AutoGE: A Tool for Estimation of Grammatical Evolution Models

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Abstract: AutoGE (Automatic Grammatical Evolution), a new tool for the estimation of Grammatical Evolution (GE) parameters, is designed to aid users of GE. The tool comprises a rich suite of algorithms to assist in fine tuning BNF grammar to make it adaptable across a wide range of problems. It primarily facilitates the identification of optimal grammar structures, the choice of function sets to achieve improved or existing fitness at a lower computational overhead over the existing GE setups. This research work discusses and reports initial results with one of the key algorithms in AutoGE, Production Rule Pruning, which employs a simple frequency-based approach for identifying less worthy productions. It captures the relationship between production rules and function sets involved in the problem domain to identify optimal grammar structures. Preliminary studies on a set of fourteen standard Genetic Programming benchmark problems in the symbolic regression domain show that the algorithm removes less useful terminals and production rules resulting in individuals with shorter genome lengths. The results depict that the proposed algorithm identifies the optimal grammar structure for the symbolic regression problem domain to be arity-based grammar. It also establishes that the proposed algorithm results in enhanced fitness for some of the benchmark problems.

1 INTRODUCTION

Grammatical Evolution (GE), since its inception twenty years back, has found wide acceptance in the research communities (Ryan et al 2018). It is a bioinspired population-based methodology from the domain of evolutionary. Its ability to produce arbitrary valid data structures and the way executable programs can be evolved has created wide-scale appeal. Moreover, due to its simple approach of evolving programs constrained through the definition of BNF grammar and the ability to adapt to domain knowledge through it makes it a valuable tool.

GE uses an innovative mapping scheme in which variable-length input genomes (also known as chromosomes or genotype) are represented in binary form and get mapped to the output program or phenotype. The values in the genotype control the choice of production rules and the resulting phenotype then gets evaluated based on the definition of fitness functions that gives a fitness score to the individuals in the population.

Although the selection and definition of fitness criteria is dependent on the problem and/or the problem domain, there exists a good body of knowledge which serves as guidelines (Koza 1993). This, however, is not the case when a user is faced with the problem of choosing a function set and defining a grammar. There is little guidance in the literature and no systematic approach exists (Wang 2005, Uy 2013).

Automatic Grammatical Evolution (AutoGE) is an initiative to create a tool that can aid users to define and identify proper grammar structures to smoothly adapt to the application under consideration. Its suite of algorithms will enable GE users to design appropriate BNF rules using the right grammar structures. This will mainly help the users in identifying appropriate terminals involved in forming production rules. The algorithm will also facilitate the selection of correct fitness function definition. Fitness functions can be composed of single, multiple or...
many objectives. They can be hierarchical in nature. As such AutoGE will serve to automate the selection of grammar structure, function sets and fitness functions depending on the nature of the underlying problem and its complexity. AutoGE’s suite of algorithms are designed in a manner to automatically assist in evolving individuals of shorter lengths thereby optimizing memory usage (Kshirsagar 2020). AutoGE’s rich suite of powerful algorithms also automatically address bloats (Bleuler 2008) through restricting tree size and tree nodes thereby reducing computational overhead and complexity (Murphy 2020).

2 BACKGROUND

2.1 Grammatical Evolution (GE)

Grammatical Evolution is a variant of Genetic Programming (GP) in which the space of possible solutions is specified through a grammar (Ryan 1998). Although different types of grammars have been used, the most commonly used is Context Free Grammar (CFG), generally written in Backus-Naur Form (BNF). GE facilitates a modular design, which means that any search engine can be used, although typically a variable-length Genetic Algorithm (GA) is employed to evolve a population of binary strings.

In GE, each population individual has a dual representation, a genotype and a phenotype. When the underlying search engine is a genetic algorithm, the genotype is a sequence of codons (a group of 8-bit substrings), while the phenotype expresses an individual’s representation in the solution space. Mapping, a key process in GE, maps a given genotype to the phenotype. While subsequently consuming each codon, it selects a production from the available set of alternative productions in a rule and builds the derivation tree. Although there are other mapping schemes (Fagan 2018), the conventional scheme follows left-most derivation.

An important measure in the mapping process is the effective genome length, which is equal to the number of codons consumed to generate a fully mapped individual (the one which does not contain any non-terminals in this phenotype). The actual genome length is the total number of codons in the genome, some of which may remain unused.

2.2 Grammar Design in GE

Since GE exploits the expressive power of grammars, it can be applied to a multitude of problem domains, for instance in Symbolic Regression (SR) where the purpose is to search the space of mathematical expressions to find a model that best fits a given dataset (Koza 1993). To construct valid and useful mathematical expressions in GE, the grammar needs to be well designed.

A grammar is formally defined as the tuple \((T, N, P, S)\) where \(T\) is a set of terminal symbols, \(N\) is a set of non-terminal symbols, \(P\) is a set of production rules, and \(S\) is the start symbol. While the set of terminals outline the building blocks of a solution, the choice of non-terminals and deciding how exactly to organize those into a set of rules and productions is a design task. By designing an appropriate grammar, one specifies the syntactic space of possible solutions.

2.2.1 Grammar Structures

Instead of designing grammar from scratch, a common approach is to utilize and adapt existing grammar designs for that domain. For example, in grammatical evolution based symbolic regression (GESR), typical grammar structures are shown in Table 1. In a mixed-arity grammar, operations of multiple arities are combined in a single rule. A contrasting design is that of arity-based grammars where productions relevant to arity-1 and arity-2 operations are grouped in separate rules. A balanced grammar version balances the probabilities of selecting recursive (non-terminating) productions and terminating production (Nicolau 2018).

It is important to note how operators and functions are represented as productions in the grammar. Besides embodying arithmetic operators, a number of common mathematical functions are represented as alternative recursive productions.

<table>
<thead>
<tr>
<th>Mixed-arity Grammar</th>
<th>Arity-based Grammar</th>
<th>Balanced Arity-based Grammar</th>
</tr>
</thead>
<tbody>
<tr>
<td>(&lt;expr&gt; ::= &lt;expr&gt;&lt;op&gt;&lt;expr&gt;))</td>
<td>(&lt;expr1::=\sin&lt;expr&gt;</td>
<td>\cos&lt;expr&gt;))</td>
</tr>
<tr>
<td>(\sin&lt;expr&gt;</td>
<td>\cos&lt;expr&gt;))</td>
<td>(\exp&lt;expr&gt;</td>
</tr>
<tr>
<td>(\exp&lt;expr&gt;</td>
<td>\pow&lt;expr&gt;,2))</td>
<td>(\sqrt&lt;expr&gt;</td>
</tr>
<tr>
<td>(\sqrt&lt;expr&gt;</td>
<td>\sqrt&lt;expr&gt;))</td>
<td>(&lt;var&gt; ::= X</td>
</tr>
<tr>
<td>(&lt;var&gt; ::= X</td>
<td>Y)</td>
<td>(&lt;var&gt; ::= X</td>
</tr>
</tbody>
</table>

# The rest is the same as arity-based
3 METHODOLOGY

We discuss our approach to rank grammar productions and subsequently pruning of unworthy productions in this section. Figure 1 depicts the overall schematic of our approach.

3.1 Production Ranking

With the correct configuration and fitness criteria, an evolutionary process is geared towards convergence. Increasingly, the evolved solutions contain more and more of the right ingredients or building blocks (in our case, grammar productions). We hypothesize that the structural composition of evolved solutions carries information that can be useful in identifying the right ingredients.

In GE, every individual in the population is composed of terminals which appear in an order defined by the derivation tree constructed during genotype to phenotype mapping. By traversing the derivation tree, it is possible to obtain a list of grammar productions used in the mapping process to generate an individual. Such a list is termed as the production-list. Once identified, the frequency of usage of each production in the production-list can be easily determined.

Productions can be weighed or ranked based on how frequently they are used in the construction of individuals in the population. As evolution proceeds, fitter individuals survive, and the productions which more frequently shape the structures are the ones that are considered to be worthy being part of the grammar. Such productions are assigned a high rank. On the contrary, productions which harm individual’s fitness such that they become extinct, generally do not enjoy high usage frequency (although rarely zero, due to hitch-hiking effects) in the population.

To test our hypothesis, we devised a simple frequency-based approach to rank productions. Since frequency counting is a trivial and efficient operation, it carries minimal overhead. The two basic production ranking schemes are:

Normalized Frequency-based Ranking (NFR): This is the simplest ranking scheme where frequencies of the productions in production-list are normalized to unity. We compute ranking scores offline, at the end of each evolutionary cycle (see Figure 1), which bears minimal overhead. Note that this does not take the fitness of individuals into consideration, rather simply the survival of production rules.

Fitness Proportionate Ranking (FPR): In this scheme, the normalized ranks are multiplied with the individual’s fitness.

An important consideration is to decide how much of the population to select for ranking. We experimented with three possible choices: 1) the whole population, 2) all unique individuals, 3) top X% of the population (we use X=20, a completely arbitrary number that seemed reasonable). Potential issues include, with the 1st option, rankings can be biased due to repeated individuals, and with the 3rd option there was a chance of pruning important productions. The second option turned out to be the best choice based on our empirical evaluations.

Once individual ranking scores have been computed, we accumulate the scores to compute run worth of a production. Figure 2 shows a sample box and whisker plot of FPR ranking for Page-1 problem. It exposes a nice picture of the utility of each production in the evolutionary cycle.

3.2 Grammar Pruning

We follow the principle of Occam’s razor which states “no more things should be presumed to exist than are absolutely necessary.” Grammar is a key model of the solution space, so the idea is to remove unnecessary or less worthy productions (or functions) from the grammar to tune the grammar design.

The key driver in grammar tuning is the pruning strategy and the algorithm. There can be a number of strategies for pruning and we look at two here. The key concept they have in common is a staged approach; that is, a small number of runs is conducted, then one or more rules are pruned, and...
then more runs are conducted. This second stage (also true for third and subsequent stages, if they exist) is a complete restart with the newly modified grammar.

The exact algorithm depends on the strategy being employed. We experimented with the following two strategies:

- **Strategy 1:** Prune for the maximum available budget. The remaining runs will verify if it was fruitful.
- **Strategy 2:** Only proceed with pruning if it results in improving mean training score at each stage. If it degrades performance, stop.

Strategy 1 has slightly less overhead but suffers from blind pruning which in many cases failed to reap any benefits. For instance, in case of Keijzer-6 problem, this strategy pruned the production carrying logarithm function, which is a vital approximating function for this problem.

Strategy 2 incorporates a feedback loop which informs on its usefulness. In our preliminary experiments, we have observed it to be yielding a much better overall outcome. Coupled with the pruning policies defined in section 4.3, our Production Rule Pruning algorithm achieved excellent results.

### 3.2.1 Production Rule Pruning Algorithm

The outlines the Production Rule Pruning (PRP) algorithm is shown in Listing 1:

```
procedure PRP():
    Prunings = Empty
    Stage = 0; AvailableBudget = 20%; PruningGen = 5
    Do full runs for PruningGen generations
    Set the training performance score $E_{trg}(0)$ and PRUNE
    While there is AvailableBudget:
        Proceed to pruning stage $i$
        Do full runs for PruningGen generations and get $E_{trg}(i)$
        If $E_{trg}(i) < E_{trg}(i-1)$: PRUNE
        If $E_{trg}(i) > E_{trg}(i-1)$: REVERT
        Decrement AvailableBudget
    PRUNE
```

**PRUNE** is the key procedure in the algorithm. It performs two important functions:

1) It analyses production ranking scores and identifies the least worthy productions. Based on the pruning policy, it identifies how many productions to prune at a given stage and returns that many productions as candidates to be pruned.

2) It removes productions from the grammar and adds them to **Prunings**, which is implemented as a stack. At each stage, pruned productions are pushed to the stack.

The **REVERT** function undoes the last pruning action by popping the last productions from **Prunings** and adding them back to the grammar. When a pruning stage reverts, the **PruningGen** is incremented from 5 to 10.

### 3.2.2 Consistency of Pruning Suggestions

The output of the PRP algorithm is pruning suggestions. In order to verify how consistent the pruning suggestions are, we ran 100 experiments on certain problems for each grammar structure and ranking scheme. Each experiment consisted of 50 independent runs evolving for 5 generations with a population size of 250. Due to space limitations, Table 2 only shows the count of experiments for which the given productions were the first, second, and third pruning suggestions for mixed-arity grammar and FPR ranking scheme.

### 4 EXPERIMENTAL SETUP

#### 4.1 Problems and Function Set

A collection of symbolic regression benchmark problems was listed in (McDermott 2012). We utilized a subset of those problems ranging from simple to more challenging ones. Among the chosen problems, there is a high variance in terms of problem difficulty, number of variables, and the sample size...
for training and test data. Table 3 lists the problems considered in this work and the original function sets. For details on the mathematical expression, training and test ranges, please refer to (McDermott 2012).

Table 2: Experimental results to assess the consistency of pruning suggestions in case of FPR ranking.

<table>
<thead>
<tr>
<th>Problem</th>
<th>Production</th>
<th>Pruning Suggestions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vlad-2</td>
<td>tan(expr)</td>
<td>99</td>
</tr>
<tr>
<td></td>
<td>log(abs(expr))</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>pow(expr^2)</td>
<td>-16</td>
</tr>
<tr>
<td>Pagie-1</td>
<td>sinh(expr)</td>
<td>99</td>
</tr>
<tr>
<td></td>
<td>log(abs(expr))</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>(-1*(expr))</td>
<td>-7</td>
</tr>
<tr>
<td>Keijzer-6</td>
<td>t(-1*(expr))</td>
<td>98</td>
</tr>
<tr>
<td></td>
<td>log(abs(expr))</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>pow(expr^2)</td>
<td>-22</td>
</tr>
<tr>
<td>Nguyen-7</td>
<td>log(abs(expr))</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>tan(expr)</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>pow(expr^2)</td>
<td>-66</td>
</tr>
</tbody>
</table>

4.1.1 Original Function Set

The function set proposed for each benchmark problem, as shown in Table 3, is referred to as Original Function Set. Note that the grammar which embodies the original function set is termed Original Grammar in this work, referenced with the letter ‘O’ in Table 4 and 5.

Choosing an appropriate function set is a key decision in applying GP as it can have a vital impact on the performance of GP (Wang 2005). However, there is not enough guidance in selecting a function set. To date, it is largely considered a decision made by domain experts. A new user trying to apply evolutionary search faces a challenge with no clear guidelines.

4.1.2 Extended Function Set

A few recent studies (e.g. Nicolau 2020) suggested that using an extended function set (even with functions that appear to be useless for a particular problem) can improve performance. Our own exploratory experiments confirm this, so we create an Extended Function Set (shown below):

\[ + \ - \ * \ / \ \sin \ \cos \ \tan \ \sinh \ \cosh \ \tanh \ e^x \ e^{-x} \ x^2 \ x^3 \ x^{-1} \ \ln(|x|) \ \forall x \ 1/x \]

It is the superset of all the original function sets. It includes arithmetic operators and all common trigonometric functions, exponentials, and power functions. Note that we do not use protected division (Keijzer 2003). The grammar which embodies the extended function set is termed Extended Grammar in this work and is referenced with the letter ‘E’ in Table 4 and 5.

Table 3: Original function sets defined with benchmarks.

<table>
<thead>
<tr>
<th>Problem</th>
<th>Original Function Set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Koza-1</td>
<td>+ - / sin cos e^x ln</td>
</tr>
<tr>
<td>Koza-2</td>
<td>+ - * / sin cos e^x</td>
</tr>
<tr>
<td>Koza-3</td>
<td>+ - * / cos e^x</td>
</tr>
<tr>
<td>Pagie-1</td>
<td>+ - * / x^2 e^x</td>
</tr>
<tr>
<td>Nguyen-7</td>
<td>+ - * / x^2 e^x sin cos</td>
</tr>
<tr>
<td>Keijzer-6</td>
<td>+ - * / x^2</td>
</tr>
</tbody>
</table>

4.2 Parameters & Fitness Function

Following evolutionary parameters were used in all experiments in this work:

- Population Size: 250
- Number of Generations: 100
- Crossover Type: One-point Crossover
- Crossover Probability: 0.9
- Mutation Probability: 0.01
- Selection Type: Tournament
- Initialization Method: Sensible Initialization
- Maximum Depth: 10
- Number of Runs: 30

The objective of the fitness function is to measure the performance of the algorithm against a predefined objective goal. The fitness of every individual is measured using Root Mean Squared Error (RMSE) against an acceptable threshold. As it is a negatively aligned metric, it is defined to minimise the fitness function. The lower the RMSE, the better the value of objective function.

4.3 Pruning Policies

For the problems we examined, the usage frequency of arithmetic operators, variables, and constant terminals was low, irrespective of the grammar structure. We therefore do not consider their corresponding productions, and the productions where the right-hand side is only composed of non-terminals (for example productions in the start rule of arity-based grammar in Table 1). This resulted in 14 prunable productions which primarily consist of extended function set excluding arithmetic operators. It is important to highlight a few other policies adopted while pruning which serve as parameters to the PRP algorithm:
We do not consume more than 20% of the computational budget on pruning. In our case, it meant consuming at most 20 generations.

Pruning takes place in stages. At a stage, prune only 10% of the productions.

In pruning runs, we evolve for 5 generations to maximize pruning. If 5 generation runs terminate with a REVERT decision and the pruning budget is remaining, we proceed with 10 generations.

Note that the grammar which results after pruning is termed **Pruned Grammar** in this work and is referenced with the letter ‘P’ in Table 4 and 5.

5 RESULTS

A summarized view of results from all 42 (14 x 3) experiments is presented in Table 4 and 5. They show the impact of using various grammar structures alongside extended functions set and pruning approach on performance (both in approximation and generalization) and mean effective genome length for the best solution as well as the whole population.

5.1 Statistical Test

We applied statistical test to validate our results and claims. Student's t-test for statistical significance with the p-value of 0.05 was used. The outcome of the significance test is also encoded in Table 4 and 5. The symbol ‘+’ indicates significant improvement, while ‘-’ is for improvement which is not statistically significant. Results from the original grammar are treated as baseline. ‘O-’ indicates that though original grammar had the best output, it was not significantly better than the extended grammar. With ‘E -’ or ‘P -’, the results are only slightly better than original grammar.

5.2 Impact of Extended Grammar

In general, for most of the problems and for all three grammar structures, using the extended grammar (representing the extended function set) significantly improved performance as well as genome size when compared with the original grammar. This observation is consistent with the outcome noted by (Nicolau 2020). Although the problem set we experimented with is limited, considering the diversity in the problem complexity and non-linearity (Vladislavleva 2009) which makes it a representative sample, we can suggest utilizing our extended function set for synthetic symbolic regression problems.

Koza highlighted that if a function set is not adequate, GP cannot find (good) solutions, but on the other hand, if a function set includes many extraneous functions, the performance is degraded (Koza 1993). Our results are contrary to this later recommendation. Besides, extending or adding more productions to the grammar adds additional dimensions to the search space, which may result in bigger individuals and lower performance. However, this is usually not the case. Finding exactly why warrants an in-depth analysis. Here we believe that production ranking can expose some clues.

5.3 Effect of Grammar Structures

It is evident that some grammar structures are more appropriate for certain types of improvement or for certain problems. Overall, arity-base grammar structure results in significant reduction in genome length, except for vlad-6 where size reductions are not
significant both for best-of-run individuals and the mean effective size in the population.

To our knowledge, many symbolic regression studies using GE or Grammar Guided Genetic Programming (GGGP) use mixed-arity grammar structure, for instance (Nicoul 2015). Even though, for many problems, the genome lengths are shortest in case of mixed-arity grammar and the reductions are also significant in several cases, the corresponding performance gains are lower as compared to simple or balanced arity-based grammars. In general, balanced arity-based grammar produced best performing individuals as compared to other structures.

### 5.4 Effect of Pruning

Pruning was applied in all 42 experiments. The number of productions pruned varied from 1 to 6, out of 14 prunable productions. Pruning achieved significantly shorter effective lengths when looking at the whole population for 6 different problems with mixed arity grammar. However, with arity-based grammar, 9 out of 14 get improvements.

Regarding performance, pruning achieves better results in only 1 problem (Keijzer-6) with mixed-arity, and 4 problems with (balanced) arity-based grammar. However, it is worth noting that in order to keep the same computational budget, trials with the pruned grammar lasted for 80 in some cases 85 generations. Had the pruned grammar also exercised for 100 generations, it is likely that it would have achieved better performance.

Figure 3 shows two sample convergence plots (for Keijzer-6 and Vladislavleva-6 problems) where grammar pruning effectively improved approximation performance when compared with original and extended grammars. The four spikes in the plot in case of pruned grammar depict that pruning runs were carried out in four stages (as explained in section 3.2) in the first 20 generations.

### 6 CONCLUSIONS

We propose a new algorithm as part of the AutoGE tool suite being developed. The proposed Production
Rule Pruning algorithm is an approach combining an extended function set and a frequency counting mechanism for ranking production rules. Together, with the choice of extended function set and pruning algorithm, AutoGE achieved significantly better genome length in 13 out of 14 problems, with the (balanced) arity-based grammar structure. Significant improvement in approximation performance for 13 problems and generalization performance for 8 out of 14 problems is observed with balanced arity-based grammar. We therefore conclude that arity-based grammar structure (simple or balanced), as opposed to commonly used mixed arity grammar, would yield better results not only in terms of shorter genome lengths but minimized errors for symbolic regression problems resulting in enhanced accuracy.

6.1 Future Work

An immediate extension to the current work is to trial symbolic problems with real-world data, and by exploring other problem domains for instance program synthesis, and Boolean logic. The PRP algorithm performance can be further enhanced by investigating other search mechanisms, for example particle swarm optimization or ant colony optimization. We aim to extend AutoGE’s suite of algorithms and to make it more robust by exploring approaches like grammar-based EDA.

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REFERENCES


