp. 1015-1022, 2009.
- 69. 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.
- 70. 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.
- 71. 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.
- 72. T. Hastie, R. Tibshirani, Non-parametric logistic and proportional odds regression, JRSS-C (Applied Statistics) 36, pp. 260–276, 1987
- 73. M. Dash, H. Liu, P. Scheuermann, K. L. Tan, Fast hierarchical clustering and its validation, Data & Knowledge Engineering 44, pp 109–138, 2003.
- 74. P. Cortez, A. M. Gonçalves Silva, Using data mining to predict secondary school student performance, In Proceedings of 5th FUture BUsiness TEChnology Conference (FUBUTEC 2008) (pp. 5–12). EUROSIS-ETI, 2008.
- 75. I-Cheng Yeh, King-Jang Yang, Tao-Ming Ting, Knowledge discovery on RFM model using Bernoulli sequence, Expert Systems with Applications **36**, pp. 5866-5871, 2009.
- 76. 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.
- 77. 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.

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492

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497

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506

507

- 78. P. Zhong, M. Fukushima, Regularized nonsmooth Newton method for multi-class support vector machines, Optimization Methods and Software 22, pp. 225-236, 2007.
- 79. 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, Phys. Rev. E 64, pp. 1-8, 2001.
- 80. M. Koivisto, K. Sood, Exact Bayesian Structure Discovery in Bayesian Networks, The Journal of Machine Learning Research 5, pp. 549–573, 2004.
- 81. 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.
- 82. T.F. Brooks, D.S. Pope, A.M. Marcolini, Airfoil self-noise and prediction. Technical report, NASA RP-1218, July 1989.
- 83. I.Cheng Yeh, Modeling of strength of high performance concrete using artificial neural networks, Cement and Concrete Research. **28**, pp. 1797-1808, 1998.
- 84. D. Harrison and D.L. Rubinfeld, Hedonic prices and the demand for clean ai, J. Environ. Economics & Management 5, pp. 81-102, 1978.
- 85. D. P. Kingma, J. L. Ba, ADAM: a method for stochastic optimization, in: Proceedings of the 3rd International Conference on Learning Representations (ICLR 2015), pp. 1–15, 2015.
- 86. K. O. Stanley, R. Miikkulainen, Evolving Neural Networks through Augmenting Topologies, Evolutionary Computation **10**, pp. 99-127, 2002.
- 87. M.J.D Powell, A Tolerant Algorithm for Linearly Constrained Optimization Calculations, Mathematical Programming 45, pp. 547-566, 1989.
- 88. F. Glover, Parametric tabu-search for mixed integer programs. Computers & Operations Research 33, pp. 2449-2494, 2006.
- 89. A. Lim, B. Rodrigues, X. Zhang, A simulated annealing and hill-climbing algorithm for the traveling tournament problem. European Journal of Operational Research **174**, pp.1459-1478, 2006.
- 90. A. Bevilacqua, A methodological approach to parallel simulated annealing on an SMP system. Journal of Parallel and Distributed Computing **62**, pp. 1548-1570, 2002.