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Neuroevolution under Unimodal Error Landscapes

An Exploration of the Semantic Learning Machine Algorithm

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Neuroevolution under Unimodal Error Landscapes

ABSTRACT

Neuroevolution is a field in which evolutionary algorithms are applied with the goal of evolving Artificial Neural Networks (ANNs). These evolutionary approaches can be used to evolve ANNs with fixed or dynamic topologies. This paper studies the Semantic Learning Machine (SLM) algorithm, a recently proposed neuroevolution method that searches over unimodal error landscapes in any supervised learning problem, where the error is measured as a distance to the known targets. SLM is compared with the topology-changing algorithm NeuroEvolution of Augmenting Topologies (NEAT) and with a fixed-topology neuroevolution approach. Experiments are performed on a total of 6 real-world datasets of classification and regression tasks. The results show that the best SLM variants outperform the other neuroevolution approaches in terms of generalization achieved, while also being more efficient in learning the training data. Further comparisons show that the best SLM variants also outperform the common ANN backpropagation-based approach under different topologies. A combination of the SLM with a recently proposed semantic stopping criterion also shows that it is possible to evolve competitive neural networks in a few seconds on the vast majority of the datasets considered.

Keywords: Semantic Learning Machine, NEAT, Neuroevolution

RESUMO

Neuro evolução é uma área onde algoritmos evolucionários são aplicados com o objetivo de evoluir Artificial Neural Networks (ANN). Estas abordagens evolucionárias podem ser utilizadas para evoluir ANNs com topologias fixas ou dinâmicas. Este artigo estuda o algoritmo de Semantic Learning Machine (SLM), um método de neuro evolução proposto recentemente que percorre paisagens de erros unimodais em qualquer problema de aprendizagem supervisionada, onde o erro é medido como a distância com os alvos conhecidos previamente. SLM é comparado com o algoritmo de alteração de topologias NeuroEvolution of Augmenting Topologies (NEAT) e com uma abordagem neuro evolucionária de topologias fixas. Experiências são realizadas em 6 datasets reais de tarefas de regressão e classificação. Os resultados mostram que as melhores variantes de SLM são mais capazes de generalizar quando comparadas com outras abordagens de neuro evolução, ao mesmo tempo que são mais eficientes no processo de treino. Mais comparações mostram que as melhores variantes de SLM são mais eficazes que as abordagens mais comuns de treino de ANN usando diferentes topologias e retro propagação. A combinação de SLM com um critério semântico de paragem do processo de treino também mostra que é possível criar redes neuronais competitivas em poucos segundos, na maioria dos datasets considerados.

Palavras-chave: Semantic Learning Machine, NEAT, Neuroevolution

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CHAPTER 1

INTRODUCTION

Accelerated by outstanding accomplishments in matching patterns in complex data, such as recognizing objects on images [4, 9, 18], interpreting natural language [11, 21] and controlling autonomous vehicles [2], Artificial Neural Networks (ANNs) have attracted enormous interest in both research and industry. Although ANNs can generate complex solutions that can substitute human operations in various tasks with superior performance in terms of accuracy and speed [23], they are essentially only built upon two simple base components: neurons and synapses (connections). Inspired by the anatomy of the human brain, neurons aggregate a set of input connections and generate one output, determined by their activation function. To create networks, neurons are connected over synapses, so that the output of one neuron serves as input for the other.

For ANNs to perform well on a certain task, it is critical to locate a combination of satisfying connection weights. For this purpose, weights are adjusted in a learning process, based on provided training data. The most relevant approach is Backpropagation [15], where the error between prediction and ground truth is distributed back recursively through adjacent connections. However, Backpropagation fails to answer the question of how to define the general topology of neurons and synapses. Devising suitable topologies is crucial, since it directly affects the speed and accuracy of the learning process [24]. Yet still, this challenge is traditionally approached with evaluating several different combinations, which is tedious and does not guarantee to converge near the global optima.

Topology and weight evolving ANNs (TWEANNs) address this issue by developing satisfactory combinations of topology and weights. TWEANNs belong to the research field of neuroevolution, an area within artificial intelligence (AI) that deals with breeding ANNs in an evolutionary process. Inspired by Darwinism, ANNs are evaluated and selected for reproduction, based on a defined fitness function. Next, chosen solutions create offspring by randomly crossing over their genetic traits. The constructed offspring are prone to further, randomly occurring mutations. Consequently, offspring can differ from their parents in terms of connection weights as well as number of neurons and connections. The breeding cycle is repeated for a certain number of generations or until a satisfying solution is found.

This paper studies the application of several neuroevolution methods to the task of supervised machine learning. Of particular interest is the study of the recently proposed Semantic Learning Machine (SLM) algorithm. Perhaps the most interesting characteristic of SLM is that it searches over unimodal error landscapes in any supervised learning problem where the error is measured as a distance to the known targets. The SLM is explored and compared against other neuroevolution methods as well as other well-established supervised machine learning techniques.

The paper is organized as follows: Chapter 2 describes the main neuroevolution methods under study; Chapter 3 outlines the experimental methodology; Chapter 4 reports and discusses the experimental results; finally Chapter 5 concludes.

CHAPTER

2

NEUROEVOLUTION WITH DYNAMIC TOPOLOGIES

This chapter briefly describes the two Topology and Weight Evolving Artificial Neural Network algorithms under study: Semantic Learning Machine and NEAT.

2.1 Semantic Learning Machine

SLM [6, 8] is a neural network construction algorithm originally derived from Geometric Semantic Genetic Programming (GSGP) [12]. A common characteristic with GSGP is that SLM searches over unimodal error landscapes, implying that there are no local optima. This means that, with the exception of the global optimum, every point in the search space has at least one neighbor with better fitness, and that neighbor is reachable through the application of the variation operators. As this type of landscape eliminates the local optima issue, it is potentially much more favorable in terms of search effectiveness and efficiency. The strength of the SLM comes from the associated geometric semantic mutation operator. This operator allows to search over the space of neural networks without the need to use backpropagation to adjust the weights of the network. As the issue of local optima does not apply, the evolutionary search can be performed by simply hill climbing. The SLM mutation operator was originally specified for neural networks with a single hidden layer [6], but it was subsequently extended to be applicable to any number of hidden layers [8]. For further details the reader is referred to [6] and [8].

2.2 NeuroEvolution of Augmenting Topologies

One of the most popular and widely used TWEANN algorithms is NeuroEvolution of Augmenting Topologies (NEAT) [19], which has been applied to various applications, such as controlling robots and video game agents [20], computational creativity [17, 22], and mass estimation optimization [1]. In NEAT genes represent connections, specifying the in-neuron, the out-neuron, the weight and whether the connection is enabled. Also, genes store the information about their historical origin in a global innovation number that is shared among all solutions for genes of the same structure (in-neuron and out-neuron). Mutation in NEAT can change both weights and topology. For adjusting the weight of existing connections, NEAT perturbs the current value with a defined weight and probability. Regarding topology mutations, NEAT can add a new connection or add a new neuron. The adding-link mutation creates a new connection gene with a random weight between two previously unconnected neurons. In the adding-node mutation, a new intermediate neuron is created between the in-neuron and the out-neuron of an existing connection. When an unprecedented topology mutation occurs, a new innovation number is assigned to the corresponding gene. For the crossover operation, both parent topologies are aligned, based on the innovation number. When constructing offspring, genes present in both parents are inherited at random with equal probability, whereas the isolated genes are always chosen from the more fit parent. During the selection process, NEAT protects innovation by speciating the population, where a solution's fitness is adjusted by diving it by the number of solutions in its species. Solutions are placed in the same species when they show high topological compatibility. The topological compatibility between solutions is calculated as a linear combination between the matching and isolated genes as well as the average connection weight difference. Over the course of the evolutionary process, solutions of initially minimal structures are augmented incrementally. For further details the reader is referred to [19].

CHAPTER 3

EXPERIMENTAL METHODOLOGY

This chapter describes the experimental settings considered to achieve the results discussed in the subsequent section of the paper, and the datasets taken into account for assessing the performance of SLM and the comparative algorithms over regression and classification problems. All datasets under study were split into training (50%), validation (30%) and testing(20%). The best parameter configuration for models under study was determined by choosing a random configuration from a grid on configurations defined in Section 3.1, training it on the training data, and evaluating the performance on the validation data. Each model was given 300 seconds for parameter tuning. Afterwards, the parameter configuration with the best performance on validation data was selected and evaluated on testing data. The training, validation and testing samples were paired for all models. This procedure was repeated 30 times on different samples for statistical validity. Performance is evaluated as the root mean squared error (RMSE).

3.1 Settings

All genetic approaches use populations of 100 individuals and stop the evolutionary process after 200 generations, if not stated otherwise. The SLM variant under study uses a optimal learning step for each application of the mutation operator, using the pseudo-inverse between prediction and target vector. The evolutionary process is stopped, based on the Error Deviation Variation (EDV) semantic stopping criterion [7]. This semantic criterion can be used to stop the search before overfitting starts to occur. The stopping criterion was tested for a threshold of 0.25 and 0.5. The mutation operator adds one neuron to each hidden layer. The added neurons connect to a random subset of previous nodes, where the subset size is taken from a uniform distribution between 1 and a defined maximum. The maximum was tested for 1, 10, 50 and 100. For the number of layers, we tested 1 to 10 layers. All hidden neurons in the last hidden layer have the hyperbolic tangent as their activation function, whereas the activation function for the remaining hidden nodes was randomly chosen from the identity function, the Sigmoid function, the rectified linear unit (ReLU) function and the hyperbolic tangent function. This guarantees that, for each application of the mutation operator, the semantic variation always lies within the interval $[-ls, ls]$, where ls represents the learning step.

The NEAT parameters can be found in Table A.1 and Table A.2. Also, we tuned the adding-node-mutation probability for 0.1 and 0.25, the adding-link-mutation probability for 0.1 and 0.25, and the compatibility threshold for 3 and 4.

We added a fixed-topology neuroevolution approach to the benchmark, where weights of an ANN are optimized, using simple Genetic Algorithms (SGA). For the SGA, we chose a tournament selection with tournament size 5, an arithmetic crossover operator and a Gaussian mutation operator with standard deviation of 0.1. We evaluated mutation rates of 0.25 and 0.5, as well as crossover rates of 0.01 and 0.1. For the hidden topology we analyzed the following topologies: one hidden layer with one hidden neuron, one hidden layer with two hidden neurons, two hidden layers with two hidden neurons each, three hidden layers with three hidden neurons each and three hidden layers with five hidden neurons each.

Furthermore, we compared the results with the ones achieved with the Multilayer Perceptron (MLP) with backpropagation and with Support Vector Machines (SVM). To that end we used the Scikit-learn framework [14]. The parameter search grid for MLP and SVM can be found in Table A.3 and Table A.4 respectively.

3.2 Classification Datasets

The following classification datasets were studied:

- German Credit Data (Credit): the dataset classifies people, described by a set of attributes, as good or bad credit risks. The dataset contains 1000 instances, 700 people with good risk and 300 people with bad risk. Each instance has 24 numerical input variables [10].

- Pima Indians Diabetes (Diabetes): the dataset classifies females of Pima Indian heritage, based on positive or negative diabetes tests. The dataset contains 768 instances, 500 negative tests, and 268 positive tests. Each instance has 8 numerical input features [10].

- Connectionist Bench (Sonar): the dataset classifies sonar signals bounced off a metal cylinder and those bounced off a roughly cylindrical rock. The dataset contains 208 observations, 111 that bounced off a metal cylinder and 97 that bounced off a rock. Each instance has 60 numerical input features [10].

3.3 Regression Datasets

The following regression datasets were studied:

- Music: The dataset relates music to its geographical origin in longitude and latitude. It contains 1059 songs from 33 countries. Each instance contains 68 categorical and numerical audio features [10, 25]. Categorical features are coerced to binary indicator variables and missing values are imputed using the median.
- Parkinson Speech (Parkinson): The dataset relates speech recordings of patients to the Unified Parkinson's Disease Rating Scale (UPDRS) score. The dataset contains 1040 recordings of 20 healthy and 20 afflicted people. Each recording has 26 numerical input features [10, 16].
- Student Performance (Student): This dataset relates students of two Portuguese schools to their final year grade on a scale from 0 to 20. It contains information about 395 students with a mean grade of 10.42. Each observation has 30 categorical and numerical features [5, 10].

Chapter 4

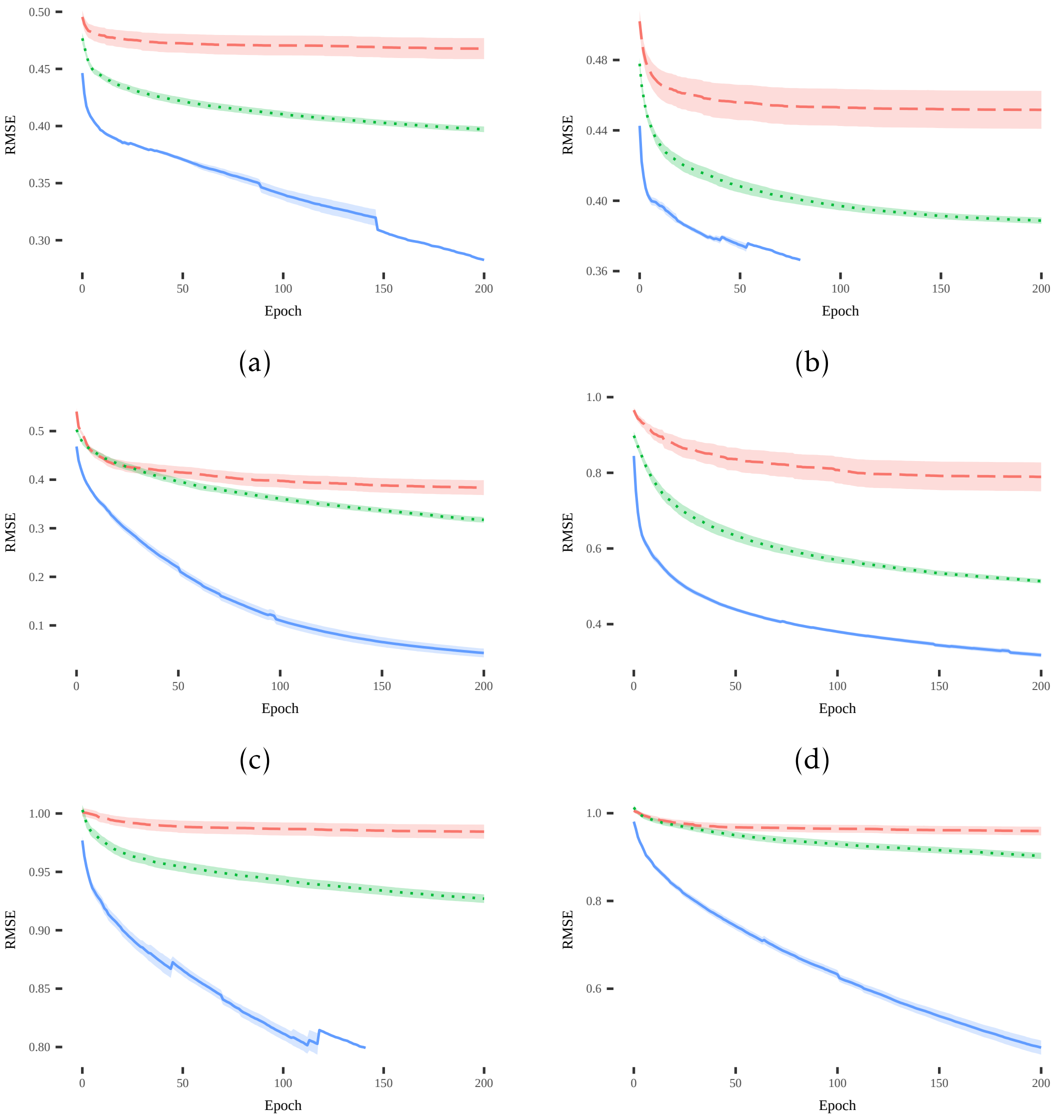
EXPERIMENTAL STUDY

This chapter presents the results obtained in the experimental phase by applying SLM and the other aforementioned ML techniques. Considering the large experimental campaign performed, we decided to present all the results on unseen data, while we limit the discussion about training performance to a few representative examples. Finally, we comment on the execution time of the SLM and we compare the resulting solutions with respect to the one obtained by NEAT, focusing on their number of nodes.

4.1 Results

The discussion starts by analyzing the plots reported from Figure 4.1(a) to Figure 4.1(f). Each plot displays the mean and standard error of the best training error (i.e., the fitness on known instances). Considering the training fitness, SLM shows the same evolution of fitness in all the considered datasets and it is the best performer among the other competitors. In some plots, like (a) and (f), the SLM produces fitness values that are not only better than the ones achieved by NEAT and SGA but it seems that fitness could improve further, if more epochs were considered. Furthermore, SGA outperforms NEAT on all displayed plots.

While results on the training set are important to understand the ability of the SLM to learn the model of the training data, it is even more important and interesting to evaluate its performance on unseen instances. Considering the plots reported from Figure 4.2(a) to Figure 4.2(f), one can see that the SLM produces good quality solutions that are able to generalize over unseen instances. In particular, the SLM presents a desirable behavior in the vast majority of problems, showing better or comparable performance with respect to the other competitors without overfitting the training data. Focusing on the other techniques, NEAT is the worst performer in 4 out of 6 datasets,



(a)

(b)

(c)

(d)

(e)

(f)

Figure 4.1: Evolution of mean and standard error of the best fitness on the training sets for the following datasets: (a) Credit; (b) Diabetes; (c) Sonar; (d) Concrete; (e) Parkinson; (f) Music. The legend for all the plots is: – – NEAT — SLM · · · SGA

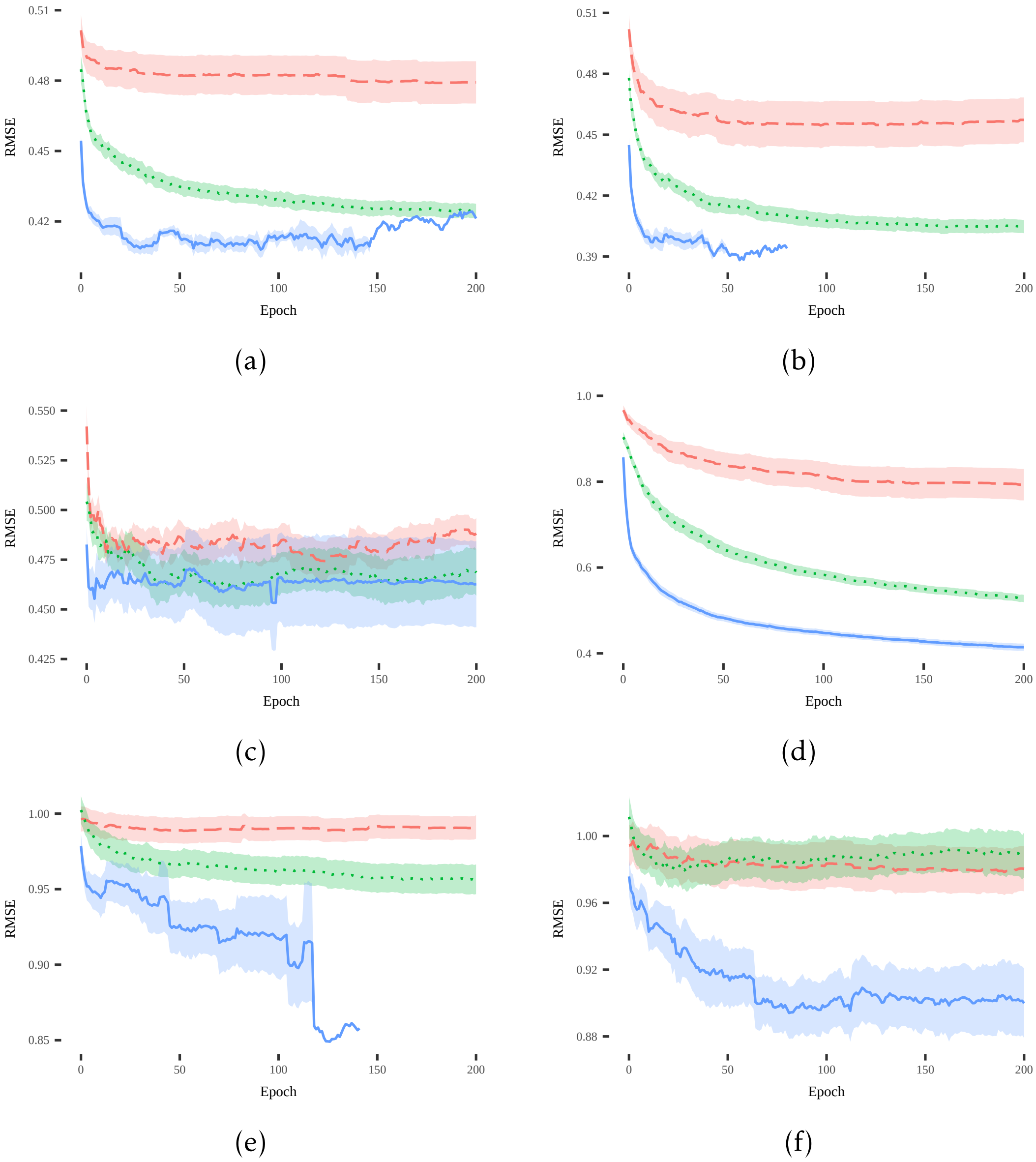
Table 4.1: Mean values for number of hidden neurons and processing time for NEAT, SGA and SLM on the Credit, Diabetes, Sonar, Concrete, Music and Parkinson dataset.

Hidden Neurons			
	NEAT	SGA	SLM
Credit	3.23	5.6	29.83
Diabetes	3.97	5.47	19.2
Sonar	5.97	6.77	168.07
Concrete	4.33	6.1	329.67
Music	3.5	5.37	99.13
Parkinson	4.63	6.43	37.7
Processing time (s)			
	NEAT	SGA	SLM
Credit	289.17	147.86	1.94
Diabetes	206.4	80.83	0.94
Sonar	118.18	278.71	8.39
Concrete	267.6	94.23	21.15
Music	668.94	435.53	10.87
Parkinson	493.62	253.2	4.09

while it achieves comparable performance with respect to the SGA in the remaining datasets. Also, plots (b) and (e) make apparent how SLM takes advantage of the EDV stopping criterion and terminates the evolutionary process before overfitting occurs. To summarize the results of this first part of the experimental phase, it is possible to state that the SLM is able to outperform SGA and NEAT with respect to the training fitness, by also producing models able to generalize over unseen instances. This is a very promising result that we are going to discuss more in the remaining part of the paper.

To that end, we reported in Figure 4.3 the results of SLM and other well-known machine learning techniques that are commonly used to solve classification and regression problems. Starting the discussion, it is possible to observe that the SLM tends to produce competitive generalization errors in all the considered datasets. Regarding MLP and SVM, the SLM obtained better results for (a) and (b), while producing comparable solutions for the remaining problems. Comparing with SGA, SLM performs better on (a) and (d), with comparable results on the remaining datasets. Most importantly, SLM is able to outperform NEAT on all the displayed datasets. Finally, by analyzing Table 4.1, it is possible to compare the number of nodes of the models obtained with the SLM , with NEAT, and SGA as well as the running time of these techniques. Although SLM produces the most complex (with the most hidden neurons) solutions, these solutions can be generated in a negligible amount of time. Compared to NEAT and SGA, SLM can develop solutions between one and two orders of magnitude faster (e.g. results on Credit).

All in all, at the end of the experimental campaign, it is possible to state that the SLM is a neuroevolution algorithm that is competitive with state of the art methods for

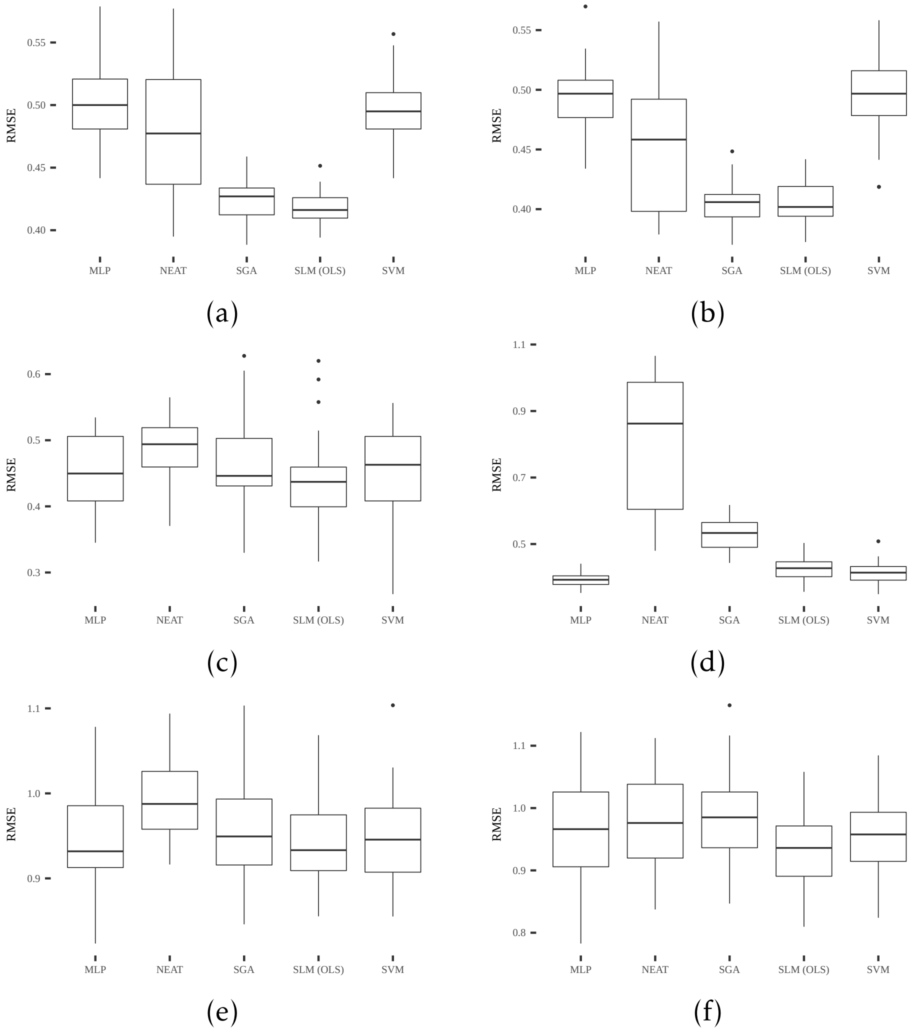


(a) (b)

(c) (d)

(e) (f)

Figure 4.2: Evolution of mean and standard error of the best fitness on the testing sets for the following datasets: (a) Credit; (b) Diabetes; (c) Sonar; (d) Concrete; (e) Parkinson; (f) Music. The legend for all the plots is: – – NEAT —— SLM · · · SGA



(a) (b) (c) (d) (e) (f)

Figure 4.3: Boxplots of generalization error for the following datasets: (a) Credit; (b) Diabetes; (c) Sonar; (d) Concrete; (e) Parkinson; (f) Music. On each box, the central mark is the median, the edges of the box are the 25^{th} and 75^{th} percentiles, and the whiskers extend to the most extreme data points, excluding outliers.

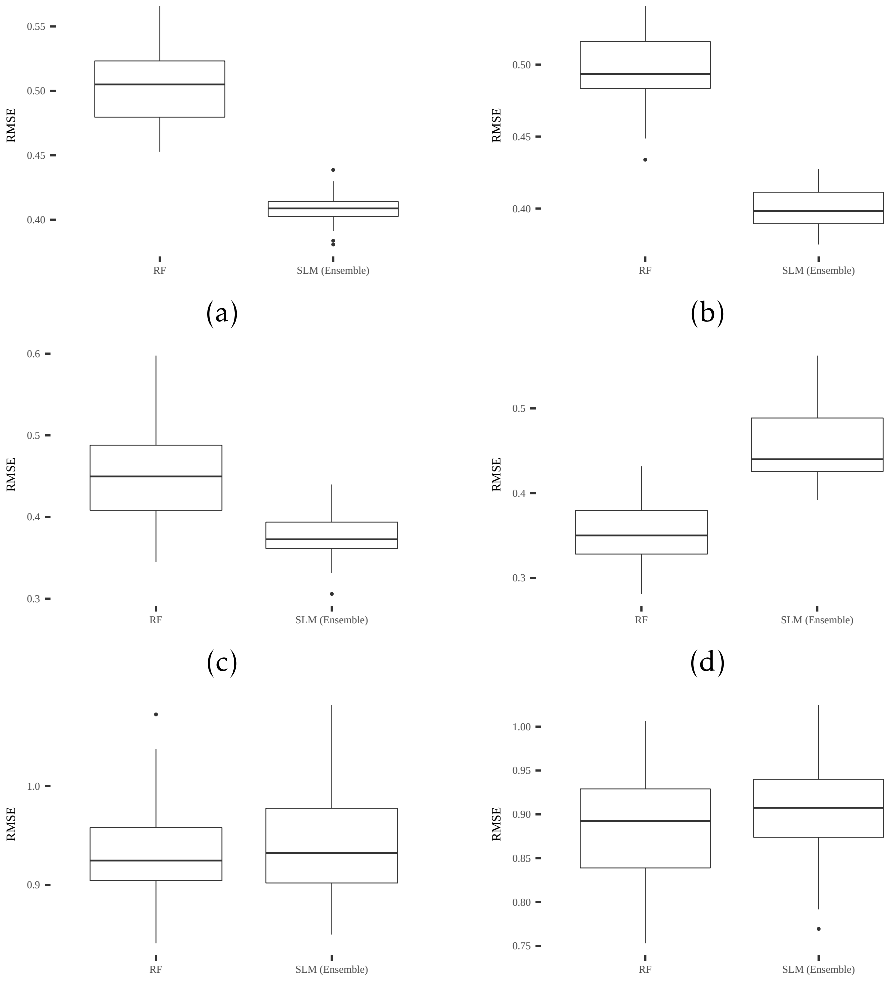
regression and classification problems and, built in a negligible amount of time and able to generalize over unseen instances. These features pave the way for future work in the area at the intersection between neuroevolution and deep learning, with the possibility of evolving the structure of deep networks in a tolerable amount of time. To assess the statistical significance of the results presented in Figure 4.3, a statistical validation was performed. The statistical validation considers, for each dataset, the SLM and compares it with the other techniques. First of all, given that is not possible to assume a normal distribution of the values obtained by running the different techniques, we ran the Shapiro-Wilk test and we considered a value of $\alpha = 0.05$. The null hypothesis of this test is that the values are normally distributed. The result of the test suggests that the alternative hypothesis cannot be rejected. Hence, the Mann-Whitney U test with paired samples is conducted for comparing the results returned by the SLM and the other considered algorithms under the null hypothesis that the SLM's median value is greater or equal to the competitive algorithm's median value, across repeated measures. Also in this test a value of $\alpha = 0.05$ was used and the Bonferroni correction was considered. Table 4.2 reports the p-values returned by the Mann-Whitney test, and **bold** is used to denote values suggesting that the alternative hypotheses cannot be rejected. According to these results, out of 10 problems, the best SLM variant outperforms (1) MLP in 2 problems; (2) NEAT in 6 problems; (3) SGA in 4 problems; (4) SVM in 3 problems. On the Credit dataset, SLM can outperform all competitors with statistical significance. In the remaining comparisons, there was no evidence of statistically significant difference between the SLM and the other competitors.

Table 4.2: P-values for Mann-Whitney U test between SLM and competitive algorithms, where the null hypothesis states that the SLM's median unseen error is greater or equal to the competitive algorithm's median unseen error.

	MLP	NEAT	SGA	SVM
Credit	**9.13E-07**	**4.89E-06**	**4.58E-02**	**9.13E-07**
Diabetes	**9.13E-07**	**6.52E-05**	7.64E-01	**9.13E-07**
Sonar	2.49E-01	**1.02E-03**	7.50E-02	3.11E-01
Concrete	1.00E+00	**9.13E-07**	**9.13E-07**	9.02E-01
Music	6.93E-02	**1.02E-03**	**5.07E-05**	**3.36E-02**
Parkinson	1.77E-01	**1.24E-06**	**4.31E-04**	1.01E-01

4.2 Ensemble Approach

The promising results obtained at the end of the experimental phase, both in terms of performance, running time and number of neurons, led us to consider a new comparison. In particular, we want to compare results achieved by considering an ensemble of SLM against the ones obtained with Random Forests (RFs) [3]. To perform this analysis, ensembles of 25 SLM models and tree predictors (for RFs) were built. The comparison was performed considering the same datasets under study as introduced in Section **??**. Figure 4.4 reports the generalization error for the 6 considered datasets. As one can see, the SLM ensemble outperforms the RFs ensemble on (a), (b) and (c), while generating comparable results in (e) and (f). These excellent results are also strengthened by the fact that the SLM ensemble model is formed by weak SLM learners that contain only a few nodes (as already discussed in the previous analysis). To statistically validate the results of this comparison the same aforementioned statistical procedure was used. The following p-values were obtained: $9.13e^{-07}$ for (a), $9.13e^{-07}$ for (b), $2.25e^{-06}$ for (c), $1.00e^{0}$ for (d), $5.25e^{-01}$ for(e) and $9.36e^{-01}$ for (f).



(a) (b)

(c) (d)

(e) (f)

Figure 4.4: Boxplots of generalization error for the following datasets: (a) Credit; (b) Diabetes; (c) Sonar; (d) Concrete; (e) Parkinson; (f) Music. On each box, the central mark is the median, the edges of the box are the 25^{th} and 75^{th} percentiles, and the whiskers extend to the most extreme data points, excluding outliers.

CHAPTER 5

CONCLUSION

This paper studied different variants of the SLM algorithm, a recently proposed neuroevolution method. Comparisons were performed against other neuroevolution methods and other well-established supervised machine learning methods. It is shown that the best SLM variants are able to outperform most of remaining methods on the majority of the 6 real-world datasets considered. Particularly interesting are the results of the SLM variation that computes the optimal mutation step for each application of the mutation operator, and that, at the same time, uses a recently proposed semantic stopping criterion to determine when to stop the search. This variant is able to evolve competitive neural networks in a few seconds on the vast majority of the datasets. An initial assessment of the usage of this SLM variant to create ensembles of neural network is also performed. This initial assessment shows that this approach is able to outperform the random forests algorithm on three out of six selected datasets.

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Appendix A

PARAMETER CONFIGURATIONS

Table A.1: First set of NEAT parameter. Parameter names and values are taken from [13]. [] defines the beginning of a configuration section, {} defines a tunable parameter from Section 3.1.

Parameter	Value
fitness_criterion	mean
fitness_threshold	10
no_fitness_termination	True
pop_size	{population_size}
reset_on_extinction	True
[DefaultSpeciesSet]	
compatibility_threshold	{compatibility_threshold}
[DefaultStagnation]	
species_fitness_func	mean
max_stagnation	15
species_elitism	1
[DefaultReproduction]	
elitism	1
survival_threshold	0.2
min_species_size	1
[DefaultGenome]	
activation_default	random
activation_mutate_rate	0.01
activation_options	sigmoid identity relu tanh
aggregation_default	sum
aggregation_mutate_rate	0
aggregation_options	sum
bias_init_mean	0
bias_init_stdev	1
bias_init_type	gaussian
bias_max_value	30
bias_min_value	-30
bias_mutate_power	0.1
bias_mutate_rate	0.01
bias_replace_rate	0.01
compatibility_disjoint_coefficient	{compatibility_disjoint_coefficient}
compatibility_weight_coefficient	{compatibility_weight_coefficient}

Table A.2: Second set of NEAT parameter. Parameter names and values are taken from [13]. [] defines the beginning of a configuration section, {} defines a tunable parameter from Section 3.1.

Parameter	Value
conn_add_prob	{conn_add_prob}
conn_delete_prob	{conn_delete_prob}
enabled_default	True
enabled_mutate_rate	0.01
enabled_rate_to_false_add	0
enabled_rate_to_true_add	0
feed_forward	True
initial_connection	partial_nodirect 0.25
node_add_prob	{node_add_prob}
node_delete_prob	{node_delete_prob}
num_hidden	1
num_inputs	{num_inputs}
num_outputs	1
response_init_mean	1
response_init_stdev	0
response_init_type	gaussian
response_max_value	30
response_min_value	-30
response_mutate_power	0
response_mutate_rate	0
response_replace_rate	0
single_structural_mutation	False
structural_mutation_surer	True
weight_init_mean	0
weight_init_stdev	1
weight_init_type	gaussian
weight_max_value	30
weight_min_value	-30
weight_mutate_power	{weight_mutate_power}
weight_mutate_rate	{weight_mutate_rate}
weight_replace_rate	0.1

Table A.3: Parameter configuration search grid for Multilayer Perceptron. Parameter names according to [14].

Parameter	Start (inclusive)	End (inclusive)	Step size (multiplicative)
alpha	10^{-6}	10^{-1}	10
learning_rate_init	10^{-6}	10^{-1}	10
hidden_layer_sizes	[(1), (2), (2, 2), (3, 3, 3), (5, 5, 5), (2, 2, 2, 2)]		
activation	['identity', 'logistic', 'tanh', 'relu']		

Table A.4: Parameter configuration search grid for Support Vector Machine. Parameter names according to [14].

Parameter	Start (inclusive)	End (inclusive)	Step size (additive)
C	0.1	1	0.1
epsilon	0.1	0.5	0.1
degree	1	4	1
gamma	0.1	0.5	0.1
coef0	0.1	0.5	0.1
kernel	[’linear’, ’poly’, ’rbf’, ’sigmoid’]		
probability	TRUE