

Cluster Analysis of a Symbolic Regression Search Space

Gabriel Kronberger and Lukas Kammerer and Bogdan Burlacu and Stephan M. Winkler and Michael Kommenda and Michael Affenzeller

Abstract In this chapter we take a closer look at the distribution of symbolic regression models generated by genetic programming in the search space. The motivation for this work is to improve the search for well-fitting symbolic regression models by using information about the similarity of models that can be precomputed independently from the target function. For our analysis, we use a restricted grammar for uni-variate symbolic regression models and generate all possible models up to a fixed length limit. We identify unique models and cluster them based on phenotypic as well as genotypic similarity. We find that phenotypic similarity leads to well-defined clusters while genotypic similarity does not produce a clear clustering. By mapping solution candidates visited by GP to the enumerated search space we find that GP initially explores the whole search space and later converges to the subspace of highest quality expressions in a run for a simple benchmark problem.

Key words: symbolic regression, grammar enumeration, approximate nearest neighbors, dimensionality reduction, clustering

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1 Introduction

Knowledge discovery systems such as Genetic Programming (GP) for symbolic regression often have to deal with a very large search space of mathematical expressions, which only grows exponentially larger with the number of input variables.

Genetic programming guides the search via selection and discovers new model structures via the action of crossover and mutation. Population diversity plays an important role in this process, as it affects the algorithm's ability to assemble existing building blocks into increasingly-fit solutions. The relationship between diversity at both the genotypic and phenotypic level has been previously explored [1], leading to a number of important insights:

- Strong exploitation of structures occurs in almost all runs
- Diversity at the structural level is quickly lost
- Encouraging different amounts of diversity can lead to better performance
- The interplay between genetic operators induces a neighborhood structure in the search space
- Fitness is positively-correlated with fitness-based (phenotypic) diversity and negatively correlated with genotypic diversity

In light of the above, we set our goal to investigate GP's ability to explore different areas of the search space by superimposing a neighborhood structure obtained via clustering of symbolic regression models generated via grammar enumeration.

In this contribution we concentrate on the distribution of models in symbolic regression search spaces. Our motivation for this work is that we hope to be able to reduce the computational effort which is required to find well-fitting symbolic regression models by precomputing a clustering of all symbolic regression models in the search space. In particular, we aim to precompute a similarity network or (equivalently) a hierarchical clustering for symbolic regression models, that is independent from a concrete dataset.

Our research questions in this work are:

1. *What is the distribution of models in a symbolic regression search space?* We are interested in identifying clusters of similar models whereby similarity could either be determined based on the model outputs (phenotypic) or similarity of the evolved expressions (genotypic).
2. *What is the distribution of solutions visited by genetic programming?* Here we are interested in the systematic search biases of GP. In particular, (i) whether there are areas of the search space that are completely ignored by GP, and (ii) how the individuals in a GP population are distributed in the search space and how this distribution changes from the beginning to the end of a GP run.

Our assumptions about the goals of symbolic regression modeling are the following. We use these assumptions as a guide for our research in symbolic regression solution methods.

- The aim of symbolic regression modeling is primarily to find compact expressions that are open for interpretation.

- Shallow expressions are preferred over deeply nested expressions.
- Models for real-world regression problems are often made up of multiple terms which capture independent effects. The independent terms can be modeled one after another.
- Interesting real-world regression problems often necessitate to capture non-linear correlations in the model. A non-linear effect is often driven by only one independent variable.
- Interactions of two or three variables are common. Interactions of more than four variables are often not relevant.
- The set of potentially relevant variables is much larger than the set of actually relevant variables. It is usually not known which individual variables or which interactions of variables are relevant.
- Measurements of input variables as well as target variables are noisy.

2 Methodology

In our journey to find answers for the research questions stated above we enumerate the complete search space (see Section 2.1) and evaluate all expressions for fixed input data. To limit the size of the search space we consider only uni-variate functions and limit the maximum length of expressions. Additionally, we use a grammar which constrains the complexity of expressions and which does not allow numeric parameters (i.e. random constants). This further reduces the search space.

For the analysis of the distribution of expressions in the symbolic regression search space (*RQ1*), our idea is to create a visual map of all expressions which hopefully allows us to identify larger clusters of similar expressions. Thus, we use the set of all evaluated expressions, identify the set of phenotypically distinct expressions and determine the phenotypically nearest neighbors for each expression (see Section 2.3). This allows us to map expressions to a two-dimensional space while preserving the local neighborhood structure of the high-dimensional space. The graph of nearest neighbors also allows us to create a clustering of all expressions. As we are interested in both – the map of phenotypically similar expressions as well as the map of genotypically similar expressions – we create a similar map based on a measure for genotypic similarity (see Section 2.2). Ideally, we expect to see similar cluster structure on both levels, assuming that expressions that are genotypically similar should also be phenotypically similar and vice-versa¹.

For the analysis of the search bias of GP (*RQ2*), the idea is to re-use the map and clusters that we generated in the first phase and analyze whether GP explores the

¹ We actually found that this assumption is wrong. We found that the search space can be split into clusters of phenotypically and genotypically similar expressions. However, we could not show that phenotypically similar expressions also are phenotypically similar and/or vice versa. This is intuitive because two highly similar expressions become dissimilar on the phenotypic level just by a multiplication with zero. Symmetrically, many different expressions can be found which produce the same output.

complete map and all clusters. Our idea is to find the phenotypically most similar expression in the pre-calculated map for each solution candidate visited by GP. For this we determine the visitation frequency for the pre-computed clusters for each generation of GP. We expect that GP visits many different clusters in the beginning and converges to the clusters with well-fitting expressions at the end of the run.

Figure 1 shows an overview of the flow of information for search space visualization and clustering. Figure 2 shows how we map GP solution candidates to the pre-computed mapping of the search space and the clusters.

A major challenge in our methodological approach is the sheer size of the search space. We have handled this challenge using state-of-the-art algorithms for dimensionality reduction and clustering which still work for datasets with millions of observations and hundreds of features (see Section 2.4). The core idea of these algorithms is the approximation of nearest neighbors using random projection trees [3].

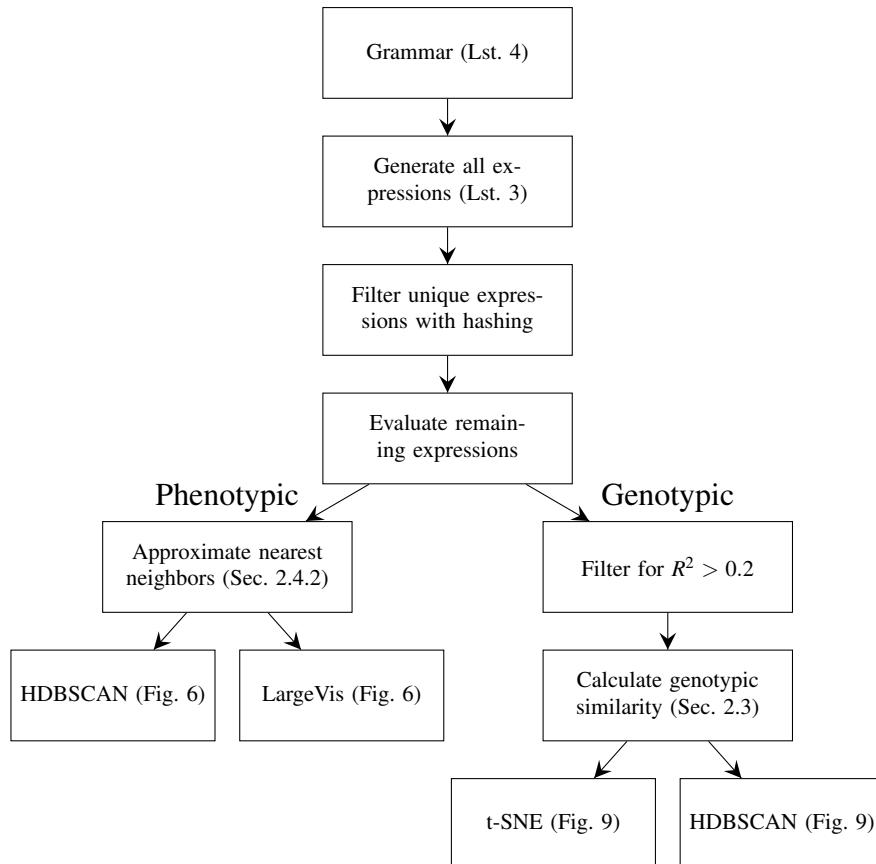


Fig. 1 Overview of the flow of information for the search space visualization and clustering (*RQ1*).

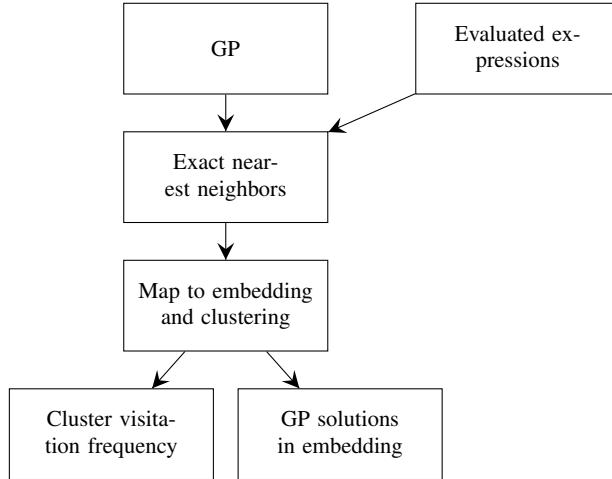


Fig. 2 Overview of the flow of information for tracking which parts of the search space are explored by GP (*RQ2*). GP solution candidates are mapped to the visualization and the clusters by finding the most similar representative.

2.1 Grammar Enumeration

We create symbolic regression models by deriving sentences from a formal grammar for expressions as shown in the listing in Figure 3. By defining a maximum sentence length and omitting numerical constants as a start, a large but finite set of all possible models – the search space – can be generated for a problem. These sentences without actual constants values can be seen as a general structure of an actual model ([5],[14]).

```

stack.push(start)

while stack not empty:
    phrase = stack.pop()
    symbol = Fetch nonterminal symbol from phrase
    for each production rule of symbol:
        create new phrase with substituted symbol

        if new phrase is a sentence:
            evaluate(new phrase)
            save(new phrase)
        else:
            stack.push(new phrase)
  
```

Fig. 3 Pseudo-code for generating all sentences of a language defined via a context-free grammar.

Given a formal grammar many mathematical identities and other phenotypically equal but genotypically different expressions are generated. This includes for example different orders of arguments in commutative operators or different representations of binomial identities. To keep the search space size manageable, we want to avoid semantic duplicates. Although it is computationally not feasible to fully prevent all semantic duplicates in such a large search space, their number can be largely reduced in two simple steps: First, the grammar is restricted, so that only one representation of relevant mathematical identities can be derived. Second, identities which cannot be prevented in the grammar are identified by hashing: semantic duplicates should have the same hash value.

Expressions derived from the restricted grammar (Figure 4) are sums of terms, which again contain variables and unary functions, such as e.g. the sine function or the inverse function. The latter can only occur once per term. Also the structures of function arguments are individually restricted.

```

G(Expr) :
Expr   -> Term "+" Expr | Term
Term   -> Factor "*" Term | Factor | "1/(" InvExpr ")"
Factor -> VarFac | ExpFac | LogFac | SinFac
VarFac -> <variable>
ExpFac -> "exp(" SimpleTerm ")"
LogFac -> "log(" SimpleExpr ")"
SinFac -> "sin(" SimpleExpr ")"

SimpleExpr -> SimpleTerm "+" SimpleExpr | SimpleTerm
SimpleTerm -> VarFac "*" SimpleTerm | VarFac

InvExpr -> InvTerm "+" InvExpr | InvTerm
InvTerm -> Factor "*" InvTerm | Factor

```

Fig. 4 The formal grammar used for grammar enumeration. In the design of the grammar, we want to allow a large set of potentially interesting expressions on the one hand, on the other hand we want to restrict the search space to disallow overly complex expressions as well as many different forms of semantically equal expressions.

Using a context-free grammar, semantic duplicates such as differently ordered terms cannot be prevented. Therefore, we additionally use a semantic hash function to identify semantically equivalent expressions. For each derived symbolic expression we calculate a hash value symbolically without evaluating the expression. Semantic duplicates are recognized by comparing the hash values of previously derived sentences. In case of a collision, the derived sentence is likely to be a semantic duplicate and therefore discarded.

The hashing function calculates the hash value recursively from a syntax tree. Each terminal symbol in the tree is assigned to a constant hash value. To cover commutativity, binary operators like multiplication or addition are flattened to n-ary operators and their arguments are ordered.

2.2 Phenotypic Similarity

For the phenotypic similarity we use Pearson's correlation coefficient of the model outputs. This allows us to determine the output similarity regardless of the offset and scale of the function values [4]. When we evaluate the expressions it is necessary to assume a range of valid input values. We use 100 points distributed on a grid in the range $(-5.0..5.0)$. All output vectors are scaled to zero mean and unit variance; undefined output values and infinity values are replaced by the average output. This preprocessing allows us to use cosine-similarity for the clustering and visualization which is supported by many implementations for approximate nearest neighbors and equivalent to Pearson's correlation coefficient for zero-mean vectors.

2.3 Genotypic Similarity

We define the genotypic similarity between two tree-based solution candidates using the Sørensen-Dice index

$$\text{GenotypicSimilarity}(T_1, T_2) = \frac{2 \cdot |M|}{|T_1| + |T_2|} \quad (1)$$

Here, M is the bottom-up mapping between T_1 and T_2 calculated using the algorithm described in [13]. We describe below the main steps of the algorithm:

1. Build a forest $F = T_1 \cup T_2$ consisting of the disjoint union between the two trees
2. Map F to a directed acyclic graph G . Two nodes in F are mapped to the same vertex in G if they are at the same height in the tree and their children are mapped to the same sequence of vertices in G . The bottom-up traversal ensures that nodes are mapped before their parents, leading to $O(|T_1| + |T_2|)$ build time for G .
3. Use the map $K : F \rightarrow G$ obtained in the previous step to build the final mapping $M : T_1 \rightarrow T_2$. This step iterates over the nodes of T_1 in level order and uses K to determine which nodes correspond to the same vertices in G . Level-order iteration guarantees that every largest unmapped subtree of T_1 will be mapped to an isomorphic subtree of T_2 .

The algorithm has a runtime complexity linear in the size of the trees regardless whether the trees are ordered or unordered.

2.4 Clustering and visualization

One of the challenges in visualizing the search space using phenotypic or genotypic similarity measures is to find a mapping of expressions to a two-dimensional space which preserves pairwise similarities as well as possible.

We use the t-SNE algorithm [7] with the distance matrices which are calculated on the basis of the previously described phenotypic or genotypic similarity measures.

The main idea behind t-SNE is to map a high-dimensional space X to a low-dimensional space Y where the distribution of pairwise similarities is preserved as much as possible. Similarity between data points $x_i, x_j \in X$ is defined as the probability that x_i would pick x_j as its neighbor. A similar probability distribution is found in Y by minimizing the Kullback-Leibler divergence between the two distributions using gradient descent. While t-SNE does not preserve distances, the visualization can potentially provide new insight into the structure of the search space for symbolic regression.

In the following we describe the visualization and clustering procedure in more detail.

2.4.1 Clustering and visualization based on genotypic similarity

The base set of $\approx 1.6 \cdot 10^5$ unique expressions obtained via grammar enumeration is unfeasibly big for the calculation of the full similarity matrix. Therefore, we further reduce this set to a feasible quantity by filtering expressions based on their R^2 value in relation to the Keijzer-4 function [4]. Figure 5 shows the distribution of R^2 values over the full set of all unique expressions. For the genotypic mapping we took only expressions with $R^2 > 0.2$.

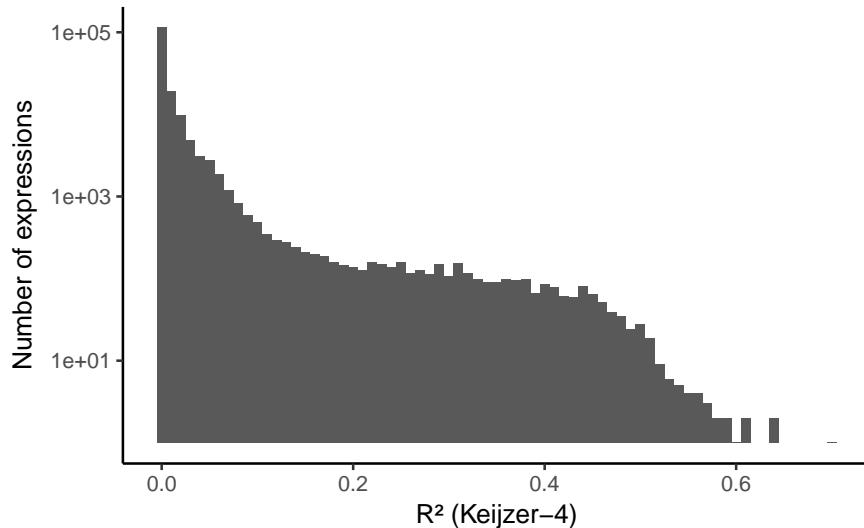


Fig. 5 Distribution of R^2 values for the Keijzer-4 function

We used the HDBSCAN algorithm [2] for clustering. We tried two approaches: (i) clustering based directly on the pre-computed similarity matrix, and (ii) clustering in the mapped 2-d space. Both approaches produced similar results.

2.4.2 Clustering and visualization based on phenotypic similarity

For the mapping based on phenotypic similarity we decided to use the complete set of the unique expressions and applied the *LargeVis* implementation [11] to produce the visualization. LargeVis relies on approximate nearest neighbor algorithms to make visualization of large-scale and high-dimensional datasets feasible. For our analysis we used the R library for LargeVis². LargeVis implements a variant of t-SNE in which the exact determination of nearest neighbors is replaced by the approximate nearest neighbors list. This has only linear runtime complexity in the number of data points. As a consequence, the asymptotic runtime of clustering and the embedding becomes linear in the number of data points.

The algorithm works in three steps. First, the lists of approximate nearest neighbors for each data points are determined using random projection trees [3]. In the second step, a sparse weighted edge matrix is calculated which encodes the nearest neighbor graph. Finally, the approximate nearest neighbor lists and the edge matrix can be used for t-SNE. LargeVis provides a variant of the HDBSCAN algorithm [8, 9] which uses the approximate nearest neighbor list.

2.5 Mapping GP solution candidates

Based on the results of the phenotypic clustering we study how GP explores the search space. For this we add a step in the GP algorithm after all individuals in the population have been evaluated. In this step, we identify the expression or cluster of expressions in the enumerated search space for each evaluated solution candidate. With this we are able to calculate a visitation density for the enumerated search space.

We expect that in the early stages of evolution GP explores many different areas of the search space, whereby over time GP should converge to the area of the search space which contains expressions which are most similar to the target function.

3 Results

In the following sections we first present our results of the clustering and visualization based on the phenotypic similarity and compare with the results of clustering

² <https://github.com/elbamos/largeVis>

and visualization based on the genotypic similarity. Then we present the results of our analysis of cluster qualities for five uni-variate functions. Finally, we present the results of the GP visitation frequency analysis.

3.1 Phenotypic mapping

Figure 6 shows a result for the visualization and clustering based on phenotypic similarity where we have used LargeVis directly on all output vectors and using cosine-similarity. Each dot represents an expression. The color indicates to which cluster an expression has been assigned. The visualization clearly shows that several clusters of similar expressions can be identified in the search space.

As a post-processing step we prepared plots for all clusters which show the outputs of all expressions within the clusters. We found that the search space includes many rather complex functions and that several clusters of interesting and similar functions are identified. Some selected plots as well as the position of the cluster center on the mapped search space are shown in Figure 6. It should be noted that the visualization does not show unique expressions which have been identified by HDBSCAN as outliers.

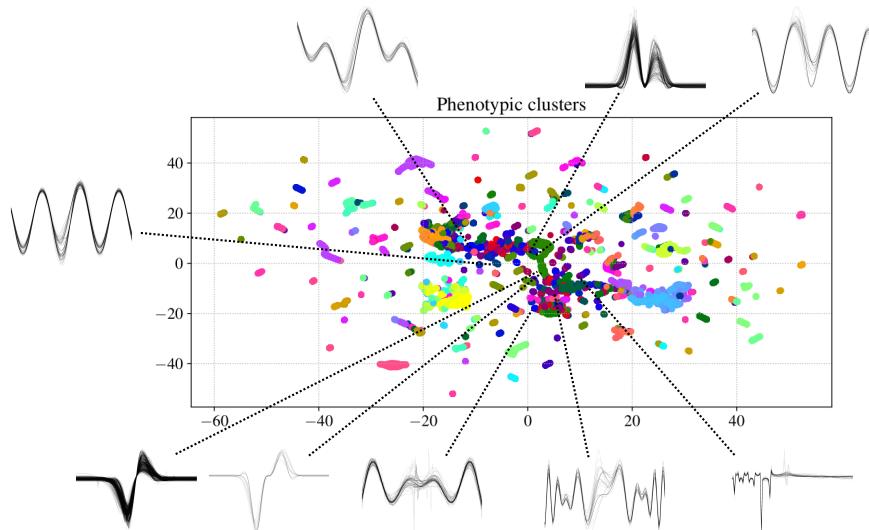


Fig. 6 Visualization of the embedding and clustering result based on phenotypic similarity. The phenotypic mapping leads to several clearly defined clusters.

Figure 7 again shows a phenotypic map. The difference to Figure 6 is that here all expressions are shown and we have used a coloring scheme based the similarity of expression outputs with the Keijzer-4 function (squared correlation R^2). The visual-

ization clearly shows that only certain areas of the search space contain expressions which are similar to the target function. Notably, there are several areas which contain expressions with large R^2 values. There are at least two potential explanations for this. First, it could be an artifact of the approximation of t-SNE. Another reason could be the fact that we have used cosine similarity for the embedding and the R^2 value for the coloring scheme. With the cosine similarity measure, two vectors that are negatively correlated are dissimilar.

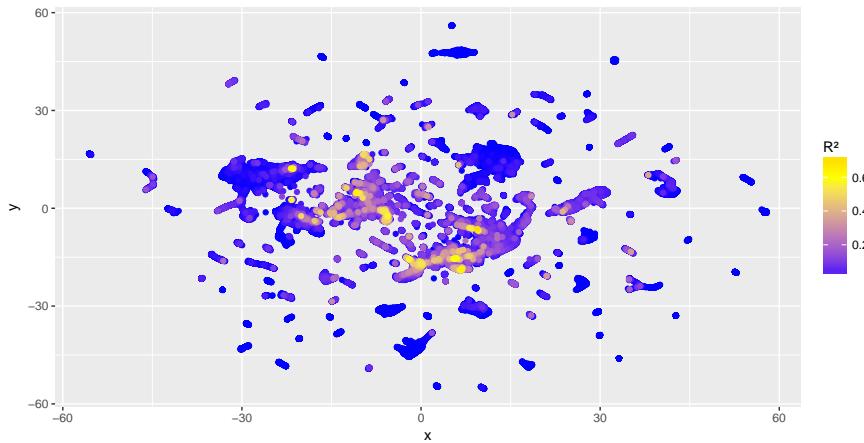


Fig. 7 All expressions in the mapped search space. We use squared correlation with the Keijzer-4 function for the coloring.

Figure 8 shows the same visualization for a different function (Pagie-1d). Compared to Figure 7 other areas of the search space are highlighted.

The results produced for the phenotypic mapping are motivating for further research. At least for the two considered examples we should be able to use a hill-climbing algorithm on the mapped search space to find well-fitting expressions. The mapping of the search space must be pre-computed only once and can be reused for potentially any target function.

3.2 Genotypic mapping

Figure 9 shows the results of t-SNE for dimensionality reduction and HDBSCAN for clustering when we use the genotypic similarity (see Section 2.3). We used HDBSCAN on the t-SNE mapped points. In comparison to the phenotypic mapping of the search space, the genotypic mapping does not produce such clearly defined clusters. In particular, in the lower sub-plot of Figure 9 no strong correlation with the quality values is visible.

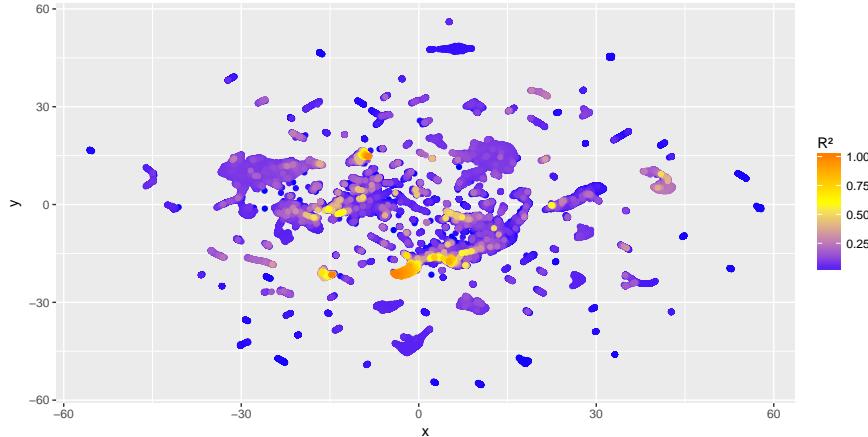


Fig. 8 All expressions in the mapped search space colored based on the squared correlation with the Pagie-1d function.

3.3 Cluster qualities for benchmark problems

To check whether the phenotypic clustering of our search space is generalizable over multiple problem instances, we use the following five uni-variate benchmark functions:

- Keijzer-4 [4]: $f(x) = x^3 e^{-x} \cos(x) \sin(x) (\sin(x)^2 \cos(x) - 1)$ for $x \in [0, 10]$
- Keijzer-9 [4]: $f(x) = \ln(x + \sqrt{x^2 + 1})$ for $x \in [0, 100]$
- Pagie-1d [10]³: $f(x) = \frac{1}{1+x^4}$ for $x \in [-5, 5]$
- Nguyen-5 [12]: $f(x) = \sin(x^2) \cos(x) - 1$ for $x \in [-1, 1]$
- Nguyen-6 [12]: $f(x) = \sin(x) + \sin(x + x^2)$ for $x \in [-1, 1]$

We average the resulting R^2 values within each cluster and rank the clusters by the average R^2 for each benchmark function independently. Figure 10 shows the average R^2 values over cluster ranks for the five benchmark functions. We find that for each of the benchmark functions a cluster with well-fitting expressions is found. Figure 11 shows plots of all functions in the best four clusters for each of the considered benchmark functions. The plots show that for the Keijzer-4 and the Pagie-1d functions the search space contains well-fitting expressions. However, for the other three functions the best clusters do not fit the target function well. This is in contrast to the calculated average R^2 values for the clusters which are relatively high (≥ 0.95) for all functions except for Keijzer-4. Here we want to stress again, that the search space clustering has been calculated independently from the target functions.

³ We have used a uni-variate variant of the benchmark function described by Pagie and Hogeweg

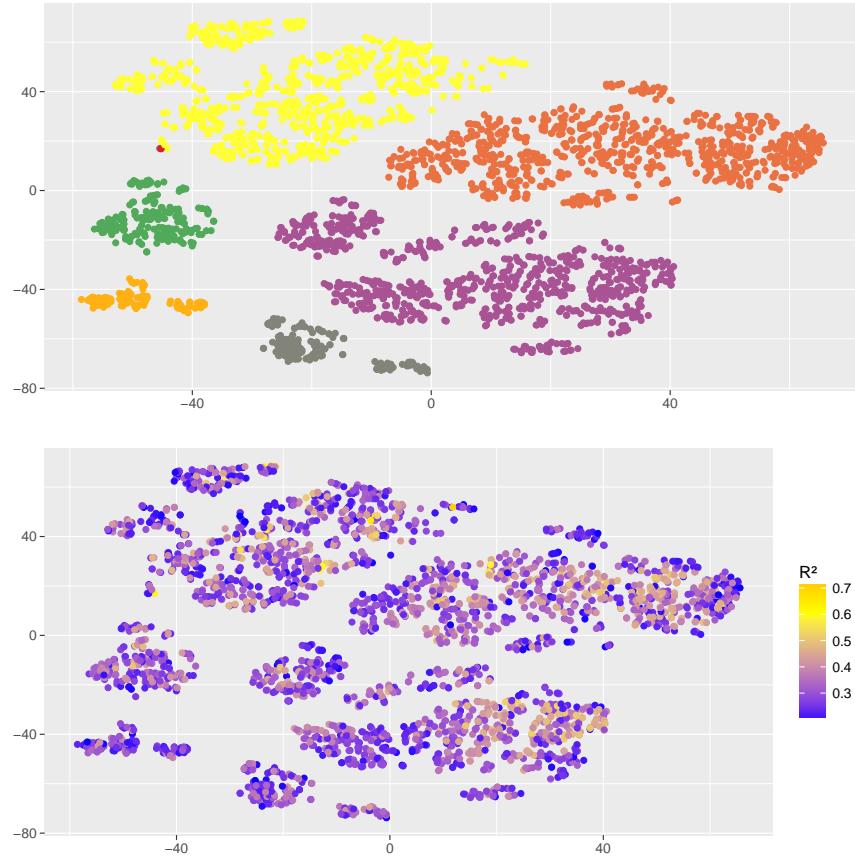


Fig. 9 Results of HDBSCAN and t-SNE with the genotypic similarity (top: coloring based on clusters; bottom: coloring based on the R^2 value with the Keijzer-4 function). The visualization of the two-dimensional mapping shows clusters of genotypically similar solutions. However, the genotypic clusters do not correlate strongly with qualities.

3.4 Mapping of GP solution candidates

We use the 2d-mapping of the search space to analyze the search bias of GP. For this we use a rather canonical GP implementation and map each evaluated solution candidate to the search space by identifying the closest representative expression in the enumerated search space. Each expression in the search space is assigned to a cluster. Therefore, we can determine which clusters of the search space are visited by GP. We have again used the Keijzer-4 function to demonstrate the concept.

Figure 12 shows the results of the analysis. In the left sub-plot the number of different clusters visited by GP are shown over generations; on the right hand side the median cluster rank (ordered by cluster quality) is shown. This clearly shows that

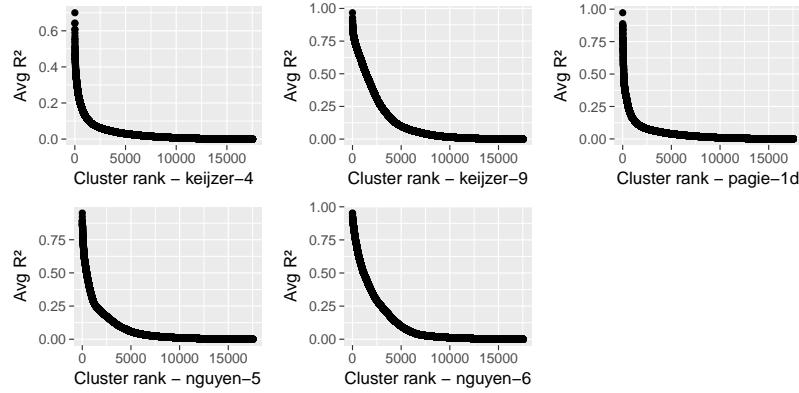


Fig. 10 Ranking of clusters by average R^2 values of expressions within all clusters. For each of the benchmark functions there are clusters which contain well-fitting expressions.

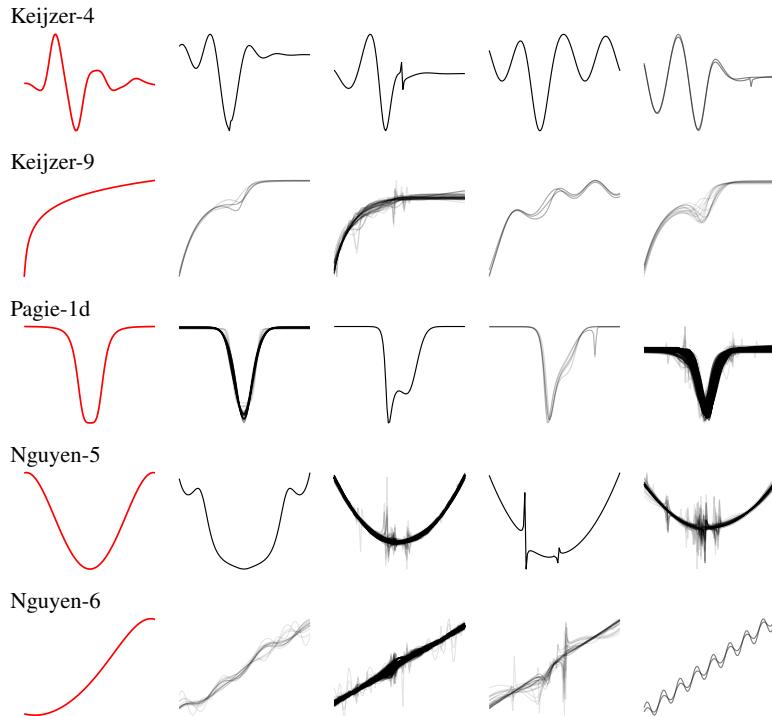


Fig. 11 The five benchmark functions and the best four clusters with the highest average R^2 for each of the functions from left to right. The average R^2 values are: 0.70 (Keijzer-4), 0.97 (Keijzer-9), 0.97 (Pagie-1d), 0.95 (Nguyen-5), and 0.95 (Nguyen-6).

in the beginning GP visits many different solution candidates and later concentrates on only a few high quality clusters.

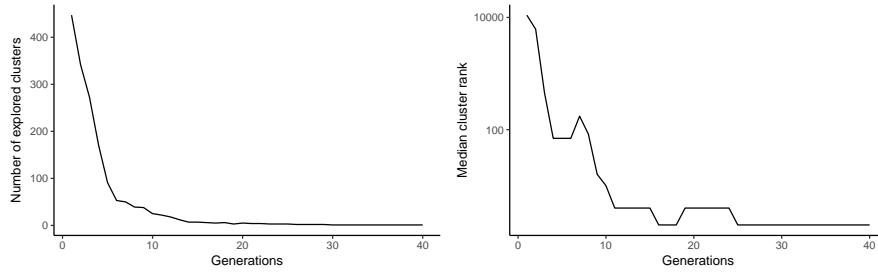


Fig. 12 The number of clusters that are visited by GP as well as the median rank (quality) of clusters over GP generations.

In Figure 13 we show the distribution of solution candidates visited by GP in more detail for the first few generations (1,2,3,4,5, and 10). It is clearly visible that within the first ten generations GP explores almost each of the 16000 clusters (population size=500 and PTC2 tree creator [6]) and quickly finds the clusters with highest quality.

4 Discussion

Our analysis so far has some limitations that merit a more detailed discussion.

- We have only looked at uni-variate models.
- The grammar is very restricted.
- Even with the limit of seven variable references, the computational effort is already rather high. When increasing the length limits the computational effort quickly becomes too big.
- The phenotypic clustering depends on the range of input values that are used when evaluating the model.
- We have completely ignored the effect of numeric constants in models, i.e. we have not used numeric constants.

In this work we have considered a search space of approximately 160000 semantically different expressions. However, in Figure 11 we see that the search space does not contain well-fitting expressions for all of the considered target functions. For a more in-depth analysis the size of the search space should be extended even for uni-variate problems.

We also found that the grammar we used produced many discontinuous functions (e.g. because of division by zero or extreme arguments to $\exp(x)$). If we assume that

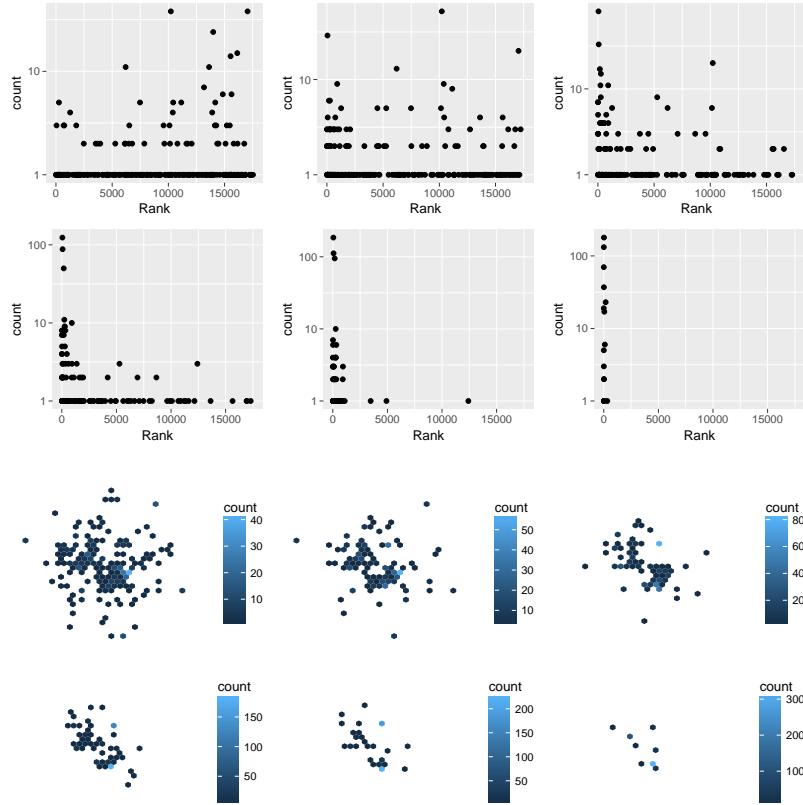


Fig. 13 More detailed visualization of the search space explored by a GP run. The plots in the first and second rows show the visitation frequency for each cluster in generations 1, 2, 3, 4, 5, 10. Clusters with lower ranks are high quality clusters. The plots in the third and fourth row show the visitation frequency in the two-dimensional phenotypic map. Within the first 10 generations GP converges to a focused area of the search space.

we are not interested in such functions then the search space could potentially be reduced massively by removing expressions leading to discontinuous functions.

If we extend the analysis to include multi-variate models, the size of the search space would increase significantly even if we use the same size restrictions. This is simply a consequence of the fact that there are more different models that can be expressed. Based on preliminary experiments, even with two or three independent variables it is possible to enumerate the search space with the same size restrictions as we used above. For more than three variables it would be necessary to use even smaller size limits.

We also need to consider that the variety of function outputs becomes much larger with increased dimensionality which could lead to a larger set of clusters.

We hypothesize that for practical problems it is usually sufficient to be able to represent two- or three-way interactions of variables as separable terms can be modeled independently. However, we cannot expect this in general.

Regarding the complexity of the grammar, we have purposefully limited the number of alternatives to be able to enumerate the full search space. It would however be rather easy to add more functions (e.g. a power or root function) as long as the complexity of the argument to the added functions is limited similarly as we have limited arguments for $\log(x)$.

A different approach that could potentially be worthwhile is to calculate the phenotypic similarity in the frequency-domain of the function.

5 Conclusion

This contribution aims to analyze the search behavior of GP in a space of hypotheses that is visualized as a 2D mapping of the search space. The idea of this approach is to enumerate the complete search space in the off-line phase independently of the regression problem to be solved. In order to do so we had to define some restrictions like the consideration of only uni-variate functions under restricting grammar assumptions. The still huge search space can be further restricted by filtering unique expressions by hashing. Once having established a mapping of the so defined search space by hierarchical clustering this off-line generated setup can be used to monitor the search behavior of different algorithms can be monitored and analyzed as demonstrated in this chapter for a relatively canonical GP implementation for the genotypic as well as for the phenotypic search space.

The ideas presented in this chapter have to be considered as very first findings of a novel approach having in mind that the restrictions on the search space delimit the generality of claimed findings. In order to achieve a deeper and more universal understanding it will be necessary to extend the approach to multi-variate models and less restrictions on the grammar of the model. Also it will be interesting to analyze the search behavior of different flavors of GP and other hypothesis search techniques.

Furthermore, the massive set of off-line generated models could be used in order to filter out an initial population for a GP run as soon as the regression problem to be tackled is available. Similar to what is done in the ANN community recently with pre-trained neural networks we could establish somehow pre-evolved initial populations for evolutionary search: In this way we could for example filter a genotypically diverse subset of model with promising correlation problems for a concrete problem in order to establish a somehow pre-evolved initial population for a GP run which is aimed to converge a lot faster in the on-line stage.

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References

1. Burke, E.K., Gustafson, S., Kendall, G.: Diversity in genetic programming: An analysis of measures and correlation with fitness. *IEEE Transactions on Evolutionary Computation* **8**(1), 47–62 (2004). DOI doi:10.1109/TEVC.2003.819263
2. Campello, R.J.G.B., Moulavi, D., Sander, J.: Density-based clustering based on hierarchical density estimates. In: J. Pei, V.S. Tseng, L. Cao, H. Motoda, G. Xu (eds.) *Advances in Knowledge Discovery and Data Mining*, pp. 160–172. Springer Berlin Heidelberg, Berlin, Heidelberg (2013)
3. Dasgupta, S., Freund, Y.: Random projection trees and low dimensional manifolds. In: *Proceedings of the 40th Annual ACM Symposium on Theory of Computing (STOC'08)*, pp. 537–546. ACM (2008)
4. Keijzer, M.: Improving symbolic regression with interval arithmetic and linear scaling. In: *European Conference on Genetic Programming*, pp. 70–82. Springer (2003)
5. Kommenda, M., Kronberger, G., Winkler, S., Affenzeller, M., Wagner, S.: Effects of constant optimization by nonlinear least squares minimization in symbolic regression. In: *Proceedings of the 15th Annual Conference Companion on Genetic and Evolutionary Computation*, pp. 1121–1128. ACM (2013)
6. Luke, S.: Two fast tree-creation algorithms for genetic programming. *IEEE Transactions on Evolutionary Computation* **4**(3), 274–283 (2000)
7. Maaten, L.v.d., Hinton, G.: Visualizing data using t-SNE. *Journal of machine learning research* **9**(Nov), 2579–2605 (2008)
8. McInnes, L., Healy, J.: Accelerated hierarchical density based clustering. In: *2017 IEEE International Conference on Data Mining Workshops (ICDMW)*, pp. 33–42 (2017). DOI 10.1109/ICDMW.2017.12
9. McInnes, L., Healy, J., Astels, S.: hdbscan: Hierarchical density based clustering. *The Journal of Open Source Software* **2**(11) (2017). DOI 10.21105/joss.00205
10. Pagié, L., Hogeweg, P.: Evolutionary consequences of coevolving targets. *Evolutionary computation* **5**(4), 401–418 (1997)
11. Tang, J., Liu, J., Zhang, M., Mei, Q.: Visualizing large-scale and high-dimensional data. In: *Proceedings of the 25th International Conference on World Wide Web, WWW '16*, pp. 287–297. International World Wide Web Conferences Steering Committee, Republic and Canton of Geneva, Switzerland (2016). DOI 10.1145/2872427.2883041
12. Uy, N.Q., Hoai, N.X., O'Neill, M., McKay, R.I., Galván-López, E.: Semantically-based crossover in genetic programming: application to real-valued symbolic regression. *Genetic Programming and Evolvable Machines* **12**(2), 91–119 (2011)
13. Valiente, G.: An efficient bottom-up distance between trees. In: *Proc. 8th Int. Symposium on String Processing and Information Retrieval*, pp. 212–219. IEEE Computer Science Press (2001)
14. Worm, T., Chiu, K.: Prioritized grammar enumeration: symbolic regression by dynamic programming. In: *Proceedings of the 15th Annual Conference on Genetic and Evolutionary Computation*, pp. 1021–1028. ACM (2013)