Simple Simultaneous Ensemble Learning in Genetic Programming

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Abstract. Learning ensembles by bagging can substantially improve the generalization performance of low-bias high-variance estimators, including those evolved by Genetic Programming (GP). Yet, the best way to learn ensembles in GP remains to be determined. This work attempts to fill the gap between existing GP ensemble learning algorithms, which are often either simple but expensive, or efficient but complex. We propose a new algorithm that is both simple and efficient, named Simple Simultaneous Ensemble Genetic Programming (2SEGP). 2SEGP is obtained by relatively minor modifications to fitness evaluation and selection of a classic GP algorithm, and its only drawback is an (arguably small) increase of the fitness evaluation cost from the classic \(O(n\ell)\) to \(O(n(\ell + \beta))\), with \(n\) the number of observations and \(\ell/\beta\) the estimator/ensemble size. Experimental comparisons on real-world datasets between supervised classification and regression show that, despite its simplicity, 2SEGP fares very well against state-of-the-art (ensemble and not) GP algorithms. We further provide insights into what matters in 2SEGP by (i) scaling \(\beta\), (ii) ablating the proposed selection method, (iii) observing the evolvability induced by traditional subtree variation.

Keywords: genetic programming, ensemble learning, machine learning, bagging, symbolic regression

1 Introduction

Learning ensembles by bagging, i.e., aggregating the predictions of low-bias high-variance estimators fitted on different samples of the training set (see Section 3.1), can improve generalization performance significantly [6,7,15,45]. Random forests are a remarkable example of this [58]. At the same time, mixed results have been found when using deep neural networks [10,19,37,58].

In Genetic Programming (GP) [32], bagging has been often found to be beneficial [3,24,30,51]. Perhaps the simplest way to build an ensemble of GP-learned estimators is to run multiple and independent classic GP evolutions that produce a single estimator each. However, since GP relies on a population of diverse estimators, it is natural to wonder whether the population can be leveraged to learn an ensemble simultaneously, and save computational resources.

Several ensemble learning GP-based approaches have been proposed so far. While we provide an overview in Section 2, we can broadly categorize current
approaches into two classes: Simple Independent Ensemble Learning Approaches (SIEL-Apps), and Complex Simultaneous Ensemble Learning Algorithms (CSEL-Algs). SIEL-Apps form an ensemble of estimators by repeating the execution of a GP algorithm that produces a single estimator. While these approaches simply require to run a same GP algorithm multiple times, they can be considered rather inefficient. On the other hand, CSEL-Algs make use of a number of novel mechanisms and respective hyper-parameters in order to obtain an ensemble in one go. A CSEL-Alg can therefore be very efficient (and effective), but it can also result rather involved to adopt in practice. Moreover, from a scientific standpoint, it may be hard to assess to what extent the mechanisms adopted in a CSEL-Alg contribute to its performance.

We propose an ensemble learning GP-based algorithm that attempts to be in between the two categories. Our algorithm, named Simple Simultaneous Ensemble Genetic Programming (2SEGP), learns an ensemble by evolving a single population, by means of minor modifications to a classic GP algorithm (e.g., as described in [48]). In particular, we only change the fitness evaluation and selection processes slightly, for a moderate computational cost increase. Moreover, 2SEGP requires only one additional hyper-parameter compared to a classic GP algorithm, i.e., the desired ensemble size.

Our experimental results on 9 real-world classification and regression datasets show that, despite its simplicity, 2SEGP is very competitive with CSEL-Algs as well as other (non-ensemble) GP algorithms that are considered to be State-of-the-Art (SoA) in recent literature. We further include experiments to gain insights into what matters in 2SEGP.

2 Related work

In this paper, we focus on ensemble learning intended as bagging (see Section 3.1), when GP is used to learn (evolve) the estimators. We do not consider ensemble learning intended as boosting, i.e., the iterative fitting of weak estimators to (weighted) residuals [11, 20, 21]. For the reader interested in boosting GP, we refer, e.g., to [17, 24, 25, 50]. Similarly, we do not consider works where, even if GP was used to decide how to aggregate the estimators, these were learned by other (machine learning) algorithms than GP [3, 4, 27, 39, 38].

We begin by considering works with SIEL-Algs. Some of the first works in this category are [24, 30]. In both works, along other contributions, the authors investigate how the prediction of the ensemble members should be weighed, e.g., by relying on the a measure of confidence [24], or by excluding extreme predictions [30]. In [25, 26, 55], further investigations are made into how GP estimators that are evolved independently should be best aggregated into an ensemble across problems of different nature. In [32], again an SIEL-App is taken, but this time using a particular estimator representation (linear combination of multiple trees), and harnessing on-line, parallel computing.

We remark that the works just discussed mainly focus on how aggregation should be conducted, rather than how to obtain an ensemble efficiently. Other
works in this category are [31,60,72], respectively for hybridization with multi-objective evolution, incomplete data, and large-scale data.

Regarding CSEL-Algs, a recent work is [69], where the algorithm Diverse Niching Genetic Programming (DivNichGP) is presented. DivNichGP makes use of bootstrap sampling each generation (see Section 5.1), and uses niching to maintain diversity during the run and also to aggregate the final ensemble. The niching process requires two dedicated hyper-parameters to be set. In [2], ensembles are composed of Pareto non-dominated estimators found by a multi-objective GP algorithm. Importantly, having multiple objectives is needed for this proposal to be applicable. The investigation proposed in [13] explores learning ensembles by spatially distributing the evolving estimators and bootstrap samples on a graph (e.g., a toroidal grid), enforcing competition in niches [59]. This algorithm requires to choose the graph and niche structure as well as node-resource allocation. Lastly, in [52] ensemble learning is realized by the simultaneous co-evolution of a population of estimators (trees), and a population of ensemble candidates (forests). For this algorithm, one needs to choose hyper-parameter settings also for the population of ensemble candidates (e.g., for variation, selection, and voting method).

It would not be fair not to acknowledge the fact that the works just mentioned provide a recommendation for default hyper-parameter settings (typically derived from preliminary experiments). Even so, we believe that these algorithms can still be considered sufficiently complex that the proposal of a simpler algorithm ensemble learning algorithm for GP, i.e., this work, remains worthwhile.

3 Our algorithm

We now describe 2SEGP, in terms of differences compared to a classic GP algorithm that returns a single estimator. We refer to [48] (Chapters 2–4) for a description of a classic, tree-based GP algorithm.

The backbone of 2SEGP consists of two aspects: (i) evaluate a same estimator according to different samples of the training set; (ii) balance the improvement across different training set samples at selection time. To achieve these aspects, we only need to modify fitness evaluation (we also describe the use of linear scaling [28] and selection, as explained in the next sections. We propose no change to variation compared to a classic GP algorithm. Our intuition is that exchanging genetic material between estimators that are best on different samples of the training set is not detrimental because these samples are themselves similar to one another. We provide insights about variation in 2SEGP in Section 7.3.

In the next section, we recall the ensemble learning setting we consider, i.e., bagging. Next, we describe the modifications to fitness evaluation and selection.

3.1 Bagging

We consider ensemble learning by bagging (bootstrap aggregating) [7]. We use traditional bootstrap, i.e., we obtain $\beta$ training sets $T_1, \ldots, T_\beta$, each with as
many observations as the original \( T = \{(x_i, y_i)\}_{i=1}^n \), by uniformly sampling from \( T \) with replacement. One run of our algorithm will produce an ensemble of \( \beta \) estimators where each estimator is the best-found on a respective training set \( T_j \), with \( j = 1, \ldots, \beta \). We aggregate predictions in a traditional manner, i.e., by majority voting (i.e., mode) for classification, and averaging for regression.

### 3.2 Fitness evaluation

To compute the fitness of an estimator in a classic GP algorithm, one needs to (i) compute the output of the estimator; (ii) compute the loss function between the output and the label. Both (i) and (ii) are performed using the original training set \( T = \{(x_i, y_i)\}_{i=1}^n \). Recall that the computation cost of (i) is \( O(\ell n) \), with \( \ell \) the size of the estimator (e.g., the number of nodes in tree-based GP), as we need to compute the \( \ell \) operations that compose the estimator for each observation. Since (ii) takes \( O(n) \) and is additive, the total cost remains \( O(\ell n) \).

We intend to compute the fitness of each estimator according to each of the training sets \( T_1, \ldots, T_\beta \), i.e., each estimator will have \( \beta \) fitness values assigned. We will use this information for selection later. A naive solution is to repeat (i) and (ii) for each \( T_j \), costing \( O(\beta \ell n) \). In fact, this would lead to the same cost of an SIEL-App. To be markedly more efficient, it suffices to consider that each training set \( T_j \) obtained by bootstrap of the original \( T \) strictly contains elements of \( T \), and therefore any \( T_j \)-specific output element will necessarily be one of the output elements computed over \( T \). Formally, let \( S_j \) be the collection of indices that identifies \( T_j \), i.e., \( S_j = [s_j^1, \ldots, s_j^n] \) s.t. \( s_j^l \in \{1, \ldots, n\} \) and \( \{(x_k, y_k)\}_{k \in S_j} = \{(x_k, y_k)\}_{k=s_j^1}^{s_j^n} = T_j \). Then one can:

1. Compute once the output of the estimator over \( T \), i.e., \( \{o_i\}_{i=1}^n \);
2. For \( j = 1, \ldots, \beta \), assemble a \( T_j \)-specific output \( \{o_k\}_{k \in S_j} \) from \( \{o_i\}_{i=1}^n \);
3. For \( j = 1, \ldots, \beta \), compute the loss \( \text{Loss}_j(\{y_k\}_{k \in S_j}, \{o_k\}_{k \in S_j}) \).

Step 1 costs \( O(\ell n) \), step 2 and step 3 cost \( O(\beta n) \), they are executed in sequence:

\[
O(\ell n) + O(\beta n) + O(\beta n) = O(n(\ell + \beta)).
\] (1)

This method is asymptotically faster than re-computing the output over each \( T_j \) whenever \( \ell + \beta < \ell \beta \)—basically in any meaningful scenario. A glance to Figure 1 is sufficient to see that \( \beta + \ell \) quickly becomes orders of magnitudes better than \( \beta \times \ell \) for growing \( \beta \) and \( \ell \).

We remark that steps 2 and 3 can be implemented in terms of \((\beta \times n)\)-dimensional matrix operations if desired. For example, in our python implementation that is available at \( \text{http://github.com/marcovirgolin/2SEGP} \) we leverage \texttt{numpy} [61].

### 3.3 Linear scaling over multiple training sets

Linear scaling [28,29] is a popular method to improve the performance of GP in regression. It consists of computing and applying two coefficients \( a, b \) to perform
an affine transformation of the output that optimally minimizes the (training) mean squared error. These coefficients are:

\[
a = \bar{y} - \bar{o}, \quad b = \frac{\sum_{i=1}^{n} (y_i - \bar{y}) \sum_{i=1}^{n} (o_i - \bar{o})}{\sum_{i=1}^{n} (o_i - \bar{o})^2},
\]

where \(\bar{y}\) (and \(\bar{o}\)) denote the arithmetic mean of the label (respectively, output) over the training set \(T\). SotA GP algorithms often include linear scaling or some other form of linear regression step \([33,34,64,65,71]\). We can readily incorporate the calculation of coefficients \(a_j, b_j\) to scale each \(T_j\)-specific output in a similar fashion to how step 3 of the previous section is performed. Again, implementation can be realized in terms of matrix operations for the sake of speed.

3.4 Selection

We employ a remarkably simple modification of truncation selection that is applied after the offspring population has been obtained by variation of the parent population, in a \((\mu + \lambda)\) fashion. Pseudocode is illustrated in Algorithm 1. Let \(n_{\text{pop}}\) be the size of both the parent and offspring populations (\(|P| = |O| = n_{\text{pop}}\)). For \(j = 1, \ldots, \beta\), we sort the merged parent-offspring population (\(Q\) of size \(2n_{\text{pop}}\)) according to best fitness value on \(T_j\), and copy the first \(n_{\text{pop}}/\beta\) top-ranking estimators to the population of selected estimators (\(P'\)).

Note that a same estimator can obtain multiple copies (i.e., because top-ranking for different training sets). Note also that this selection ensures weakly monotonic fitness decrease across all training sets \(T_j\). Lastly, the computational complexity is determined by sorting the population \(\beta\) times and copying estimators, i.e., \(O(\beta n_{\text{pop}} \log n_{\text{pop}} + n_{\text{pop}} \ell)\). Since the cost of fitness evaluation over the entire population is \(n_{\text{pop}}\) times Equation (1), the larger the training set at hand in terms of number of observations \(n\), the less the cost of selection matters. We provide insights on the use of this selection method in Section 7.2.
Algorithm 1: Our simple extension of truncation selection.

input: \( P \) (parent population), \( O \) (offspring population), \( \beta \) (ensemble size)
output: \( P' \)

1. \( Q = P \cup O \);
2. \( P' \leftarrow \emptyset \);
3. for \( j \in 1, \ldots, \beta \) do
   4. sort \( Q \) according to the \( j \)th fitness value;
   5. for \( k \in 1, \ldots, n_{\text{pop}}/\beta \) do
      6. \( P' \leftarrow P' \cup \{Q_k\} \);
4. return \( P' \);

4 Experimental setup

We attempt to (mostly) reproduce the experimental settings used in [51], to
which we compare in terms of classification. Specifically, we use \( n_{\text{pop}} = 500 \), the
selection method described in Section 3.4, and variation by subtree crossover
and subtree mutation with equal probability (0.5). Random node selection for
crossover and mutation is done by uniform depth as proposed in [47], to oppose
bloat. If variation produces an offspring with more than 500 nodes, the offspring
is discarded and the parent is cloned.

We use ramped half-and-half initialization with tree heights 2–6 [48]. The
function set is \{+, −, ×, ÷, √, log\}, with the last three operators implementing
protection by, respectively, \( \tilde{\times}(a, b) := a \times \text{sign}(b)/(|b| + \epsilon) \), \( \tilde{\sqrt{x}} := \sqrt{|x|} \), \( \tilde{\log}(x) := \log(|x| + \epsilon) \); with \( \text{sign}(0) := 1 \) and \( \epsilon = 10^{-10} \). Alongside the features, the terminal
set includes ephemeral random constants [48] (albeit [51] chose not to) with
values sampled from \( U(-5, 5) \), as ephemeral random constants can substantially
boost performance [48, 64]. We need only on one additional hyper-parameter
compared to classic GP, i.e., the ensemble size \( \beta \). We set \( \beta = 0.1 n_{\text{pop}} = 50 \) as a
rule of thumb (see Section 7.1 for results with other settings).

We perform z-score data standardization as advised in [14]. In (binary)
classification, the label is either 0 or 1. We include linear scaling for both regression
and classification tasks. In our case it is plausible to apply linear scaling in classifi-
cation (prior to rounding the output of an estimator to the nearest class)
because we only consider binary classification problems (as in [51]). We also
include results without linear scaling for classification.

A run consists of 100 generations. We conduct 40 independent runs to account
for the randomness of both GP and training-test splitting, for which we use
70\%/30\% as in [51, 71]. Statistical significance of the results is evaluated by
means of pairwise non-parametric Mann-Whitney \( U \) tests, using \( p \)-value \(< 0.05 \)
and Holm-Bonferroni correction [23, 42]. In particular, we say that an algorithm
is among the best ones if no other exists that performs significantly better.
5 Competing algorithms and datasets

Classification. For classification problems, we consider results that were kindly provided by the authors of [51]. Specifically, we focus on the best-performing ensemble algorithm “ensemble GP with weighted voting” (eGPw); the best-performing non-ensemble algorithm “Multidimensional Multiclass GP with Multidimensional Populations” (M3GP), and classic GP (cGP) (see their Table 4). M3GP in particular can be considered a SotA GP-based feature construction approach, and in [51] is found to outperform most of the other (GP and non-GP) algorithms, including random forest.

We further include our own re-implementation of “Diverse Niching Genetic Programming” (DivNichGP), made by following [69], and that we make available at https://github.com/marcovirgolin/DivNichGP. For DivNichGP, we maintain equal subtree crossover and mutation probability, but also allow reproduction to take place, with a rate of 5% as in [69]. DivNichGP internally uses tournament selection: we set this to size 8 (as for our cGP for regression, described below). For DivNichGP’s niching mechanism, we use the same distance threshold of 0 and maximal niche size of 1 as in [69]. Since DivNichGP uses a validation set to aggregate the ensemble, we build a pseudo-validation set by taking the out-of-bag observations of the last used training bootstrap sample. All the other settings are as in Section 4.

The datasets we consider for classification are the five real-world datasets used in [51] that are readily available from the UCI repository [16]. We refer to [51] for details on these datasets.

Regression. For regression, we report the (median) results from [71] (see their Table 7), where test error of SotA GP regression algorithms is shown. These algorithms are “Evolutionary Feature Synthesis” (EFS) [1], “Genetic Programming Toolbox for The Identification of Physical Systems” (GPTIPS) [54,53] (and a modified version mGPTIPS that uses settings similar to those of EFS), and “Geometric Semantic Genetic Programming with Reduced Trees” (GSGP-Red) [44,13]. We refer to [71] for what settings were chosen.

We further include a home-baked version of cGP that uses tournament selection of size 8 (we also tried 4 but it performed worse in preliminary experiments), all other settings being as in Section 4. We consider again our re-implementation of DivNichGP. Like for 2SEGPG, we use linear scaling in cGP and DivNichGP as it is typically helpful in regression (see, e.g., [65]).

Next, we consider two algorithms from our own works on improving variation. The first is the GP version of the Gene-pool Optimal Mixing Evolutionary Algorithm (GP-GOMEA) [64,67]. GP-GOMEA uses a form of crossover that preserves high-mutual information patterns. Since GP-GOMEA requires relatively large population sizes to infer meaningful patterns but converges quickly, we shift resources between population size and number of generations, i.e., we set $n_{pop} = 5000$ and use only 10 generations. Moreover, GP-GOMEA uses a fixed tree template representation: we set the template height to 7 so that up
to 255 nodes can be hosted (half the maximum allowed size for the other algorithms). Lastly, we include our linear scaling-enhanced version of the semantic operator Random Desired Operator \[47,70\], named RDO_{+LS} \times \text{LS} \times \text{LS} \times \text{LS} \times \text{LS} \times \text{LS} \times \text{LS}

uses a form of semantic-driven mutation based on intermediate estimator outputs and a library of pre-computed subtrees. We use the “population-based” library, re-computed every generation, storing up to 500 subtrees, up to 12 deep.

We remark that while the generational costs of 2SEGP is only marginally larger than the one of cGP, the same is not always true for the competing SotA algorithms (we refer to the respective papers for details).

The datasets we consider are the four real-world UCI datasets of \[71\].

### 6 Results on real-world benchmark datasets

#### 6.1 Classification

Table 1 shows the accuracy obtained by eGPw, M3GP, DivNichGP, cGP, and of course 2SEGP, the latter with and without linear scaling. At training time, M3GP is significantly best on three out of five datasets, while 2SEGP is second-best. Compared to eGPw and DivNichGP, which also evolve ensembles, 2SEGP performs better (on Heart significantly so), except for on Parks when linear scaling is disabled. This is the only dataset where we observe a substantial drop in performance when linear scaling is turned off.

In terms of test accuracy, due to generalization gaps, only a few results are significantly worse than others. On BCW and Heart, all algorithms are equally good. Compared to M3GP, SEGP is significantly better on Parks, but worse on Sonar. On Heart, M3GP is no longer superior, as substantial performance is lost when testing. It can further be noted that DivNichGP, possibly because it uses a validation set to choose the final ensemble, exhibits slightly (but not significantly) better generalization than 2SEGP on Heart and Iono. Overall, 2SEGP reaches high and competitive accuracy on all datasets.

**Table 1.** Median accuracy (higher is better) on the UCI datasets of \[51\] obtained by 2SEGP, 2SEGP w/o linear scaling (w/oLS), DivNichGP, eGPw, M3GP, and cGP. Bold results are best, i.e., not significantly worse than any other.

| Algorithm   | Training | Test  |
|-------------|----------|-------|
|             | BCW      | Heart | Iono | Parks | Sonar | BCW      | Heart | Iono | Parks | Sonar |
| 2SEGP (ours) | 0.992    | 0.976 | 0.948 | 0.959 | 0.971 | 0.802 | 0.896 | 0.938 | 0.746 |
| w/oLS (ours) | 0.995    | 0.958 | 0.880 | 0.813 | 0.957 | 0.790 | 0.896 | 0.815 | 0.730 |
| DNGP        | 0.974    | 0.907 | 0.955 | 0.930 | 0.956 | 0.815 | 0.901 | 0.924 | 0.730 |
| eGPw        | 0.983    | 0.907 | 0.884 | 0.923 | 0.956 | 0.790 | 0.830 | 0.822 | 0.762 |
| M3GP        | 0.971    | 0.970 | 0.932 | 0.981 | 1.000 | 0.957 | 0.778 | 0.871 | 0.897 | 0.810 |
| cGP         | 0.964    | 0.825 | 0.773 | 0.842 | 0.769 | 0.961 | 0.784 | 0.745 | 0.797 | 0.714 |
6.2 Regression

Table 2 shows the results of 2SEGP, DivNichGP, GP-GOMEA, $RDO_{\text{+LS}}^x$, cGP, and the algorithms from of [71] (from their Table 7, test only) in terms of Root Mean Squared Error (RMSE). 2SEGP always outperforms DivNichGP significantly except for on ENH at training time, and cGP except for on ENC at test time. 2SEGP is also competitive with the SotA algorithms, as it is only significantly worse than GP-GOMEA and $RDO_{\text{+LS}}^x$ on ENH when testing. On ASN, 2SEGP is not matched by any other algorithm. Interestingly, our implementation of cGP achieves rather good results on most datasets, and performs better in terms of median than several of the SotA algorithms from [71].

We remark that the hyper-parameter settings for 2SEGP (and also DivNichGP, cGP, GP-GOMEA, and $RDO_{\text{+LS}}^x$) were chosen by following [51], where classification was pursued. As will be shown in Section 7.1 solely increasing $\beta$ can lead to better results.

Table 2. Median RMSE (smaller is better) on the UCI datasets of [71] obtained by the considered algorithms. Median results of GPTIPS, mGPTIPS, EFS, and GSGP-Red are reported from [71]. Bold results are best, i.e., not significantly worse than any other (the algorithms from [71] are excluded from this comparison). Underlined results are best in terms of median-only (across all algorithms).

| Algorithm            | Training | Test    |
|----------------------|----------|---------|
|                      | ASN CCS  | ENC ENH | ASN CCS  | ENC ENH |
| 2SEGP (ours)         | 2.901 5.820 1.602 0.918 | 3.195 6.565 1.801 1.013 |
| DNGP                 | 3.197 6.582 1.849 1.201 | 3.371 7.108 2.018 1.239 |
| GP-GOMEA             | 3.221 6.326 1.605 0.786 | 3.361 6.716 1.705 0.810 |
| $RDO_{\text{+LS}}^x$| 3.501 6.445 1.688 0.835 | 3.564 6.826 1.744 0.863 |
| cGP                  | 3.216 6.265 1.795 1.257 | 3.345 6.842 1.936 1.273 |
| GPTIPS               | - - - - | 4.138 8.762 2.907 2.538 |
| mGPTIPS              | - - - - | 4.003 7.178 2.278 1.717 |
| EFS                  | - - - - | 3.623 6.429 1.640 0.546 |
| GSGP-Red             | - - - - | 12.140 8.798 3.172 2.726 |

7 Insights

In this section, we provide insights regarding 2SEGP. We begin by investing the role of $\beta$ in terms of prediction error and time, including when the ensemble is formed by an SIEL-App. We proceed by investigating our selection method by ablation. Last but not least, we peek into the effect of variation in 2SEGP, which we left untouched. We will focus our analysis on the UCI regression datasets.
We consider how sensitive the performance of 2SEGP is to the setting of $\beta$, especially when compared to learning the ensemble by using independent cGP evolutions, i.e., by a classic SIEL-App. For 2SEGP, we scale $\beta$ (approx.) exponentially, i.e., $\beta = 5, 25, 50, 100, 250, 500$. For our SIEL-App, we use $\beta = 1, 2, \ldots, 10$, as running times of sequential executions quickly become prohibitive. We also include cGP in the comparison. All settings are as before (Section 4).

Figure 2 shows the distribution of test RMSE against the average time taken when using different $\beta$ settings. Results on the training set (not shown) follow the same trends. Regarding the time cost, of course the time taken by SIEL-App to form an ensemble of size $\beta$ is approximately $\beta$ times the time of performing a single evolution (we address parallelism potential in the last paragraph of this section). With 2SEGP, large ensembles can be evolved in a fraction of the time taken by SIEL-App, as can be expected from Equation 1.

Fig. 2. Distribution of test RMSE (25th, 50th, 75th percentiles) over the average time taken to obtain an ensemble by 2SEGP (in red) and a classic SIEL-App (in blue); or to obtain a single estimator by cGP (in black). For 2SEGP, $\beta$ is scaled approximately exponentially (from left to right $\beta$ is 5, 25, 50, 100, 250, 500). For SIEL-App, $\beta$ is scaled linearly (from left to right, $\beta$ is 1, 2, 3, $\ldots$, 10).
Larger ensembles tend to generalize better than smaller ensembles, however increasing $\beta$ leads to diminishing returns. Statistical tests between pairwise configurations of $\beta$ for 2SEGP reveal that most test RMSE distributions are not significantly different from each other ($p$-value $\geq 0.05$ except, e.g., between $\beta = 5$ and $\beta = 500$ on CCS; and between $\beta = 5$ and $\beta = 250$ on ENH).

We can compare 2SEGP and SIEL-App for the same value $\beta = 5$ by looking at the first red point and the fifth blue point respectively, in each plot. Interestingly, while 2SEGP uses only a fraction of computational resources required to learn the ensemble compared to SIEL-App, the (distribution of) ensembles obtained by SIEL-App do not outperform the ensembles obtained by 2SEGP.

SIEL-App can already perform similarly to cGP with $\beta = 2$, of course for double the time cost. Yet, 2SEGP can obtain an ensemble of size 50 within the same time (3rd red dot), which is normally significantly better than both cGP and SIEL-App (with $\beta = 2$). In general, given a same time limit, poor runs for 2SEGP are often better or similar to median runs of SIEL-App, thanks to the former obtaining a much larger ensemble. A downside of 2SEGP is that it obtains larger inter-run variation compared to SIEL-App (but because the latter uses a new $n_{\text{pop}}$ for each estimator).

Interestingly, $\beta = 500 = n_{\text{pop}}$ works well on CCS, despite the fact that this setting could be considered somewhat extreme. At the same time, using $\beta = 500$ can also make results worse (e.g., on ENH). This confirms the hypothesis stated in [13] that setting $\beta = n_{\text{pop}}$ can lead to poor performance because the resources for the evolution of each estimator are insufficient.

We remark that if the population size (which we now denote by $|P|$ for readability) and/or the number of generations ($G$) required by SIEL-App are reduced as to make SIEL-App match the computational expensiveness of 2SEGP, then SIEL-App performs poorly. This can be expected because, if we assume $\ell$ to be the average estimator size across the entire evolution, then we get:

Time cost of SIEL-App = time cost of 2SEGP,

$$\beta G_{\text{SIEL-App}} |P|_{\text{SIEL-App}} n = G_{\text{2SEGP}} |P|_{\text{2SEGP}} n (\beta + \ell) \quad \text{(from Equation (1))},$$

$$G_{\text{SIEL-App}} |P|_{\text{SIEL-App}} = G_{\text{2SEGP}} |P|_{\text{2SEGP}} \frac{\beta + \ell}{\beta \ell}.$$

For example, if we assume $\ell = 100$, and we set $\beta = 50$, $G_{\text{2SEGP}} = 100$, and $|P|_{\text{2SEGP}} = 500$, then a possible setting for SIEL-App is $|P|_{\text{SIEL-App}} = 100$ and $G_{\text{SIEL-App}} = 15$ (or vice versa); if we use the same settings as above but reduce the ensemble size to $\beta = 5$, then a possible setting for SIEL-App is $|P|_{\text{SIEL-App}} = 105$ and $G_{\text{SIEL-App}} = 100$ (or vice versa). With the former setting, we found SIEL-App to be incapable of producing competitive results. With the latter setting, SIEL-App performed better, but still significantly worse than 2SEGP and cGP on all four datasets.

Finally, it is important to consider that with SIEL-App each ensemble member can be evolved completely in parallel. For example, if $k\beta$ cores are available, one could evolve a $\beta$-sized ensemble $\beta$ parallel evolutions that are each parallelized on $k$ cores. Nevertheless, with 2SEGP, resources for parallelism can be
fully invested into one population, which can consequently be increased in size if desired. We leave an assessment of how SIEL-App and 2SEGP compare in terms of the interplay between population size and parallel compute to future work.

### 7.2 Ablation of selection

We look into ablating our selection method by removing the partitioning of the population into $\beta$ truncations. By doing that, we can no longer select $n_{\text{pop}}/\beta$ top-ranking estimators according to a specific $T_j$. We thus consider:

1. Survival according to truncation (Trunc) or tournament (Tourn) selection, based on the best fitness value among any $T_j$—We call this strategy “Push further What is Best” (PWB);

2. Like the previous point, but according to worse fitness value among any $T_j$—We call this strategy “Push What Lacks behind” (PWL).

Table 3 shows the comparison of our selection method with the ablated versions on the UCI regression datasets. It can be noted that the ablated versions perform worse than our selection, with some exceptions for tournament selection with size 8 on ENC or ENH. In fact, the performance of tournament selection is the closest to the one of our selection. Using PWB or PWL leads to mixed results across the datasets, except when tournament selection with size 8 is used, where PWL is always better in terms of median results.

**Table 3.** Median test RMSE of our selection and the ablated versions. Tournament selection is run with sizes 4 and 8. Bold results are best (no other is significantly better).

| Selection | ASN | CCS | ENC | ENH |
|-----------|-----|-----|-----|-----|
| Ours      | 3.105 | 6.565 | 1.801 | 1.013 |
| Trunc$^{\text{PWB}}$ | 3.728 | 7.351 | 2.183 | 1.613 |
| Trunc$^{\text{PWL}}$ | 3.687 | 7.355 | 2.154 | 1.592 |
| Tourn$^{\text{PWB}}_4$ | 3.531 | 7.018 | 1.972 | 1.302 |
| Tourn$^{\text{PWL}}_4$ | 3.578 | 7.010 | 1.950 | 1.342 |
| Tourn$^{\text{PWB}}_8$ | 3.440 | 7.044 | 1.938 | **1.154** |
| Tourn$^{\text{PWL}}_8$ | 3.382 | 6.911 | 1.876 | **1.014** |

Figure 3 shows how the fitness values of the ensemble evolves for ASN using our selection method, and the two PWB ablated versions, in one run chosen at random (we cannot display averages over multiple runs because particular trends cancel out). It can be seen that ablated truncation performs worse than the other two, and that our selection leads to smallest RMSEs. At the same time, our selection leads to rather uniform decrease of best-found RMSEs across the training set samples. Conversely, when using Tourn$^{\text{PWB}}_4$, some RMSE remain large compared to the rest, e.g., notably for $T_7$, $T_{40}$, and $T_{47}$. 


These results confirm that our selection method, where balance is maintained across the training sets, is important to obtaining a well-performing ensemble. Since tournament selection performs rather well, and in particular better than simple truncation selection, it would be worth studying whether our selection method can be improved by incorporating tournaments in place of truncations, or SotA selection methods such as $\epsilon$-lexicase selection [36,35].

7.3 Variation within the single population

In our experiments, we relied on classic subtree crossover and subtree mutation, without incorporating any modification thereof. Our intuition being that $T_j$ and $T_k$ are (loosely speaking) correlated, thus an estimator that is good on $T_j$ is probably also decent on $T_k$. To gain an understanding into whether using classic variation across the entire population is a good idea, we look at evolvability [63], expressed in terms of frequency with which the $i$th offspring obtained by variation is more fit than the respective $i$th parent. We consider two aspects:

1. Within-$T_j$ improvement: frequency of successful variation in terms of producing an offspring that has better $j$th fitness value than the parent;
2. Across-$T_j$'s improvement: frequency of successful variation in terms of producing an offspring that has better $k$th $\neq$ $j$th fitness value than the parent.
Figure 4 shows the average ratios of improvement across 30 runs for the first 10 generations of a random run on ASN. As can be seen, not only across-$T_j$'s improvements are frequent, they are more frequent than within-$T_j$ improvements (we observe the same in other runs). In other words, classic variation is already able to make the population improve across different training sets.

Fig. 4. Frequency of producing offspring with smaller RMSE than their parents for the first 10 generations of a random run on ASN (darker is better).

The result of this experiment corroborates our proposal of leaving classic variation untouched for the sake of simplicity. Nevertheless, improvements may be possible by incorporating (orthogonal) SotA variation methods [44,47,64], or strategies for restricted mating and speciation [18,41,57].

8 Conclusions and future work

We proposed 2SEGP, a simple GP algorithm for simultaneous ensemble learning when bagging, that adopts a single population and performs a single evolution. The algorithm is different from a classic GP implementation only in terms of fitness evaluation and selection processes, and requires a marginal increment of the computation cost. At the same time, learning an ensemble with 2SEGP is markedly more efficient than running independent GP evolutions. Our experimental results on classification and regression datasets show that, despite its simplicity, 2SEGP performs on par with more complex ensemble learning and SotA GP algorithms.

In the future, it could be interesting to investigate how 2SEGP can be integrated with SotA variation and selection methods. Moreover, 2SEGP could be improved by leveraging more advanced prediction aggregation methods (e.g., as
in [55] than simple majority voting or averaging. Knowledge of ensemble learning algorithms of different nature could also be transferred to 2SEGP [49,50]. The adaptation of 2SEGP to other types of representations than those typical of GP such as, e.g., neural networks of evolving topology [57], could also represent an interesting endeavor. Lastly, we remark that by learning an ensemble of many estimators, we loose a potential advantage of GP, i.e., the interpretability of the final solution [9,22,66,68]. Nevertheless, future work could consider the integration of feature importance and prediction confidence estimation, which are also important aspects to gain insights useful to trust machine learning [12,31,37].

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