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# A Multi-Population Hybrid Genetic Programming System

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Dissertation presented as partial requirement for obtaining the Master's degree in Advanced Analytics

NOVA Information Management School
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# A MULTI-POPULATION HYBRID GENETIC PROGRAMMING SYSTEM

by

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# ABSTRACT

In the last few years, geometric semantic genetic programming has incremented its popularity, obtaining interesting results on several real life applications. Nevertheless, the large size of the solutions generated by geometric semantic genetic programming is still an issue, in particular for those applications in which reading and interpreting the final solution is desirable. In this thesis, a new parallel and distributed genetic programming system is introduced with the objective of mitigating this drawback. The proposed system (called MPHGP, which stands for Multi-Population Hybrid Genetic Programming) is composed by two types of subpopulations, one of which runs geometric semantic genetic programming, while the other runs a standard multi-objective genetic programming algorithm that optimizes, at the same time, fitness and size of solutions. The two subpopulations evolve independently and in parallel, exchanging individuals at prefixed synchronization instants. The presented experimental results, obtained on five real-life symbolic regression applications, suggest that MPHGP is able to find solutions that are comparable, or even better, than the ones found by geometric semantic genetic programming, both on training and on unseen testing data. At the same time, MPHGP is also able to find solutions that are significantly smaller than the ones found by geometric semantic genetic programming.

# KEYWORDS

Machine Learning; Statistics; Computational Intelligence; Genetic Programming; Genetic Algorithm; Evolutionary Algorithm; Optimization Algorithm; Optimization Problem; Overfitting; Semantic Awareness; Multi-Objective System; Hybrid Genetic Programming; Parallel and Distributed;

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# 1 INTRODUCTION

Genetic Programming (GP) [Koz92] is a machine learning algorithm (typically used for supervised problems) that aims at finding programs - mathematical functions or computer programs - that best map inputs to outputs. It is called “genetic” due to the inspiration it takes from evolutionary biology. GP in fact belongs to the Evolutionary Computation class of algorithms.

A GP algorithm evolves a population of individuals (i.e. the programs) over the course of a prefixed number of generations. The evolution within a generation is carried out by the selection phase and the variation phase. The selection phase selects individuals (i.e. programs) based on their fitness into the variation phase - where fitness is captured by a set of objective functions to be optimized.

The variation phase is a means to search for fitter individuals by manipulating the ”genome” of the individuals - i.e. the genotypic (or syntactic) content of the program. In standard GP this is typically a crossover with a randomly selected crossover point or a mutation with a randomly selected mutation point. For a tree-based representation of programs, both these operations replace subtrees of a parent which consequently results in a new offspring. It should be noted that there are several other possible crossover and mutation operators. Each of these programs is considered to be an individual and a population of individuals is evolved for a prefixed number of generations. At the end of the evolution, the algorithm returns the fittest individual.

In recent years, many efforts to improve GP were undertaken [VCS14]. In particular, Moraglio et al. [MKJ12] found variation operators that have known effects on the semantics of the offspring individuals [Van17] - where semantics are defined by the vector of outputs of a program on the different training data. These operators constitute Geometric Semantic Genetic Programming (GSGP). The geometric semantic (GS) crossover and GS mutation operators are correspondingly defined as:

$$T_{XO} = T_R.T_1 + (1 - T_R).T_2$$

and

$$T_{MU} = ms.(T_{R1} - T_{R2}) + T$$

Where $ms$ is the mutation step constant; $R$, $R_1$ and $R_2$ are random real functions with codomain [0,1]; and $T$, $T_1$ and $T_2$ represent parents of the offspring. The semantics of a crossover offspring are the result of a geometric mean of the semantics of its parents, hence, regarding distance to the global optimum, the offspring cannot be worse than the worst of its parents.

GS mutation corresponds to a ball mutation that induces a unimodal fitness landscape [Van17] in supervised learning problems. A unimodal fitness landscape is that which is constituted by a single local optimum: the global optimum. To convince oneself of this property, any individual that is not the global optimum in the semantic space has at least one neighbor whose semantics are closer to the target values. To put it simply, there is virtually no risk of the algorithm being stuck in the non-existent local optima. It must be noted, this is one of the reasons this work opted to undertake only GS mutation, therefore excluding GS crossover.

However, GSGP comes at a cost regarding size of found solutions: GS operators take the entirety of the nodes of the parents to produce the offspring. This results in a linear size growth if using GS mutation and exponential growth if using GS crossover. In order to circumvent this issue, an efficient implementation of GSGP proposed by Castelli et al. [Cas+13] (which is used in this thesis) allowed for the application of GSGP in real-world datasets [Van+13]. It essentially puts aside building the genotypic constitution of individuals, thus evolving the population using only the semantics which are obtainable by the definition of the GS operators. Despite this, offline reconstruction (i.e. after evolution) still remains a problem due to the large size of GSGP individuals. Even when possible, readability and interpretability of the model produced by GSGP remains an issue.

In contrast, GP is not aggressive in size growth, at least by construction of its variation operators. Nevertheless, GP can incur in bloat, which is defined as the growth in size of the program without an improvement in fitness. In spite of GP facing the bloat issue, its solutions are yet acknowledged as parsimonious enough for readability and interpretability, being considered one of its main advantages [Koz10]. It is worth mentioning that such property of GP solutions ”shines” when bloat-limiting methods are used [SC09] [Tru+16] or when fitness and size are conjointly optimized in a multi-objective framework [VSD09].

Regarding performance of GSGP *versus* GP, it is important to note that GP is semantically blind in its crossover and mutation operators as they perform random operations on the syntax of individuals. This makes it frequently unable to find solutions that are competitive with those found by GSGP in terms of training error. In terms of unseen error, there is indication for the potentially better generalization ability [Van17] of GSGP on three pharmacokinetic datasets [Van+13] that are presented in this work as well.

The proposition of Multi-Population Hybrid Genetic Programming (MPHGP) algorithm is to be able to capitalize on the advantages of GP and GSGP and improve upon some shortcomings of the two. It essentially incorporates in its subpopulations GP and GSGP in an effort to make them complement each other. What is intended to capture with MPHGP is the generalization ability and optimization power of GSGP and the parsimoniousness of GP for readability and interpretability. This goal was not entirely achieved in the work presented in this thesis.

The remainder of this thesis is organized as follows: firstly the implementation of MPHGP is described, as well as how to properly configure GP and GSGP subpopulations; secondly results of MPHGP experiments are discussed starting from the simplest MPHGP configuration possible with just two subpopulations, followed by increasing this number and briefly discussing computational performance; lastly this thesis concludes with proposing research paths and closing remarks.

# 2 MULTI-POPULATION HYBRID GENETIC PROGRAMMING

The proposed MPHGP system presented here has two types of subpopulations, one running multi-objective genetic programming (MOGP) and another one running GSGP. The former optimizes size and training error and the latter optimizes only training error. Each subpopulation is assigned to a thread and evolution is carried out by running each in parallel. MPHGP is completely implemented in Java, which carries out and handles parallelism with the class Thread. The synchronization instants correspond to moments of migration between the subpopulations. These are prefixed by the migration frequency parameter $f$, i.e. migration moments occur every $f$ generations, thus each subpopulation evolves independently during $f$ generations.

Following Fernández et al. [FTV03], the migration direction is configured as a ring for any number of subpopulations. This means that if there are two subpopulations, the ring configuration corresponds to a simple exchange of individuals between the two subpopulations. If the number of subpopulations is, for instance, three, then subpopulation 1 sends its best individuals to subpopulation 2; subpopulation 2 to 3; and finally, subpopulation 3 sends migrants to subpopulation 1.

In order to provide a comparative framework, this work considers standalone versions denoted by MOGP and GSGP. The hybrid system is denoted by MPHGP (Multi-Population Hybrid Genetic Programming) and to refer its subpopulations, the terms sub-MOGP and sub-GSGP are employed. MOGP, GSGP and MPHGP run with a population size of 400 individuals each. Thus, if MPHGP has two subpopulations, this means that sub-MOGP and sub-GSGP run with 200 individuals each. All these variants are initialized using Ramped-Half-Half-Initialization [Koz92].

The migration policy is *best-to-worst*, meaning that the individuals selected to migrate replace the worst in their destination subpopulation. In order to keep the size of the overall population of MPHGP constant, a copy of these best individuals remains in the origin subpopulation, so as to not waste the genetic material found by the evolution of that subpopulation. Except where noted, the selection of best individuals to migrate changes according to the optimization criteria of the subpopulation: in sub-GSGP, this means simply picking the fittest; in sub-MOGP, to follow a multi-objective policy, this means picking the fittest starting from the best pareto front. Other migration policies, such as *random-to-random* or *best-to-random* are not explored in this thesis.

In a view to address cross-domain robustness of the approaches, these three GP variants are tested in 5 real-world symbolic regression problems described by Table 2.1. The problems %F, PPB and LD50 [Arc+07] pertain to problems in pharmacokinetics research aiding drug discovery - respectively to human-oral bioavailability, plasma protein binding level and toxicity. These problems use as input a set of molecular descriptors of a potential new drug. The Concrete [CVS13] problem pertains to predicting the strength of this material according to its features and the Energy [Cas+15] problem refers to predicting the energy consumption using as input meteorological data of that and previous days, for instance. All of these problems have already been used in previous GP studies. These problem sets cover different degrees of dimensionality as proxies to their level of difficulty. Finally, to address optimization and generalization ability, these datasets are split into 70% for training data and 30% for unseen (test) data and the median Root Mean Square Error (RMSE) of 30 independent runs is reported.

It ought to be noted that the %F dataset faces criticism due to the presence of raw data and missing data that ideally would be cleaned up and transformed beforehand. This cannot be the case for this thesis. From the perspective of developing a machine learning technique, it is preferable to observe its behavior with a hard dataset. Moreover, GP is a machine learning technique that performs data transformations and feature selection with its evolutionary process. Such behavior ought to be nurtured - namely, its ability to work around hard data - when designing new approaches to GP.

## 2.1 Intra-population Configuration

As it is known, GP faces the bloat problem, which is why a multi-objective GP (MOGP) that optimizes both size and training error - using Pareto-based NSGA-II [Deb+02] - was chosen to be included in MPHGP. Furthermore, no depth limit could be applied to MOGP, as it would make it incapable of interacting with GSGP

| Dataset | # Features | # Instances |
|---:|---:|---:|
| Bioavailability (%F) [Arc+07] | 241 | 206 |
| Protein Plasma Binding Level (PPB) [Arc+07] | 626 | 131 |
| Toxicity (LD50) [Arc+07] | 626 | 234 |
| Concrete [CVS13] | 8 | 1029 |
| Energy [Cas+15] | 8 | 768 |

**Table 2.1.:** Description of the test problems. For each dataset, the number of features (independent variables) and the number of instances (observations) are reported.

individuals whose depth is well beyond a traditional depth limit of 17. For example, a depth limit mechanism works by rejecting an offspring if its depth is beyond the limit (and keeping one of the parents as replacement) and only accepting otherwise. Enabling depth limits would mean making sub-MOGP be a storing subpopulation that would just return sub-GSGP individuals from previous migration instants. Furthermore, MOGP that includes size as an objective to be minimized is aggressive in reducing size of individuals: notice how an individual with only one node is in the first pareto front regardless of its uselessness in capturing the complexities of the dataset and its training error. The selection mechanism - pareto rank selection (NSGA-II) - is thus going to consider such small individuals as among the fittest.

GSGP uses the aforementioned efficient implementation [CSV15] and has a crossover rate of 0. This is justified because geometric semantic mutation does not increase size as dramatically as geometric semantic crossover would, making MPHGP testable in useful time - notice that GSGP individuals have to be built at each migration instant and that MOGP cannot work on these individuals offline! Note that GS mutation builds up from a single individual rather than from two entire individuals. This is also convenient in offline rebuilding of the fittest individual after an evolution has ended, and, in the context of MPHGP, at migration instants: with only mutation, each individual has only a single parent, and after $g$ generations, the fittest individual will have $g$ ascendants to look up in the offline records. [1] In the opposite extreme case of only crossover, each individual will have two parents, meaning that the winning champion will have to be rebuilt upon $2^g$ parents and looking up such an amount of individuals is an expensive task itself. For this reason, crossovers are handled by sub-MOGP only, which will be in charge of making crossovers between sub-GSGP individuals and its own small individu-

[1] I.e. the hash tables storing the references to relevant individuals in the history of the evolution of GSGP, random trees generated along generations and the respective variation operations performed.

| Parameter | MOGP | GSGP |
|---|---|---|
| Objectives | training error and size | training error |
| Crossover Rate | 0.9 | 0 |
| Elitist Survival | 5 | 5 |
| Tournament Size | 15 | 15 |
| Parent Selection Method | Pareto Rank Selection | Tournament Selection |
| Mutation Step | - | 1.0 |
| Bounded Mutation | - | Yes |
| Migrant Selection | multi-objective | single-objective |

**Table 2.2.:** Synthesis of the parameter tuning for the tested 2-Population Hybrid Genetic Programming (MPHGP-2) system. In order to provide a comparative basis, standalone MOGP (with 400 individuals) and standalone GSGP (with 400 individuals as well) follow the same tuning as the one reported here for the MPHGP-2 subpopulations, each of which with a size of 200 individuals. Multi-objective migrant selection means picking the fittest from the first pareto rank, then from the second pareto rank and so on.

als.

The cosine function is included along with protected division, multiplication, addition and subtraction operators. Generally it improves fitness, generalization ability and reduces size. Please refer to Figures A.1 to A.5 and Tables A.1 to A.5, where standalone MOGP and GSGP are measured against their equivalents without the cosine operator. It is observed that regardless of the dataset, the cosine operator allowed for a reduction in size for GSGP while improving or retaining training error and (or) unseen error - except for the exquisite LD50 dataset. Differences are not notable in MOGP due to the aforementioned issue that it cherishes a small number of nodes excessively, which may have hindered this algorithm from actually taking advantage from the cosine function the way GSGP did. For this reason, the cosine was opted to be included in the MOGP subpopulations of MPHGP, a context in which sub-MOGPs will definitely be operating with individuals of greater sizes that they receive from sub-GSGPs.

To evaluate MPHGP, standalone versions of the subpopulations were run. Thus, standalone MOGP with 400 individuals and standalone GSGP with 400 individuals serve as reference to evaluate MPHGP against, where MPHGP is constituted by a subpopulation running MOGP (sub-MOGP) with 200 individuals and with a subpopulation running GSGP (sub-GSGP) with 200 individuals. When increasing the number of subpopulations of MPHGP, its overall population size remains constant. Table 2.2 describes the configuration and tuning of MOGP, GSGP and, by inheritance, that of the subpopulations of MPHGP.

The number of elite survivors is unusually high and fixed at 5. Considering the case of MOGP, which has a tendency of being blind to optimization quality in favor of lower size, this is meant to keep the fittest individuals in place of the smallest of the new generation with no comparable quality - hence, the selection of elites and deletion of the worst individuals was purely single-objective even in MOGP. In the case of GSGP, this is based on the idea of growth along generations: individuals from previous generations are expected to be smaller than those of the current generation [CVP15]. Elitism in GSGP is used not only under the perspective of keeping solutions of better fitness but also of keeping other solutions that may slow down size growth.

Similarly to the number of elite survivors, the tournament size is high as well. It follows the rule of 7.5% of subpopulation size with a minimum constraint of 3 individuals - this pertains to a higher number of subpopulations, which is mentioned in Section 2.4. For a 2-population MPHGP, this equates to 15 individuals. Regarding MOGP (remind that it uses ”pareto rank selection” from NSGA-II), in the event that very small solutions are randomly drawn to the selection phase, it is desirable that such solutions do not have an excessively higher probability of being selected than solutions of better optimization quality, and increasing tournament size is equivalent to approximating to a uniform density function. In the case of GSGP, this increases the chances of finding the fittest solution, given tournament selection.

## 2.2 Inter-Population Parameter Tuning

For the analysis of a 2-population MPHGP system, the effect of varying two migrational parameters is discussed in this section. The first one is the migration frequency $f$, which is defined as the number of generations that each subpopulation uses to evolve independently from the other one. The second parameter to be discussed is the migration rate $r$, the percentage of the subpopulation size that determines the integer number of migrants. For instance, if the MPHGP system is split into two subpopulations, each will have a size of 200 individuals. Then, for a migration rate of 0.15, MOGP will send its best 0.15 * 200 = 30 individuals to GSGP and this subpopulation in its turn will return its fittest 30 individuals to MOGP. This study covers migration frequencies $\{$25, 50, 100$\}$ that result correspondingly to $\{$12, 6, 3$\}$ migration instants in 300 generations; and migration rates $\{$0.05, 0.15, 0.25, 0.35$\}$ that correspond to $\{$15, 30, 45, 60$\}$ individuals migrating from each subpopulation. This results in 12 combinations of migration parameters that were ran for the 5 datasets across 30-independent runs.[2]

For each dataset, Figures A.6 to A.10 show on the left-hand side line plots for the median training and unseen errors, where unseen errors are portrayed by dotted lines; and a right-hand side plot for the size. Each row in each these figures pertains to a migration frequency $f$ and all migration rates are plotted together. One observes that migration rates are generally ineffective in median terms, at least for a given migration frequency.

To further look into this matter, matrices of $p$-values for the Wilcoxon Rank-Sum test - testing whether two samples come from the same distribution - between the results of two migrational parameter combinations are provided in Tables A.6 to A.25. If one wants to check for the statistical significance of effects of migration rate for a given migration frequency, one only needs to look at the "blocks" in the diagonal of these tables. In most cases, there is close to no difference in varying the migration rate for a fixed migration frequency. The "blocks" standing outside the diagonal represent cross-frequency $p$-values. In these cases, the difference is more noticeable, indicating the higher impact of varying migration frequencies.

Overall the combination $f = 50$ and $r = 0.15$ seemed to obtain the best results across the datasets. For this reason and the sake of simplicity, the migrational parameters are generally fixed to these values and the analysis in the following sections is to be seen as one of *coeteris paribus*.

## 2.3 2-Population Hybrid Genetic Programming

The work included in this section is already published and was presented by the author in an international conference [VG17]. The results presented pertain to migration frequency 50 and migration rate 0.15 for a MPHGP with two subpopulations, except where noted. In this section it is attempted the study of MPHGP against the standalone MOGP and GSGP versions as well as the exercise of studying the relationship between GSGP and MOGP subpopulations of MPHGP - these are denoted as sub-MOGP and sub-GSGP in the introspection Figures A.16 to A.21.

The reported results show that MPHGP is able to at least retain the best training and unseen errors from the subpopulations. In some cases, improvement on one

[2] Please note that this resulted in $12 * 30 * 5 = 1800$ runs just for MPHGP results pertaining to this section.

of these measures can be observed. General statements cannot be made about the obtained size of solutions for a 2-population hybrid system.

In the Bioavailability case (Fig. A.11 and Table A.26) MPHGP retained the training error and improved both unseen error and size. To understand how the algorithm got to this outcome, it is useful to look into the behaviour of each subpopulation in Fig. A.16. Note that MPHGP picks the best individual on training error from the two subpopulations to be reported, and each subpopulation reports only its best individual on training error to be reported as well. The first migration event takes place after evolving generation 50, at which point sub-GSGP is leading on training error, thus these fitter individuals emigrate to sub-MOGP, which causes not only sub-MOGP to improve its fitness but also to take in the size of these individuals, causing the spike in its median size at generation 50.

It is after this moment that sub-MOGP takes over the lead of MPHGP, suggesting that its NSGA-II selection mechanism and standard variation operators are more suitable for the sub-GSGP individuals at this moment of the evolution of MPHGP. Leadership in training error is important to help determine what way size will shift to at each migration event. With this notion in mind, one can observe that size of sub-GSGP shifted downwards at migration instants of generation 100 and 150: it is because sub-GSGP applied its operators on the fitter and smaller individuals that came from sub-MOGP and updated its best individual accordingly. For the remaining generations, sub-GSGP takes back the leadership and does not stem away from its size evolution trajectory anymore as sub-MOGP becomes a passive participant of MPHGP.

This aspect is important to the success of a basic hybrid system: each subpopulation ought to be an active participant in the evolution process and this is verified with the exchange of leadership in fitness between the subpopulations. To put it in other terms, what use would be of MPHGP if sub-GSGP led throughout the entire evolution? Is MOGP contributing at all in this case? Would it not be better to run only GSGP instead with offline reconstruction of individuals and end the run sooner instead of forcing MOGP to build large individuals? One has to ensure active participation of all subpopulations in MPHGP to reach the goals of this algorithm.

In the case of the PPB dataset (Fig. A.12 and Table A.27), at the end of 300 generations, MPHGP almost retains the median training error of GSGP, is identical to GSGP in median terms of unseen error and achieved effective size reduction. In introspection (Fig. A.17), it is observed that, unlike the Bioavailability case, sub-

MOGP has the lead before the first migration instant, and concedes it indefinitely to sub-GSGP from this moment onwards. The main observation one can make is that there is only one size reduction event that takes place in the evolution of MPHGP: at the first migration instant (generation 50) when sub-MOGP dominates in training error and in size. As no fitter and smaller individuals from sub-MOGP arise in the remaining generations of the evolution of MPHGP, sub-GSGP runs on its own and sub-MOGP merely becomes a follower. MPHGP finds a more parsimonious solution (in terms of size) than GSGP due to this single occurrence. Refer to Table A.27 for the statistical significance of these results.

In the Toxicity dataset, MPHGP was only better in terms of training error - Fig. A.13 and Table A.28. In fact the best performing algorithm for 300 generations was MOGP with the lowest reported median unseen error and size. When looking into introspection (Fig. A.18), it is verified that GSGP played the passive role throughout all of the 300 generations. It is also observable that the spikes in size occurred only with the migration moments every 50 generations, meaning that the fittest on training error from MPHGP lied in the sub-MOGP. Further proof that MPHGP gravitated towards solutions of MOGP lies in Table A.28, where one can observe that MPHGP does not differ significantly from MOGP.

Finally for the Concrete and Energy datasets, statistically significant size reduction was not achieved by employing the base MPHGP. A special strategy - denoted by MPHGP* - to be able to achieve this result with two subpopulations can be synthesized by force-feeding sub-MOGP individuals into sub-GSGP. For this goal, two changes were applied to MPHGP:

- The selection of emigrants in sub-MOGP is single objective on training error, so as to increase the chances of these individuals of being selected in sub-GSGP.
- Sub-GSGP only sends one individual to sub-MOGP.

Moreover, migration rate of sub-MOGP* is increased to 0.35. The Concrete dataset achieved always the same results in median terms for size, training error and unseen error. However, looking at the box plot of size in Fig. A.14, one can quickly observe that the distribution of MPHGP* results differ from those of GSGP and MPHGP in that the 25% quantile drops. The Rank-Sum test in Table A.29 proves that the distribution of size results of MPHGP* is statistically different than that of GSGP. Introspecting the behavior of MPHGP and MPHGP* in the Concrete dataset (Fig. A.19), there is visibly no difference in median terms between the two.

This suggests that in the case of MPHGP*, sub-MOGP* individuals were being more frequently mutated and performant in sub-GSGP*, even becoming the fittest in some runs. If this is the case, then there is support for MPHGP: there is no full reliability on the first migration instant nor on the hope that MOGP leads at such moment. This means that another way to improve MPHGP could be to properly tune or find better algorithms for each of the subpopulations.

For the Energy dataset (Fig. A.15 and Table A.30), MPHGP* had its migration frequency dropped to 25 (Figures A.20 and A.21, respectively) in order to take advantage of the leadership of sub-MOGP* at this moment of the evolution, causing sub-GSGP* to "reset" the size of its fittest individual after the first migration instant. In fact, the difference in size between MPHGP* and MPHGP and GSGP is due to this single "reset" and one can observe that despite this gap, the growth trend of MPHGP is identical to that of GSGP. Yet significant size decrease was achieved as showed in Table A.30.

This closes the study of a 2-population MPHGP system. In general, this system with basic configurations was able to keep the performance in training and unseen error of the standalone versions, or even improve in some cases. With regards to size, this strategy is not robust, which justified running MPHGP* with its tweaks. Nonetheless, active participation (leadership exchange on training error) of all subpopulations is important for the effectiveness of a basic MPHGP algorithm on reducing size of found solutions when two different subpopulations are evolving individuals in different size ranges. In other words, it is necessary to ensure that subpopulations run on par with each other in terms of training error in order to achieve the important "collaboration" between them. The case of the Concrete dataset showed that, in spite of having sub-MOGP be a passive participant, sub-MOGP can still influence sub-GSGP to bring down the size of solutions.

## 2.4 Increasing Number of Subpopulations

The work in this section was done at a time later than the paper [VG17] submission to CEC2017, but could as well be part of another paper to be published. As mentioned before, specific strategies were used for the Concrete and Energy datasets with two subpopulations: migrant selection in MOGP is single objective on training error and GSGP only sends one individual to MOGP. As this strategy proved already that it can be effective, baseline MPHGP was chosen to run for all datasets in an attempt to verify the potential robustness of only increasing the number of subpopulations.

| Number of Subpopulations | Subpopulation Size | Tournament Size | Elite Survivors | Migrants |
|---|---|---|---|---|
| 2 | 200 | 15 | 5 | 30 |
| 4 | 100 | 7 | 5 | 15 |
| 8 | 50 | 3 | 5 | 7 |
| 20 | 20 | 3 | 5 | 3 |
| 40 | 10 | 3 | 5 | 1 |

**Table 2.3.:** Changes in subpopulation size, tournament size, number of elite survivors and number of migrants according to the increasing number of subpopulations. Overall population remains constant at 400 individuals. Tournament size obeys to the rule of 7.5% of subpopulation size with a floor constraint of 3. Number of migrants obeys to the constant migration rate $r = 0.15$. It is attempted to study the impact of only changing the number of subpopulations.

The number of subpopulations tested were 4, 8, 20 and 40. In order to capture the effect of varying only this parameter as much as possible, only tournament size was adapted for each number of subpopulations and is determined by a rule of [0.075 * subpopulation size] subject to a minimum of three. In order to have a clear picture of how these runs were performed, please refer to Table 2.3. Increasing the number of subpopulations generally proved to be effective in reducing the size of the solutions found.

For the Bioavailability dataset (Fig. A.22, Table A.31), and for an increasing number of subpopulations, median training error increased slightly, but generalization ability of the solutions found by MPHGP was kept and their respective sizes decreased. This can be considered a successful experiment that is also verified for the PPB (Fig. A.23, Table A.32) and Energy datasets (Fig. A.26, Table A.35). The effect of decreasing size seems to reach a plateau at 8 subpopulations for the Bioavailability and PPB datasets. Since increasing the distribution of the population yet retains the generalization ability, one may state that 40 subpopulations is optimal for the cases of Bioavailability, PPB and Energy, as computation time decreases as discussed in section 2.5.

In other datasets the story differs. For the Toxicity dataset (Fig. A.24, Table A.33), overfitting increased with an increasing number of subpopulations as well as the size of the solutions found. Finally, for the Concrete dataset (Fig. A.25, Table A.34) a pure trade off is verified with the size of solutions decreasing in detriment of their performance. In cases such as this one it is impossible to determine the optimal number of subpopulations, however, knowing that increasing it decreases size, this may be a starting point depending on how much one values interpretability over performance.

Focusing on the achievement of size reduction and following the argument given in Section 2.3, a possible explanation is that sub-GSGPs with smaller search space - that is, smaller subpopulation sizes - evolve at a slower pace, which puts them more on par with sub-MOGPs. This allows sub-GSGPs to welcome sub-MOGPs more receptively and ultimately capitalize on individuals of lower size. Looking at the results in a positive light, no special tweaks from MPHGP* were necessary to find statistically significant smaller solutions. In the specific case of the Toxicity dataset, in which sub-MOGP has more optimization power than sub-GSGP, increasing the number of subpopulations increased the relevance of sub-GSGP in optimizing fitness, which is why MPHGP tended to solutions of higher size.

## 2.5 Running Times

The results in this section correspond to the following available data on running times:

- MOGP-ß, standalone multi-objective GP, optimizing training error and size, without the cosine operator.
- GSGP-ß, standalone single objective Geometric Semantic Genetic Programming, without the cosine operator.
- MPHGP*-2, the MPHGP with two subpopulations, where MOGP selects migrants on training error only and GSGP only sends one individual to MOGP. With $f = 5$ and $r = 0.5$.
- The remaining MPHGPs are those of Section 2.4, with the number of subpopulations increasing.
- For the Energy dataset, the migration frequency is set to 25; for the remaining datasets it is set to 50.

As mentioned before, increasing the number of subpopulations reduces the size of the best found solution, which contributes to having less nodes being evaluated per average individual in the population. Furthermore, subpopulations run in parallel until the prefixed migration instant, which means that more computation is being performed simultaneously, in the sense that instead of having one thread going over each of 400 individuals sequentially, there are, for instance, 20 threads going sequentially over just 20 individuals at the same time.

These two factors both contribute to the decreasing computation time with increasing number of subpopulations as verified in Fig. A.27 and in Fig. A.36. The only exception would be for the Toxicity dataset - which always yielded better results with MOGP for 300 generations - where the size of the best found individual increased with the number of subpopulations, by tending to sub-GSGP solutions.

Generally, the more data instances a dataset has, the longer it will take to complete a run. For example, note the largest dataset in instances, Concrete. Increasing the number of subpopulations had the effect of reducing the size of solutions found, which allowed for faster running times. Moreover, these lower running times make the option of cross-validation a more realistic undertaking, at least for the datasets presented in this work.

# 3 CONCLUSION

This thesis proposed a hybrid model to combine a multi-objective GP and GSGP, two subpopulations that run independently until a prefixed migration instant or synchronization moment when the two subpopulations exchange individuals. The experimental results on five real-world symbolic regression problems show that MPHGP is able to retain the advantageous properties of any of the algorithms while finding statistically significant smaller solutions, namely, than GSGP.

There are caveats to this work however. Firstly, while MPHGP was able to decrease size, such solutions remain yet greater than desirable for the interpretability and readability in any of the problems. Thus, this work ought to be seen as one of first step in that direction.

Moreover, the increase in size of MPHGP solutions as generations go by follow the same trend as GSGP for a 2-Population Hybrid system, except for the Bioavailability (%F) dataset. Increasing the number of subpopulations helped getting away from such trend, mainly because of the compacter search-space of each subpopulation, which ”allowed” for the subpopulations to be on par with each other more frequently, thus exchange of individuals was more valuable.

Secondly, the bar was lowered with using only mutation in GSGP: size growth is linear, as well as the number of ascendants of an individual. This allowed for the reconstruction of individuals to be trivial at each migration instant. This decision was undertaken for the sake of executing runs in useful time in a setting where MOGP would be responsible for crossovers. Hence, the crossover was never semantically aware and that is a case to be covered when the challenge of dealing with exponential growth is well handled.

Some may argue that this is just extra work on top of GSGP. Without a doubt, sub-GSGP was doing all the work on its own in some cases, but not in the cases where the number of subpopulations was higher, as mentioned before. However this extra work proved to be worthwhile: while MPHGP retains train and unseen errors of GSGP, in some cases it boosted one of these measures![3] Such a fact would have gone unnoticed without this extra work and it shows that sub-GSGP and sub-MOGP can complement each other.

Future work includes new research paths. Notice that there are several GP variants out there that can be included in a hybrid system and it is yet to be known how well they would interact in such environment or how well they would benefit or benefit from GSGP. In specific, some of the most sophisticated known algorithms of simplification of mathematical expressions [ZZS05] ought to be included among the subpopulations of MPHGP. Given the results presented by this work, it is a given that these simplification algorithms will not be carrying out such a task by themselves!

An ambitious future work is to define a dynamic and versatile parallel and distributed hybrid GP system. While this work was rather parsimonious in the parameter configuration, ideally one can build a hybrid system that subjects to evolution number and size of subpopulations; algorithms executed in different subpopulations; and respective parameters. As a result, these would change during the run according to specific criteria.

[3] Fig. A.13 for an example of a boost on training error; Fig. A.11 for an example of a boost on unseen error.

# A APPENDIX: FIGURES AND TABLES OF RESULTS

## A.1 COSINE VS. NO COSINE

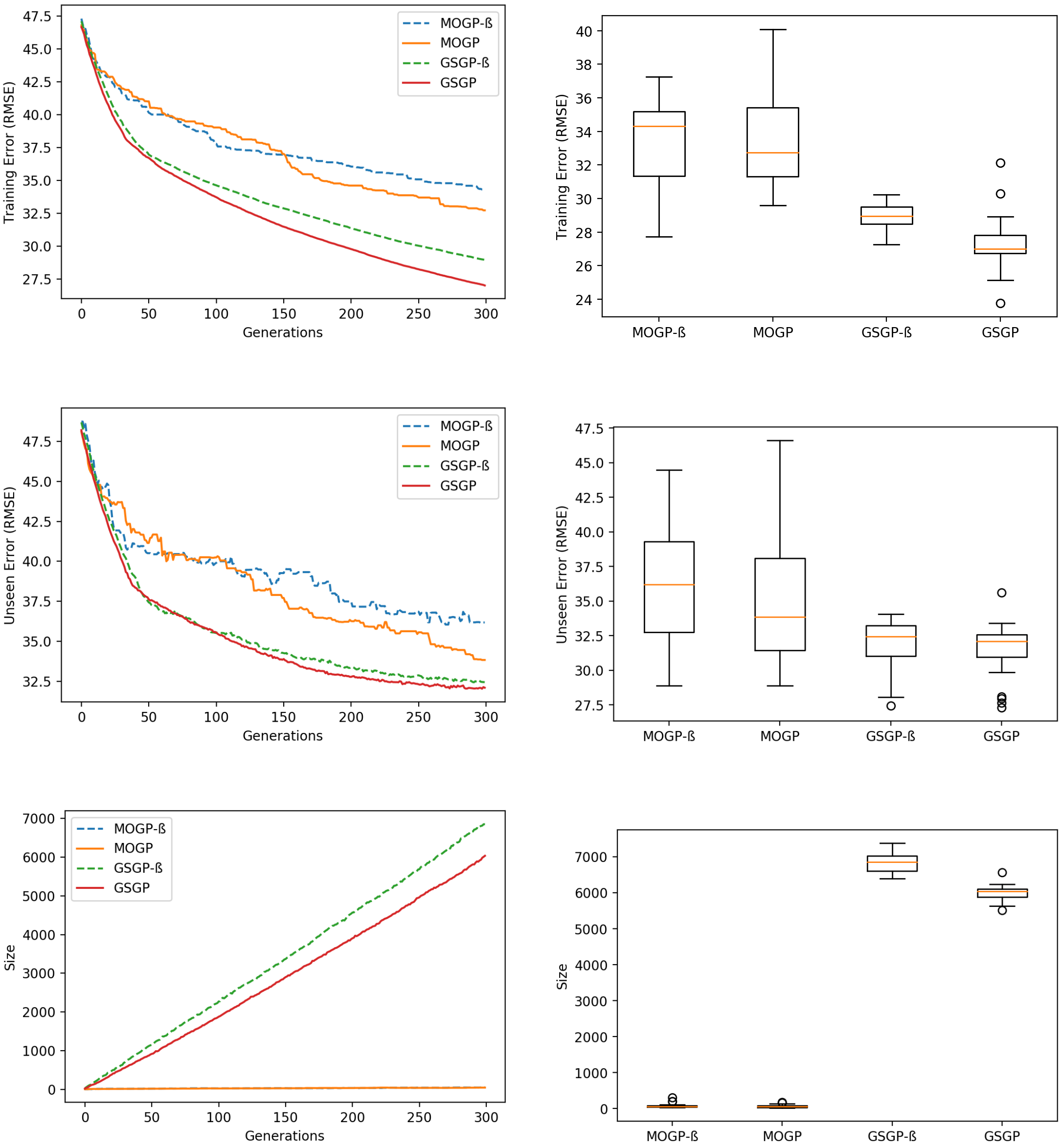


**Figure A.1.:** Bioavailability (%F) - standalone MOGP and GSGP (with the cosine function); and standalone MOGP-ß and GSGP-ß (without the cosine function).

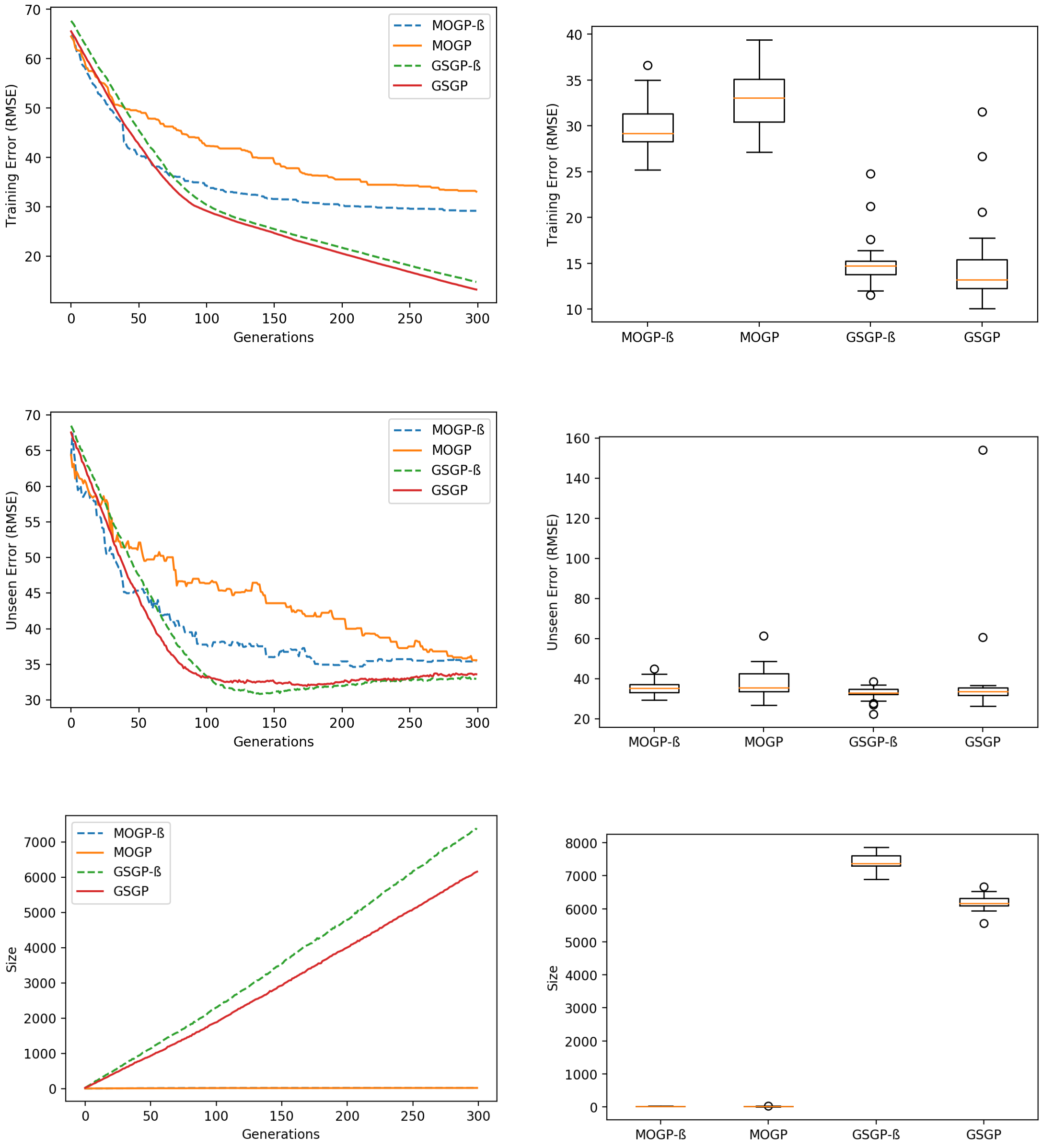


**Figure A.2.:** PPB - standalone MOGP and GSGP (with the cosine function); and standalone MOGP-ß and GSGP-ß (without the cosine function).

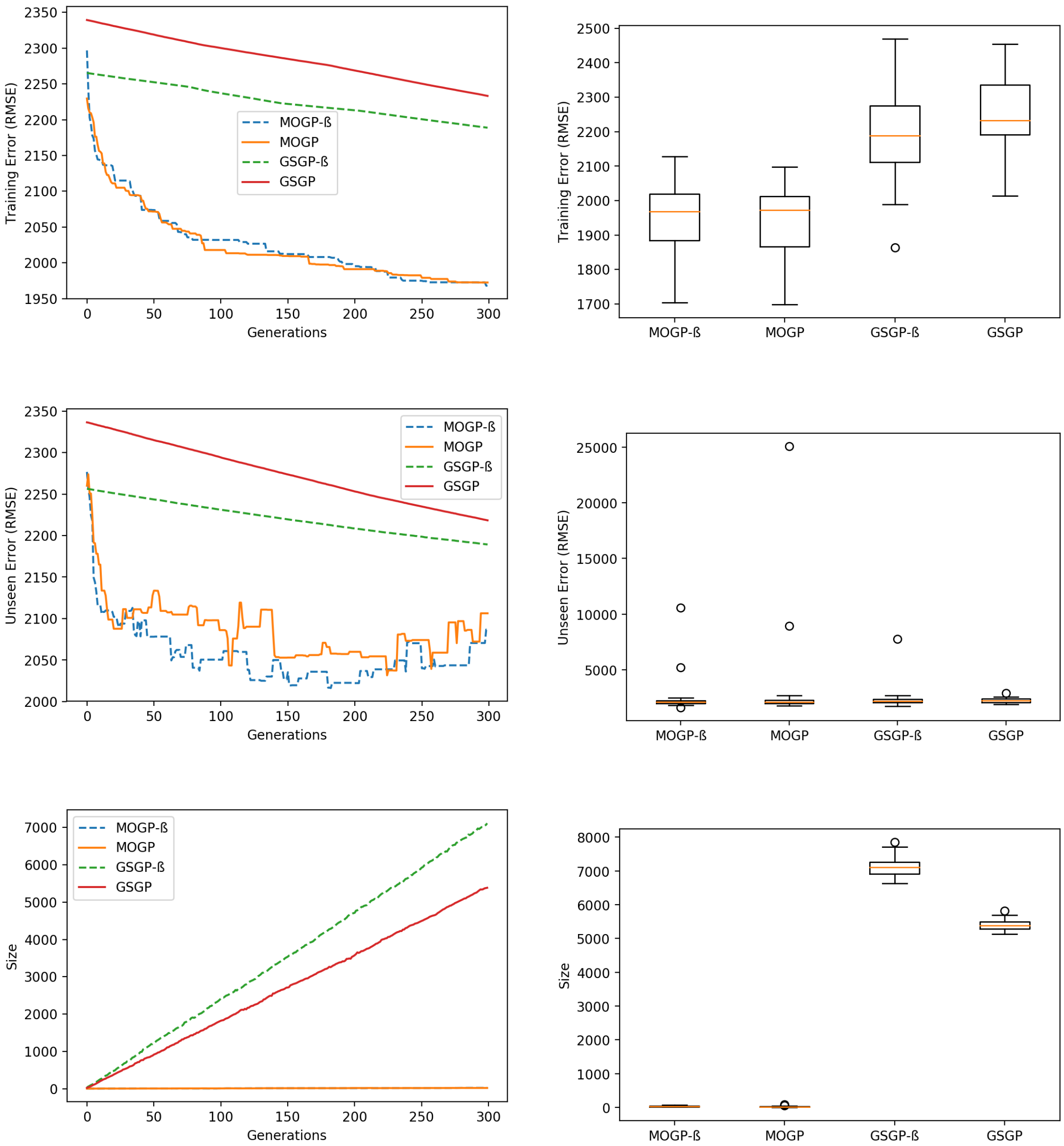


**Figure A.3.:** Toxicity (LD50)- standalone MOGP and GSGP (with the cosine function); and standalone MOGP-ß and GSGP-ß (without the cosine function).

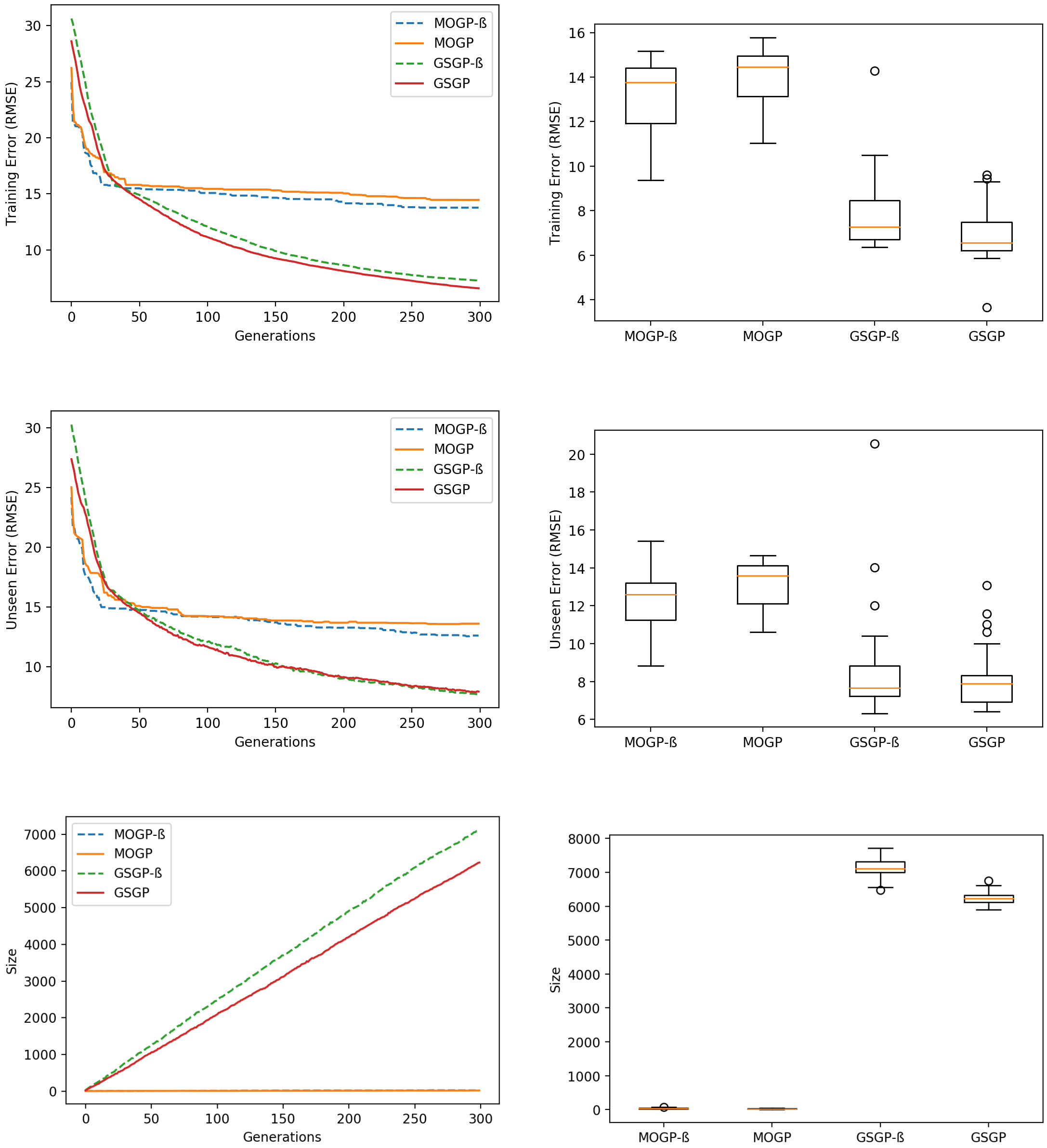


**Figure A.4.:** Concrete - standalone MOGP and GSGP (with the cosine function); and standalone MOGP-ß and GSGP-ß (without the cosine function).

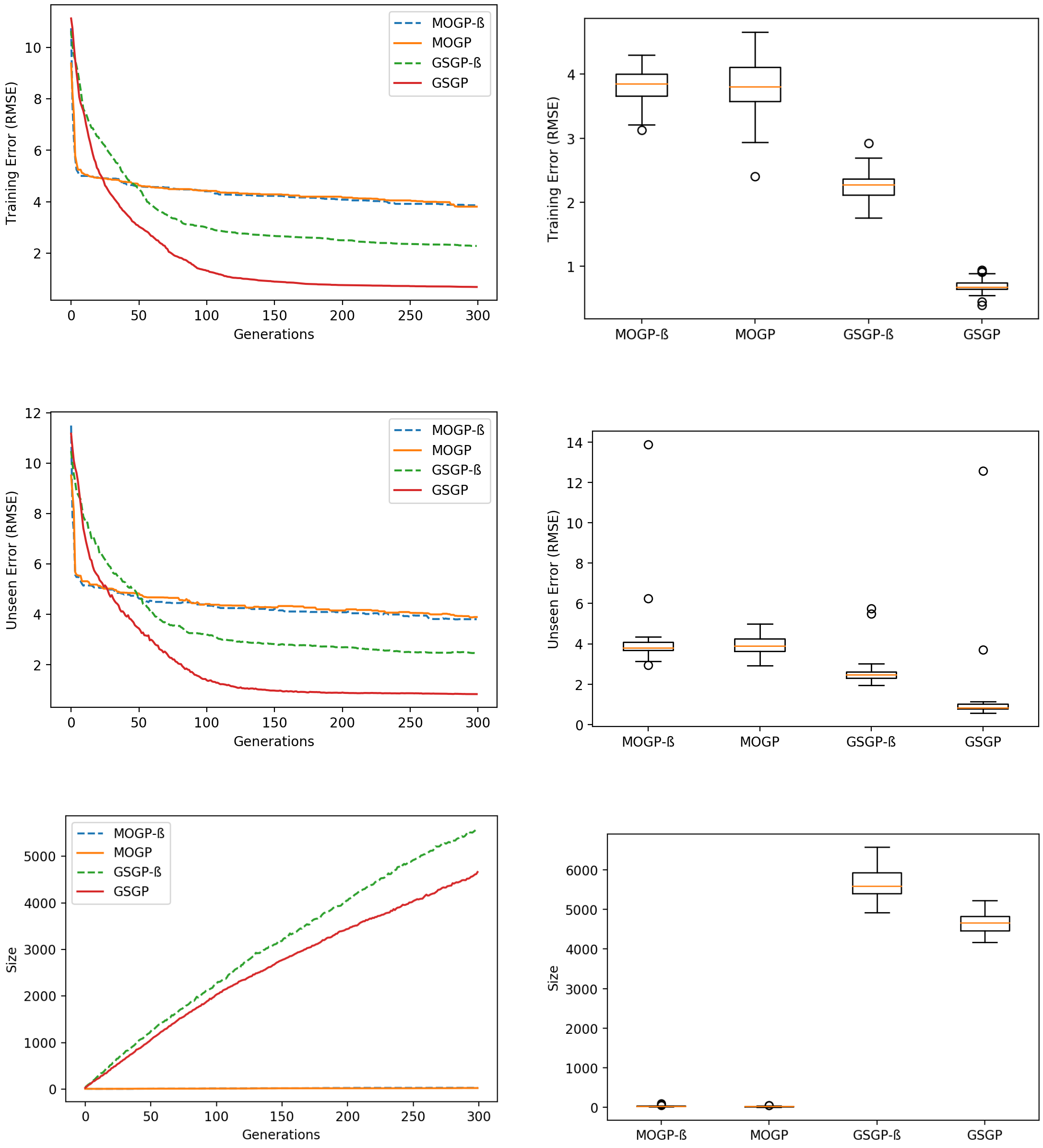


**Figure A.5.:** Energy - standalone MOGP and GSGP (with the cosine function); and standalone MOGP-ß and GSGP-ß (without the cosine function).

| %F | Train | Unseen | Size |
|---|---|---|---|
| MOGP-ß vs MOGP | 0.74987 | 0.22102 | 0.50378 |
| GSGP-ß vs GSGP | 2.84E-05 | 0.13591 | 1.92E-06 |

**Table A.1.:** Bioavailability (%F) - Statistical significance of cosine function according to $p$-values Wilcoxon Rank-Sum tests. Significance at 5% is highlighted in light grey, stating that the distribution of results differs.

| PPB | Train | Unseen | Size |
|---|---|---|---|
| MOGP-ß vs MOGP | 0.00057 | 0.44052 | 0.13779 |
| GSGP-ß vs GSGP | 0.06871 | 0.17138 | 1.73E-06 |

**Table A.2.:** PPB - Statistical significance of cosine function according to $p$-values Wilcoxon Rank-Sum tests. Significance at 5% is highlighted in light grey, stating that the distribution of results differs.

| LD50 | Train | Unseen | Size |
|---|---|---|---|
| MOGP-ß vs MOGP | 0.97539 | 0.81302 | 0.11080 |
| GSGP-ß vs GSGP | 0.00148 | 0.29894 | 1.73E-06 |

**Table A.3.:** Toxicity (LD50) - Statistical significance of cosine function according to $p$-values Wilcoxon Rank-Sum tests. Significance at 5% is highlighted in light grey, stating that the distribution of results differs.

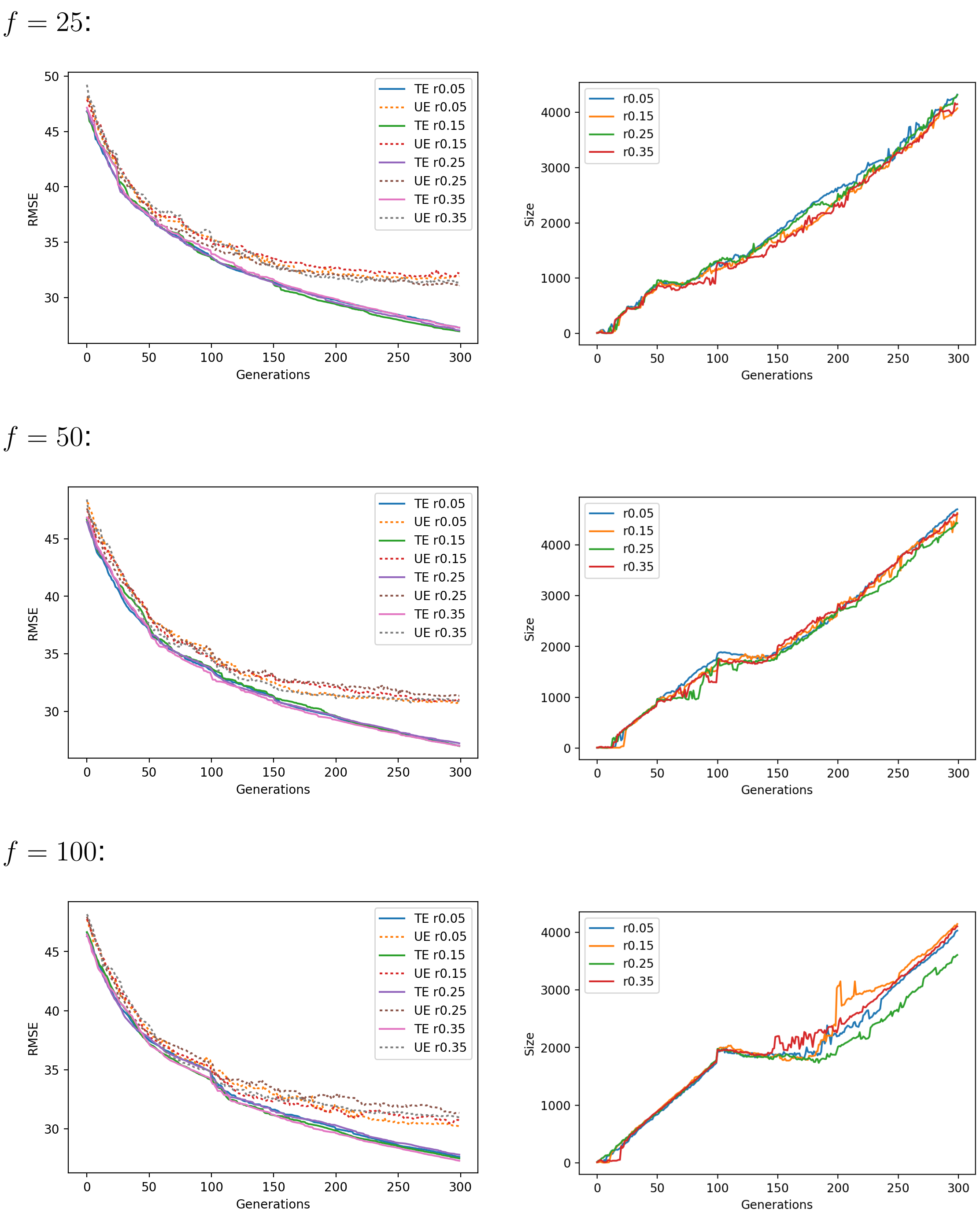
| Concrete | Train | Unseen | Size |
|---|---|---|---|
| MOGP-ß vs MOGP | 0.01852 | 0.02564 | 0.06408 |
| GSGP-ß vs GSGP | 0.01752 | 0.65833 | 1.73E-06 |

**Table A.4.:** Concrete - Statistical significance of cosine function according to $p$-values Wilcoxon Rank-Sum tests. Significance at 5% is highlighted in light grey, stating that the distribution of results differs.

| Energy | Train | Unseen | Size |
|---|---|---|---|
| MOGP-ß vs MOGP | 0.95899 | 0.71889 | 0.03222 |
| GSGP-ß vs GSGP | 1.73E-06 | 0.00003 | 1.73E-06 |

**Table A.5.:** Energy - Statistical significance of cosine function according to $p$-values Wilcoxon Rank-Sum tests. Significance at 5% is highlighted in light grey, stating that the distribution of results differs.

## A.2 Inter-Population Parameter Tuning

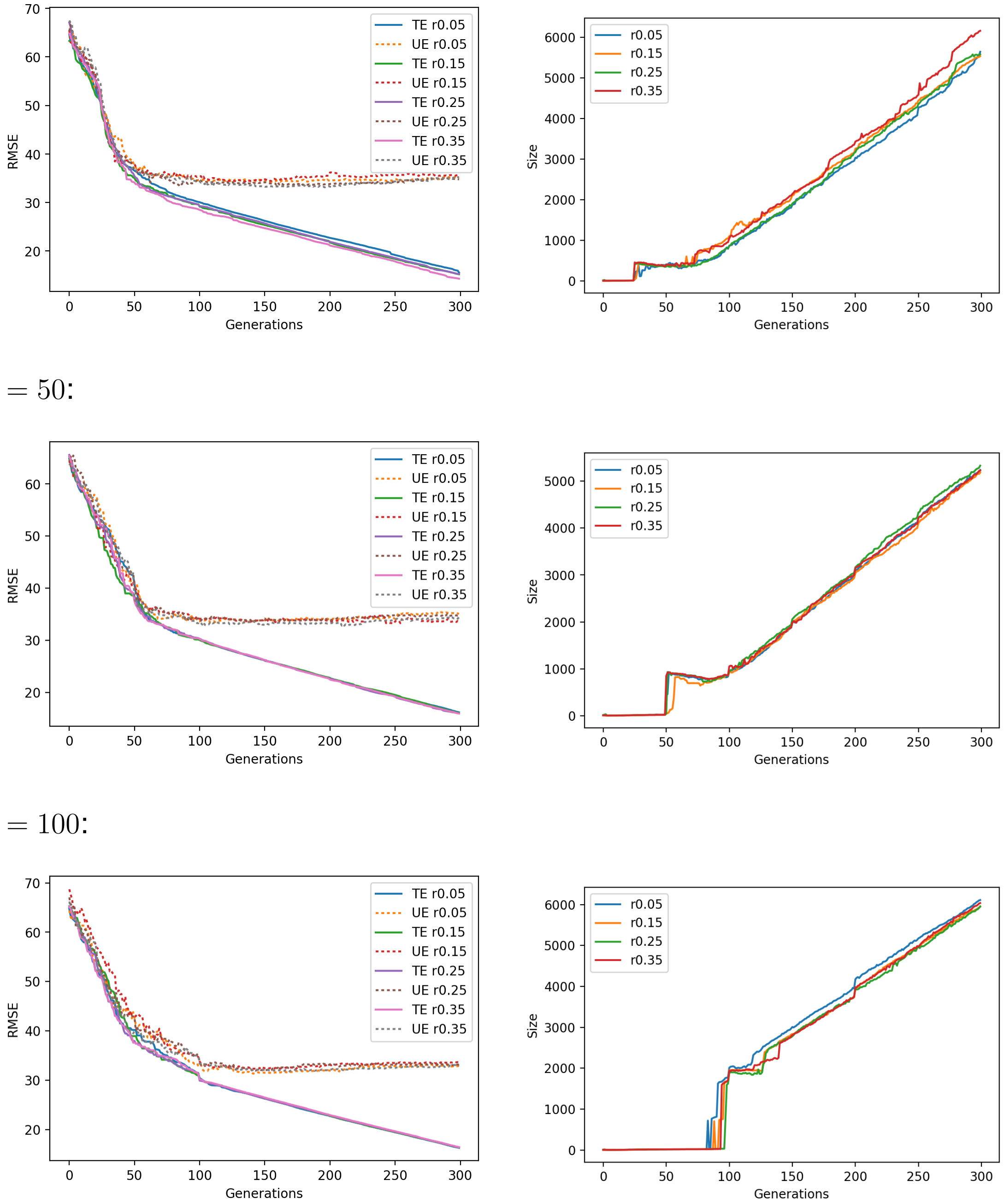


$f = 25$:

$f = 50$:

$f = 100$:

**Figure A.6.:** Bioavailability (F%) - Comparison of combinations of migrational parameters: first column plots training error (TE) together with unseen error (UE) and the second plots size. Each row pertains to a migration frequency $f$ from the set $\{25, 50, 100\}$. In each plot, every tested migration rate $r$ in the set $\{0.05, 0.15, 0.25, 0.35\}$ is present.

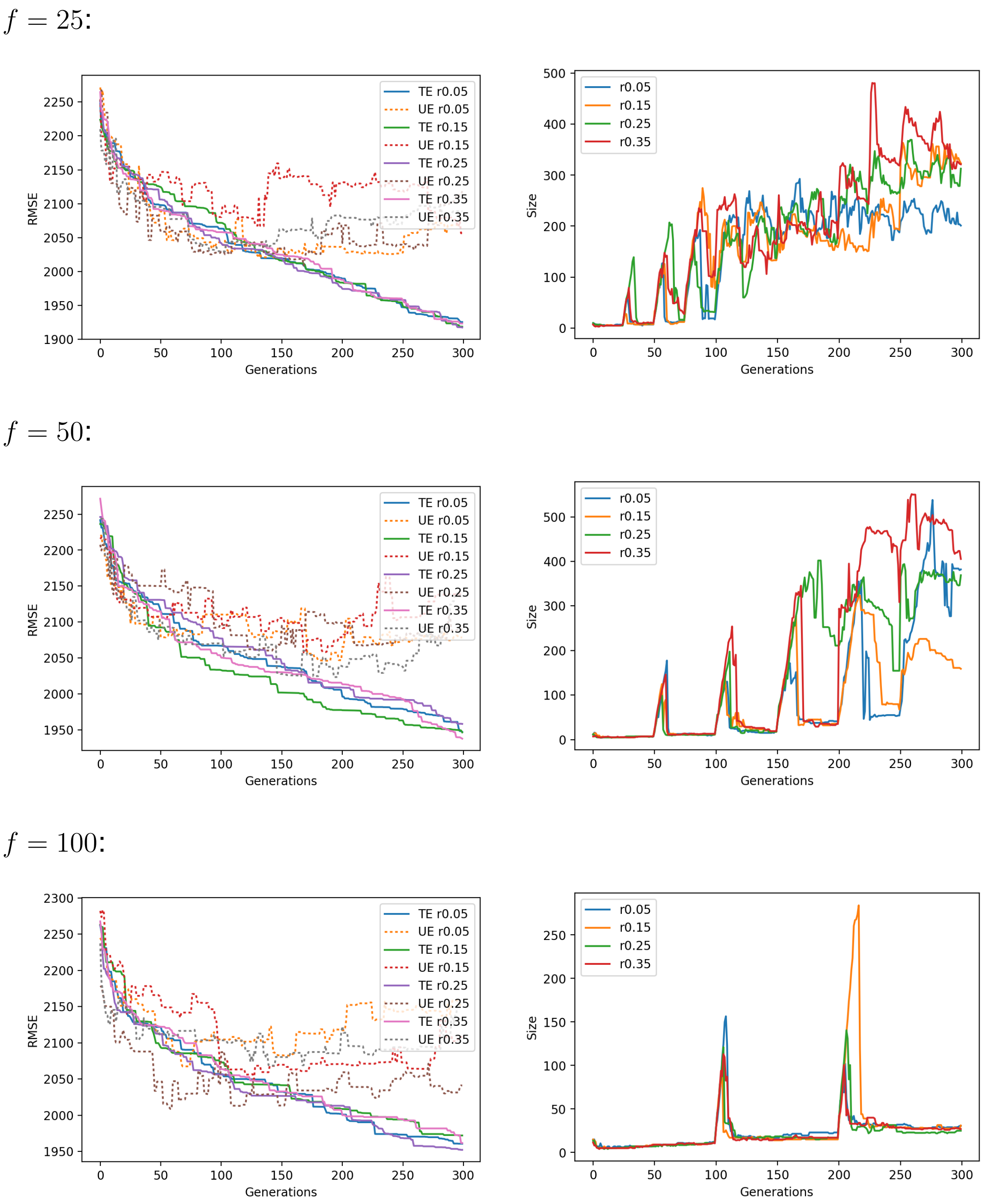


$f = 25$:

$f = 50$:

$f = 100$:

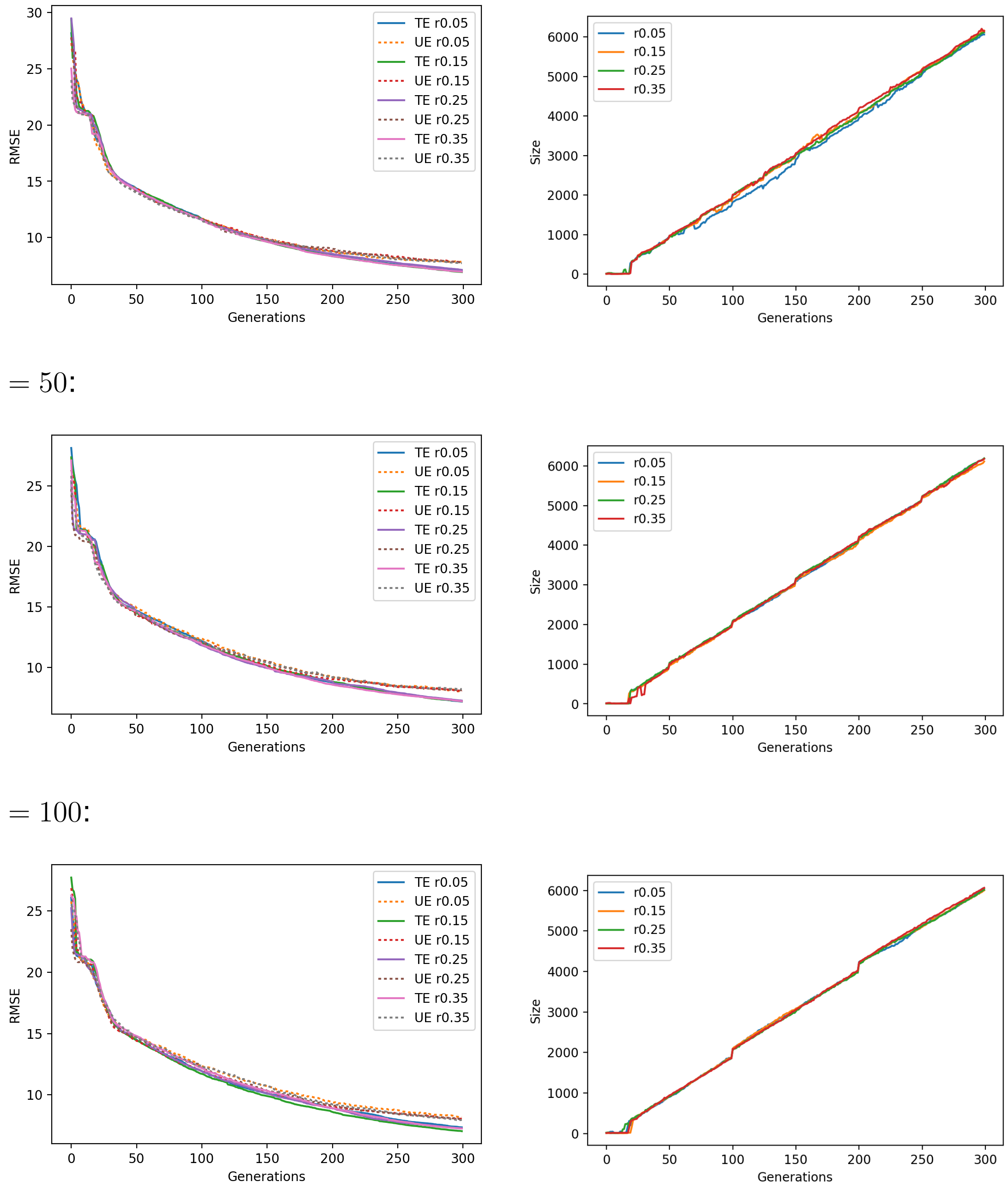
**Figure A.7.:** PPB - Comparison of combinations of migrational parameters: first column plots training error (TE) together with unseen error (UE) and the second plots size. Each row pertains to a migration frequency $f$ from the set $\{25, 50, 100\}$. In each plot, every tested migration rate $r$ in the set $\{0.05, 0.15, 0.25, 0.35\}$ is present.


$f = 25$:

$f = 50$:

$f = 100$:

**Figure A.8.:** Toxicity (LD50) - Comparison of combinations of migrational parameters: first column plots training error (TE) together with unseen error (UE) and the second plots size. Each row pertains to a migration frequency $f$ from the set $\{25, 50, 100\}$. In each plot, every tested migration rate $r$ in the set $\{0.05, 0.15, 0.25, 0.35\}$ is present.

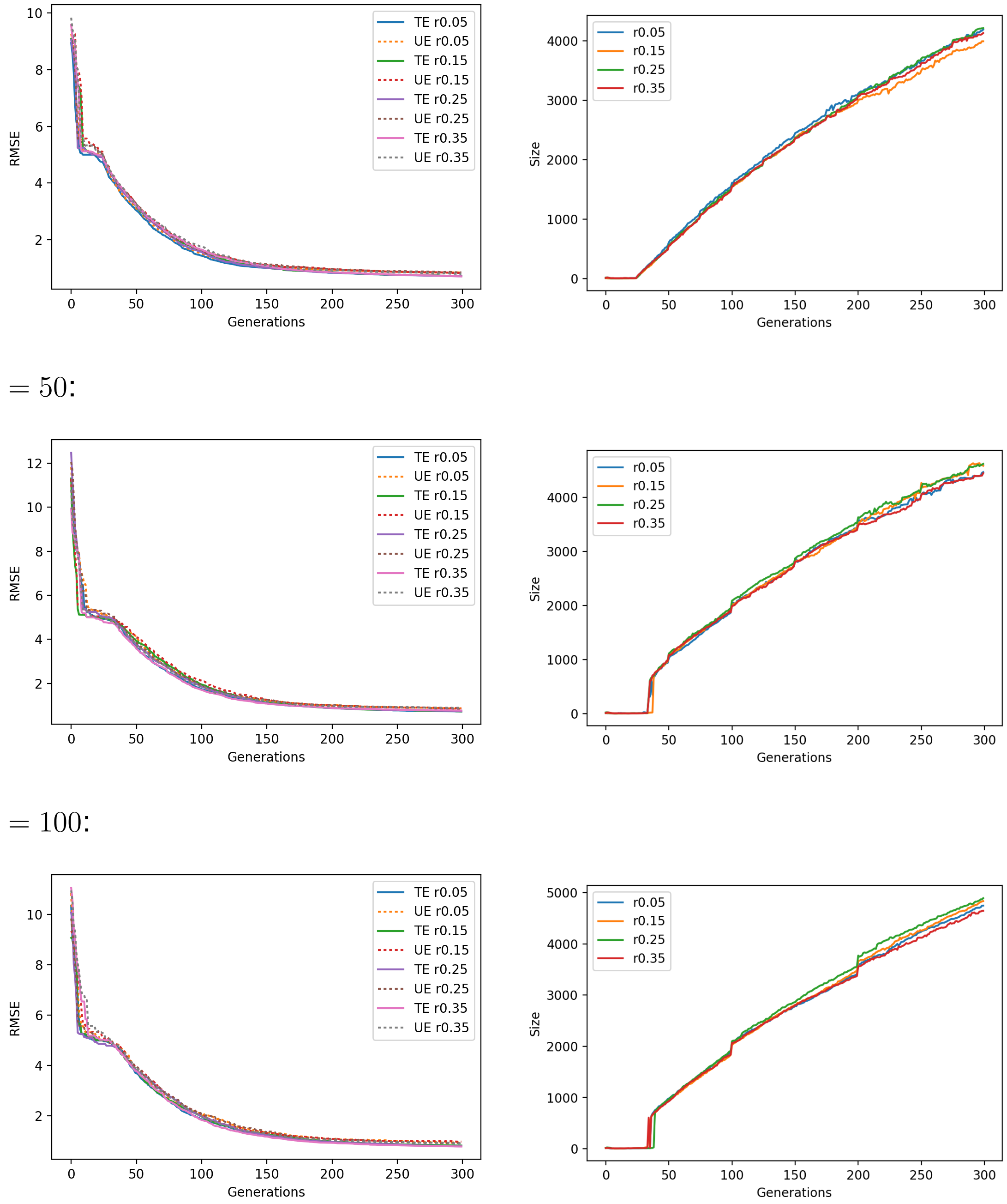


$f = 25$:

$f = 50$:

$f = 100$:

**Figure A.9.:** Concrete - Comparison of combinations of migrational parameters: first column plots training error (TE) together with unseen error (UE) and the second plots size. Each row pertains to a migration frequency $f$ from the set $\{25, 50, 100\}$. In each plot, every tested migration rate $r$ in the set $\{0.05, 0.15, 0.25, 0.35\}$ is present.


$f = 25$:

$f = 50$:

$f = 100$:

**Figure A.10.:** Energy - Comparison of combinations of migrational parameters: first column plots training error (TE) together with unseen error (UE) and the second plots size. Each row pertains to a migration frequency $f$ from the set $\{25, 50, 100\}$. In each plot, every tested migration rate $r$ in the set $\{0.05, 0.15, 0.25, 0.35\}$ is present.

| $f$ | | 25 | | | | 50 | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.41653 | 0.00129 | 0.02703 | 0.01108 | 0.00499 | 0.02304 | 0.01397 |
| | 0.15 | 0.47795 | - | 0.22888 | 0.18462 | 0.11561 | 0.13591 | 0.10639 | 0.12044 |
| | 0.25 | 0.58571 | 0.97539 | - | 0.68836 | 0.47795 | 0.81302 | 0.92626 | 0.61431 |
| | 0.35 | 0.32857 | 0.08972 | 0.21336 | - | 0.53044 | 0.39333 | 0.64352 | 0.34935 |
| 50 | 0.05 | 0.57165 | 0.08972 | 0.23694 | 0.99179 | - | 0.62884 | 0.33886 | 0.89364 |
| | 0.15 | 0.55774 | 0.09777 | 0.19152 | 0.92626 | 0.64352 | - | 0.55774 | 0.97539 |
| | 0.25 | 0.78126 | 0.08590 | 0.06268 | 0.84508 | 0.86121 | 0.74987 | - | 0.95899 |
| | 0.35 | 0.99179 | 0.24519 | 0.29894 | 0.79710 | 0.81302 | 0.73433 | 0.65833 | - |
| 100 | 0.05 | 0.02564 | 0.00468 | 0.00773 | 0.04950 | 0.04070 | 0.06871 | 0.05193 | 0.11093 |
| | 0.15 | 0.14139 | 0.00567 | 0.01044 | 0.21336 | 0.04950 | 0.11561 | 0.10201 | 0.08590 |
| | 0.25 | 0.00039 | 0.00241 | 0.00316 | 0.01397 | 0.01657 | 0.02183 | 0.00984 | 0.01397 |
| | 0.35 | 0.28021 | 0.12544 | 0.17138 | 0.44052 | 0.58571 | 0.45281 | 0.59994 | 0.41653 |

**Table A.6.:** Bioavailability (%F) - Wilcoxon Rank-Sum test on training error and unseen error. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on training error and above for unseen error. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ | | 25 | | | | 50 | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.42242 | 0.76552 | 0.06711 | 0.72656 | 0.84506 | 0.90992 | 0.62881 |
| | 0.15 | 0.85313 | - | 0.69589 | 0.37088 | 0.38705 | 0.28477 | 0.49722 | 0.30850 |
| | 0.25 | 0.84508 | 0.45281 | - | 0.13320 | 0.88821 | 0.89362 | 0.99179 | 0.97538 |
| | 0.35 | 0.45901 | 0.51705 | 0.21715 | - | 0.22877 | 0.12795 | 0.07268 | 0.20974 |
| 50 | 0.05 | 0.38203 | 0.24519 | 0.86121 | 0.09570 | - | 0.98359 | 1.00000 | 0.93442 |
| | 0.15 | 0.74987 | 0.39333 | 0.84508 | 0.11800 | 0.86121 | - | 0.91808 | 0.97538 |
| | 0.25 | 0.90993 | 0.47795 | 0.92626 | 0.14704 | 0.55774 | 0.81302 | - | 0.96718 |
| | 0.35 | 0.44052 | 0.25364 | 0.84508 | 0.15886 | 0.84508 | 0.78126 | 0.51705 | - |
| 100 | 0.05 | 0.89364 | 0.74986 | 0.26230 | 0.99179 | 0.44052 | 0.41653 | 0.81302 | 0.54401 |
| | 0.15 | 0.82901 | 0.87740 | 0.50957 | 0.81302 | 0.34935 | 0.61431 | 0.81302 | 0.68836 |
| | 0.25 | 0.01522 | 0.02849 | 0.00585 | 0.01657 | 0.00241 | 0.00567 | 0.02703 | 0.00064 |
| | 0.35 | 0.84508 | 0.61431 | 0.88551 | 0.23694 | 0.92626 | 0.70356 | 0.74987 | 0.90993 |

**Table A.7.:** Bioavailability (%F) - Wilcoxon Rank-Sum test on size and depth. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on size and above for depth. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.03872 | 0.00129 | 0.12044 | 0.00411 |
| | 0.15 | 0.03501 | 0.06564 | 0.53044 | 0.03872 |
| | 0.25 | 0.42843 | 0.79710 | 0.51705 | 0.67328 |
| | 0.35 | 0.38203 | 0.20589 | 0.89364 | 0.17138 |
| 50 | 0.05 | 0.65833 | 0.99179 | 0.28021 | 0.81302 |
| | 0.15 | 0.71889 | 0.65833 | 0.45281 | 0.71889 |
| | 0.25 | 0.37094 | 0.19152 | 0.65833 | 0.58571 |
| | 0.35 | 0.28948 | 0.45281 | 0.39333 | 0.61431 |
| 100 | 0.05 | - | 0.79710 | 0.25364 | 0.65833 |
| | 0.15 | 0.41653 | - | 0.17791 | 0.79710 |
| | 0.25 | 0.42843 | 0.13591 | - | 0.06268 |
| | 0.35 | 0.25364 | 0.79710 | 0.02849 | - |

**Table A.8.:** Continuation of Table A.6.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.65089 | 0.84507 | 0.00425 | 0.94260 |
| | 0.15 | 0.80221 | 0.35996 | 0.04714 | 0.14700 |
| | 0.25 | 0.43627 | 0.58876 | 0.00602 | 0.37091 |
| | 0.35 | 0.46876 | 0.20957 | 0.07568 | 0.03498 |
| 50 | 0.05 | 0.75386 | 0.72123 | 0.00683 | 0.35456 |
| | 0.15 | 0.90532 | 0.95079 | 0.02242 | 0.56659 |
| | 0.25 | 0.75382 | 0.98359 | 0.01478 | 0.95899 |
| | 0.35 | 1.00000 | 0.51697 | 0.00219 | 0.58131 |
| 100 | 0.05 | - | 0.41741 | 0.00845 | 0.41052 |
| | 0.15 | 0.78126 | - | 0.00107 | 0.71884 |
| | 0.25 | 0.00727 | 0.01319 | - | 0.00083 |
| | 0.35 | 0.62884 | 0.55773 | 0.00468 | - |

**Table A.9.:** Continuation of Table A.7.

| $f$ |  | 25 |  |  |  | 50 |  |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.70356 | 0.15886 | 0.42843 | 0.12544 | 0.12544 | 0.07865 | 0.00211 |
|  | 0.15 | 0.41653 | - | 0.50383 | 0.49080 | 0.15886 | 0.01319 | 0.08221 | 0.00411 |
|  | 0.25 | 0.05984 | 0.58571 | - | 0.44052 | 0.70356 | 0.20589 | 0.41653 | 0.15886 |
|  | 0.35 | 0.04277 | 0.18462 | 0.38203 | - | 0.41653 | 0.09368 | 0.30861 | 0.10201 |
| 50 | 0.05 | 0.23694 | 0.04492 | 0.00642 | 0.00211 | - | 0.47795 | 0.45281 | 0.28948 |
|  | 0.15 | 0.29894 | 0.06871 | 0.00532 | 0.00120 | 0.74987 | - | 0.79710 | 0.54401 |
|  | 0.25 | 0.31849 | 0.09368 | 0.03327 | 0.00083 | 0.68836 | 0.45281 | - | 0.55774 |
|  | 0.35 | 0.26230 | 0.04492 | 0.00642 | 0.00077 | 0.79710 | 0.92626 | 0.81302 | - |
| 100 | 0.05 | 0.28021 | 0.03501 | 0.00138 | 0.00062 | 0.94261 | 0.97539 | 0.36004 | 0.74987 |
|  | 0.15 | 0.04492 | 0.00338 | 0.00009 | 0.00022 | 0.10639 | 0.16503 | 0.02564 | 0.21336 |
|  | 0.25 | 0.07190 | 0.01108 | 0.00039 | 0.00003 | 0.26230 | 0.41653 | 0.01108 | 0.23694 |
|  | 0.35 | 0.03160 | 0.00773 | 0.00077 | 0.00002 | 0.22888 | 0.11561 | 0.01752 | 0.34935 |

**Table A.10.:** PPB - Wilcoxon Rank-Sum test on training error and unseen error. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on training error and above for unseen error. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ |  | 25 |  |  |  | 50 |  |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.56463 | 0.37518 | 0.12798 | 0.87333 | 0.91837 | 0.92623 | 0.96718 |
|  | 0.15 | 0.74987 | - | 0.81300 | 0.12738 | 0.39330 | 0.29484 | 0.32510 | 0.19070 |
|  | 0.25 | 0.57865 | 0.42843 | - | 0.51038 | 0.30364 | 0.41115 | 0.31461 | 0.16491 |
|  | 0.35 | 0.27116 | 0.03242 | 0.27116 | - | 0.06290 | 0.10861 | 0.01687 | 0.01751 |
| 50 | 0.05 | 0.13591 | 0.31849 | 0.05984 | 0.00873 | - | 0.57827 | 0.30841 | 0.87102 |
|  | 0.15 | 0.04492 | 0.10201 | 0.09367 | 0.01245 | 0.36004 | - | 0.55765 | 0.98274 |
|  | 0.25 | 0.18462 | 0.70356 | 0.10862 | 0.00773 | 0.97539 | 0.51705 | - | 0.58122 |
|  | 0.35 | 0.17791 | 0.30861 | 0.02010 | 0.00138 | 0.82901 | 0.82901 | 0.84508 | - |
| 100 | 0.05 | 0.67328 | 0.27114 | 0.74987 | 0.25364 | 0.08589 | 0.05575 | 0.08221 | 0.08972 |
|  | 0.15 | 0.16503 | 0.17137 | 0.12544 | 0.00499 | 0.95899 | 0.50383 | 0.90993 | 0.90993 |
|  | 0.25 | 0.12798 | 0.16503 | 0.19861 | 0.00439 | 0.83703 | 0.89364 | 0.67328 | 0.64352 |
|  | 0.35 | 0.12044 | 0.21336 | 0.09368 | 0.00773 | 0.87740 | 0.97539 | 0.50383 | 0.87740 |

**Table A.11.:** PPB - Wilcoxon Rank-Sum test on size and depth. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on size and above for depth. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.00138 | 0.01245 | 0.00642 | 0.00439 |
| | 0.15 | 0.00062 | 0.00226 | 0.00089 | 0.00053 |
| | 0.25 | 0.00049 | 0.00873 | 0.01397 | 0.00211 |
| | 0.35 | 0.00019 | 0.01657 | 0.00873 | 0.00211 |
| 50 | 0.05 | 0.00120 | 0.01752 | 0.06871 | 0.01752 |
| | 0.15 | 0.00468 | 0.26230 | 0.04950 | 0.07865 |
| | 0.25 | 0.01957 | 0.13591 | 0.13591 | 0.07865 |
| | 0.35 | 0.06564 | 0.49080 | 0.34935 | 0.24519 |
| 100 | 0.05 | - | 0.37094 | 0.27116 | 0.42843 |
| | 0.15 | 0.08972 | - | 0.41653 | 0.54401 |
| | 0.25 | 0.46528 | 0.58571 | - | 0.99179 |
| | 0.35 | 0.17138 | 0.54401 | 0.87740 | - |

**Table A.12.:** Continuation of Table A.10.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.03589 | 0.71887 | 0.85416 | 0.86265 |
| | 0.15 | 0.13855 | 0.57859 | 0.78122 | 0.39328 |
| | 0.25 | 0.25169 | 0.77335 | 1.00000 | 0.39896 |
| | 0.35 | 0.58875 | 0.12470 | 0.17454 | 0.11786 |
| 50 | 0.05 | 0.01912 | 0.36530 | 0.49059 | 0.82895 |
| | 0.15 | 0.05059 | 0.38139 | 0.98273 | 0.77012 |
| | 0.25 | 0.00411 | 0.27097 | 0.26918 | 0.84500 |
| | 0.35 | 0.02061 | 0.54468 | 0.90173 | 1.00000 |
| 100 | 0.05 | - | 0.31021 | 0.12090 | 0.08250 |
| | 0.15 | 0.04950 | - | 0.41478 | 0.30628 |
| | 0.25 | 0.04950 | 1.00000 | - | 0.72050 |
| | 0.35 | 0.15286 | 0.83703 | 0.92626 | - |

**Table A.13.:** Continuation of Table A.11.

| $f$ |  | 25 |  |  |  | 50 |  |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.23694 | 0.00984 | 0.10639 | 0.20589 | 0.03160 | 0.05446 | 0.12044 |
|  | 0.15 | 0.17138 | - | 0.33886 | 0.62884 | 0.92626 | 0.81302 | 0.71889 | 0.47795 |
|  | 0.25 | 0.06871 | 0.41653 | - | 0.45281 | 0.40483 | 0.71889 | 0.37094 | 0.94261 |
|  | 0.35 | 0.12544 | 0.36004 | 0.78126 | - | 0.53044 | 0.57165 | 0.62884 | 0.90993 |
| 50 | 0.05 | 0.01852 | 0.02849 | 0.00211 | 0.00468 | - | 0.05710 | 0.73433 | 0.78126 |
|  | 0.15 | 0.87740 | 0.11093 | 0.08590 | 0.05446 | 0.14139 | - | 0.26230 | 0.25364 |
|  | 0.25 | 0.37094 | 0.07865 | 0.05984 | 0.03327 | 0.28948 | 0.92626 | - | 0.78126 |
|  | 0.35 | 0.47795 | 0.64352 | 0.22888 | 0.25364 | 0.06564 | 0.27116 | 0.67328 | - |
| 100 | 0.05 | 0.00411 | 0.00211 | 0.00014 | 0.00014 | 0.50383 | 0.03872 | 0.04070 | 0.00532 |
|  | 0.15 | 0.00120 | 0.00024 | 0.00001 | 0.00002 | 0.51705 | 0.00468 | 0.00411 | 0.00138 |
|  | 0.25 | 0.00567 | 0.00028 | 0.00024 | 0.00017 | 0.38203 | 0.00211 | 0.02183 | 0.00567 |
|  | 0.35 | 0.02431 | 0.00642 | 0.00077 | 0.00567 | 0.62884 | 0.03872 | 0.19861 | 0.00499 |

**Table A.14.:** Toxicity (LD50) - Wilcoxon Rank-Sum test on training error and unseen error. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on training error and above for unseen error. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ |  | 25 |  |  |  | 50 |  |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.33879 | 0.27930 | 0.01395 | 0.57857 | 0.93106 | 0.14141 | 0.07349 |
|  | 0.15 | 0.46883 | - | 0.24514 | 0.16963 | 0.90175 | 0.29878 | 0.45555 | 0.10468 |
|  | 0.25 | 0.25363 | 0.33368 | - | 0.65747 | 0.45881 | 0.07517 | 0.72653 | 0.51696 |
|  | 0.35 | 0.04716 | 0.15583 | 0.78916 | - | 0.33870 | 0.04600 | 0.95078 | 0.61416 |
| 50 | 0.05 | 0.14704 | 0.22182 | 0.70356 | 0.99179 | - | 0.55366 | 0.87111 | 0.20574 |
|  | 0.15 | 0.58879 | 0.99179 | 0.42843 | 0.25364 | 0.34935 | - | 0.16970 | 0.06116 |
|  | 0.25 | 0.10201 | 0.15285 | 0.41653 | 0.55772 | 0.73433 | 0.22102 | - | 0.68832 |
|  | 0.35 | 0.03242 | 0.03327 | 0.38203 | 0.24519 | 0.61431 | 0.13059 | 0.92626 | - |
| 100 | 0.05 | 0.00027 | 0.00004 | 0.00003 | 0.00003 | 0.00053 | 0.00083 | 0.00019 | 0.00009 |
|  | 0.15 | 0.09368 | 0.06268 | 0.04716 | 0.03501 | 0.11560 | 0.04277 | 0.01591 | 0.06267 |
|  | 0.25 | 0.01108 | 0.02183 | 0.00873 | 0.00773 | 0.00439 | 0.01903 | 0.00705 | 0.00453 |
|  | 0.35 | 0.01566 | 0.01566 | 0.01245 | 0.01107 | 0.04099 | 0.04276 | 0.00984 | 0.01688 |

**Table A.15.:** Toxicity (LD50) - Wilcoxon Rank-Sum test on size and depth. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on size and above for depth. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.04070 | 0.09777 | 0.18462 | 0.01245 |
| | 0.15 | 0.74987 | 0.50383 | 0.70356 | 0.46528 |
| | 0.25 | 0.81302 | 0.87740 | 0.13591 | 0.97539 |
| | 0.35 | 0.61431 | 0.61431 | 0.50383 | 0.50383 |
| 50 | 0.05 | 0.51705 | 0.19152 | 0.92626 | 0.08590 |
| | 0.15 | 0.74987 | 0.64352 | 0.11093 | 0.45281 |
| | 0.25 | 0.34935 | 0.64352 | 0.59994 | 0.22888 |
| | 0.35 | 0.27116 | 0.46528 | 0.45281 | 0.31849 |
| 100 | 0.05 | - | 0.71889 | 0.34935 | 0.95899 |
| | 0.15 | 0.71889 | - | 0.30861 | 0.78126 |
| | 0.25 | 0.70356 | 0.81302 | - | 0.06564 |
| | 0.35 | 0.59994 | 0.45281 | 0.20589 | - |

**Table A.16.:** Continuation of Table A.14.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.00017 | 0.05698 | 0.01588 | 0.01317 |
| | 0.15 | 0.00007 | 0.03239 | 0.01653 | 0.01478 |
| | 0.25 | 0.00003 | 0.01851 | 0.01106 | 0.00772 |
| | 0.35 | 0.00004 | 0.01477 | 0.00466 | 0.00984 |
| 50 | 0.05 | 0.00066 | 0.07348 | 0.01074 | 0.03138 |
| | 0.15 | 0.00077 | 0.04272 | 0.02739 | 0.04425 |
| | 0.25 | 0.00015 | 0.00704 | 0.00749 | 0.00388 |
| | 0.35 | 0.00011 | 0.01173 | 0.00284 | 0.01319 |
| 100 | 0.05 | - | 0.30125 | 0.83684 | 0.98273 |
| | 0.15 | 0.36370 | - | 0.22232 | 0.58819 |
| | 0.25 | 0.74207 | 0.27480 | - | 0.93645 |
| | 0.35 | 0.67323 | 0.33581 | 0.62872 | - |

**Table A.17.:** Continuation of Table A.15.

| $f$ |  | 25 |  |  |  | 50 |  |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.79710 | 0.40483 | 0.45281 | 0.28948 | 0.00984 | 0.09368 | 0.09777 |
|  | 0.15 | 0.87740 | - | 0.61431 | 0.99179 | 0.20589 | 0.00258 | 0.08590 | 0.17791 |
|  | 0.25 | 0.23694 | 0.42843 | - | 0.44052 | 0.38203 | 0.12044 | 0.41653 | 0.53044 |
|  | 0.35 | 0.53044 | 0.64352 | 0.42843 | - | 0.07190 | 0.01245 | 0.12044 | 0.03501 |
| 50 | 0.05 | 0.01957 | 0.04277 | 0.07521 | 0.01566 | - | 0.12044 | 0.41653 | 0.33886 |
|  | 0.15 | 0.00684 | 0.01245 | 0.23694 | 0.03160 | 0.89364 | - | 0.38203 | 0.84508 |
|  | 0.25 | 0.04492 | 0.09777 | 0.53044 | 0.03001 | 0.76552 | 0.65833 | - | 0.45281 |
|  | 0.35 | 0.02304 | 0.08590 | 0.36004 | 0.06871 | 0.87740 | 0.57165 | 0.92626 | - |
| 100 | 0.05 | 0.00604 | 0.01397 | 0.17791 | 0.00642 | 0.50383 | 0.67328 | 0.28948 | 0.68836 |
|  | 0.15 | 0.04716 | 0.05193 | 0.20589 | 0.01957 | 0.74987 | 0.90993 | 0.55774 | 0.94261 |
|  | 0.25 | 0.01657 | 0.01957 | 0.26230 | 0.00727 | 0.94261 | 0.94261 | 0.67328 | 0.64352 |
|  | 0.35 | 0.00927 | 0.05193 | 0.06871 | 0.01044 | 0.53044 | 0.45281 | 0.29894 | 0.39333 |

**Table A.18.:** Concrete - Wilcoxon Rank-Sum test on training error and unseen error. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on training error and above for unseen error. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ |  | 25 |  |  |  | 50 |  |  |  |
|---|---|---|---|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.77030 | 0.74983 | 0.14125 | 0.82896 | 0.97412 | 0.53709 | 0.91835 |
|  | 0.15 | 0.89364 | - | 0.57161 | 0.34128 | 0.90933 | 0.90528 | 0.57156 | 0.93964 |
|  | 0.25 | 0.73433 | 0.82901 | - | 0.49720 | 0.49718 | 0.85310 | 0.86120 | 0.86263 |
|  | 0.35 | 0.08221 | 0.31849 | 0.19861 | - | 0.60361 | 0.51628 | 0.78116 | 0.45891 |
| 50 | 0.05 | 0.51705 | 0.14139 | 0.19861 | 0.06268 | - | 0.99091 | 0.42353 | 0.71305 |
|  | 0.15 | 0.59994 | 0.27116 | 0.46528 | 0.13591 | 0.97539 | - | 0.45885 | 0.49544 |
|  | 0.25 | 0.59994 | 0.53044 | 0.50383 | 0.13059 | 0.47795 | 0.92625 | - | 0.32832 |
|  | 0.35 | 0.24519 | 0.12543 | 0.45281 | 0.06871 | 0.90178 | 0.59994 | 0.42843 | - |
| 100 | 0.05 | 0.61431 | 0.09570 | 0.15286 | 0.01175 | 0.59994 | 0.46528 | 0.30861 | 0.61431 |
|  | 0.15 | 0.71889 | 0.04716 | 0.40483 | 0.00873 | 0.81302 | 0.44663 | 0.42842 | 0.86121 |
|  | 0.25 | 0.28021 | 0.06123 | 0.15286 | 0.00684 | 0.61431 | 0.14992 | 0.08590 | 0.11561 |
|  | 0.35 | 0.25364 | 0.39332 | 0.33368 | 0.01437 | 0.82100 | 0.31988 | 0.19152 | 0.69594 |

**Table A.19.:** Concrete - Wilcoxon Rank-Sum test on size and depth. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on size and above for depth. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.05984 | 0.17138 | 0.10639 | 0.11561 |
| | 0.15 | 0.03001 | 0.30861 | 0.04277 | 0.08972 |
| | 0.25 | 0.28948 | 0.27116 | 0.39333 | 0.19152 |
| | 0.35 | 0.01480 | 0.03327 | 0.01319 | 0.01852 |
| 50 | 0.05 | 0.13591 | 0.50383 | 0.39333 | 0.26230 |
| | 0.15 | 0.90993 | 0.39333 | 0.73433 | 0.95899 |
| | 0.25 | 0.45281 | 0.99179 | 0.65833 | 0.68836 |
| | 0.35 | 0.97539 | 0.92626 | 0.70356 | 0.31849 |
| 100 | 0.05 | - | 0.87740 | 0.84508 | 0.89364 |
| | 0.15 | 0.78126 | - | 0.81302 | 0.86121 |
| | 0.25 | 0.78126 | 0.97539 | - | 0.57165 |
| | 0.35 | 0.92626 | 0.74987 | 0.42843 | - |

**Table A.20.:** Continuation of Table A.18.

| $f$ | | 100 | | | |
|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.41383 | 0.02959 | 0.89129 | 0.38694 |
| | 0.15 | 0.46515 | 0.07336 | 0.64339 | 0.24288 |
| | 0.25 | 0.88819 | 0.18709 | 0.65830 | 0.82034 |
| | 0.35 | 0.47520 | 0.08161 | 0.44021 | 0.82893 |
| 50 | 0.05 | 0.90519 | 0.06827 | 0.65719 | 0.69848 |
| | 0.15 | 0.51619 | 0.04882 | 0.72200 | 0.50111 |
| | 0.25 | 0.82868 | 0.40421 | 0.20397 | 0.62123 |
| | 0.35 | 0.84888 | 0.13514 | 0.27444 | 0.81969 |
| 100 | 0.05 | - | 0.34593 | 0.24501 | 0.82829 |
| | 0.15 | 0.92248 | - | 0.02361 | 0.28831 |
| | 0.25 | 0.54401 | 0.56463 | - | 0.29345 |
| | 0.35 | 0.87740 | 0.86121 | 0.74986 | - |

**Table A.21.:** Continuation of Table A.19.

| $f$ | | 25 | | | | 50 | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.45281 | 0.73433 | 0.19861 | 0.99179 | 0.36004 | 0.73433 | 0.46528 |
| | 0.15 | 0.79710 | - | 0.21336 | 0.40483 | 0.29894 | 0.14139 | 0.28948 | 0.03872 |
| | 0.25 | 0.89364 | 0.86121 | - | 0.14704 | 0.99179 | 0.67328 | 0.94261 | 0.62884 |
| | 0.35 | 0.41653 | 0.50383 | 0.70356 | - | 0.22888 | 0.02304 | 0.12544 | 0.02703 |
| 50 | 0.05 | 0.21336 | 0.15286 | 0.10201 | 0.06871 | - | 0.47795 | 0.55774 | 0.30861 |
| | 0.15 | 0.28021 | 0.23694 | 0.09368 | 0.06564 | 0.81302 | - | 0.76552 | 0.55774 |
| | 0.25 | 0.20589 | 0.15886 | 0.08972 | 0.09368 | 0.90993 | 0.92626 | - | 0.57165 |
| | 0.35 | 0.24519 | 0.16503 | 0.15286 | 0.07190 | 0.78126 | 0.81302 | 0.84508 | - |
| 100 | 0.05 | 0.00045 | 0.00104 | 0.00642 | 0.00017 | 0.03501 | 0.01566 | 0.01319 | 0.01480 |
| | 0.15 | 0.00016 | 0.00004 | 0.00057 | 0.00045 | 0.01480 | 0.00411 | 0.00773 | 0.01657 |
| | 0.25 | 0.00361 | 0.00083 | 0.00604 | 0.00241 | 0.05710 | 0.01566 | 0.04716 | 0.02564 |
| | 0.35 | 0.02564 | 0.00727 | 0.00984 | 0.00684 | 0.19152 | 0.28021 | 0.31849 | 0.09368 |

**Table A.22.:** Energy - Wilcoxon Rank-Sum test on training error and unseen error. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on training error and above for unseen error. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ | | 25 | | | | 50 | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $r$ | 0.05 | 0.15 | 0.25 | 0.35 | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | - | 0.01747 | 0.67311 | 0.90993 | 0.08965 | 0.06406 | 0.05317 | 0.20967 |
| | 0.15 | 0.06294 | - | 0.02180 | 0.05973 | 0.00225 | 0.00124 | 0.00120 | 0.00159 |
| | 0.25 | 0.68080 | 0.00567 | - | 0.97538 | 0.02815 | 0.06561 | 0.00704 | 0.14430 |
| | 0.35 | 0.76552 | 0.15886 | 0.64351 | - | 0.14412 | 0.13052 | 0.06561 | 0.33365 |
| 50 | 0.05 | 0.07521 | 0.00241 | 0.47795 | 0.26230 | - | 0.92247 | 0.81194 | 0.66536 |
| | 0.15 | 0.04716 | 0.00104 | 0.13591 | 0.14139 | 0.92626 | - | 0.72119 | 0.46213 |
| | 0.25 | 0.03327 | 0.00066 | 0.05446 | 0.07190 | 0.42842 | 0.44052 | - | 0.42989 |
| | 0.35 | 0.17791 | 0.00148 | 0.76552 | 0.46528 | 0.96719 | 0.54401 | 0.33368 | - |
| 100 | 0.05 | 0.00258 | 0.00007 | 0.03001 | 0.03872 | 0.07521 | 0.08972 | 0.28021 | 0.02849 |
| | 0.15 | 0.00233 | 0.00001 | 0.02183 | 0.01044 | 0.02564 | 0.09570 | 0.27565 | 0.00873 |
| | 0.25 | 0.00031 | 0.00003 | 0.00727 | 0.00684 | 0.00499 | 0.00773 | 0.07190 | 0.01319 |
| | 0.35 | 0.03327 | 0.00277 | 0.20589 | 0.16503 | 0.32857 | 0.82901 | 0.87740 | 0.39333 |

**Table A.23.:** Energy - Wilcoxon Rank-Sum test on size and depth. Null hypothesis assumes that two samples (of results) come from the same distribution. Below the marked diagonal lie the p-values for tests on size and above for depth. At 5% significance level, the cases which reject the null hypothesis is highlighted in light grey. The purpose is to visualize the impact of varying migrational parameters.

| $f$ |  | 100 |  |  |  |
|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.03872 | 0.01957 | 0.04492 | 0.05710 |
|  | 0.15 | 0.00338 | 0.00053 | 0.00211 | 0.00642 |
|  | 0.25 | 0.05193 | 0.04950 | 0.05984 | 0.17791 |
|  | 0.35 | 0.00111 | 0.00089 | 0.01175 | 0.00338 |
| 50 | 0.05 | 0.04950 | 0.00183 | 0.02183 | 0.02849 |
|  | 0.15 | 0.05710 | 0.01175 | 0.14704 | 0.29894 |
|  | 0.25 | 0.04277 | 0.01566 | 0.05193 | 0.12044 |
|  | 0.35 | 0.05193 | 0.05710 | 0.17791 | 0.22102 |
| 100 | 0.05 | - | 0.70356 | 0.30861 | 0.46528 |
|  | 0.15 | 0.90993 | - | 0.31849 | 0.45281 |
|  | 0.25 | 0.70356 | 0.54401 | - | 0.90993 |
|  | 0.35 | 0.22888 | 0.19861 | 0.51705 | - |

**Table A.24.:** Continuation of Table A.22.

| $f$ |  | 100 |  |  |  |
|---|---|---|---|---|---|
|  | $r$ | 0.05 | 0.15 | 0.25 | 0.35 |
| 25 | 0.05 | 0.00360 | 0.00945 | 0.00059 | 0.01396 |
|  | 0.15 | 0.00015 | 0.00004 | 0.00002 | 0.00061 |
|  | 0.25 | 0.00119 | 0.00071 | 0.00014 | 0.00326 |
|  | 0.35 | 0.00566 | 0.00349 | 0.00096 | 0.02430 |
| 50 | 0.05 | 0.04274 | 0.01610 | 0.00622 | 0.07513 |
|  | 0.15 | 0.02893 | 0.01073 | 0.00133 | 0.17288 |
|  | 0.25 | 0.06445 | 0.06966 | 0.01608 | 0.39902 |
|  | 0.35 | 0.00584 | 0.00103 | 0.00025 | 0.03869 |
| 100 | 0.05 | - | 0.75373 | 0.09968 | 0.98358 |
|  | 0.15 | 0.81302 | - | 0.52349 | 0.29401 |
|  | 0.25 | 0.11093 | 0.82901 | - | 0.25333 |
|  | 0.35 | 0.19151 | 0.01752 | 0.07865 | - |

**Table A.25.:** Continuation of Table A.23.

## A.3 2-Population Hybrid Genetic Programming

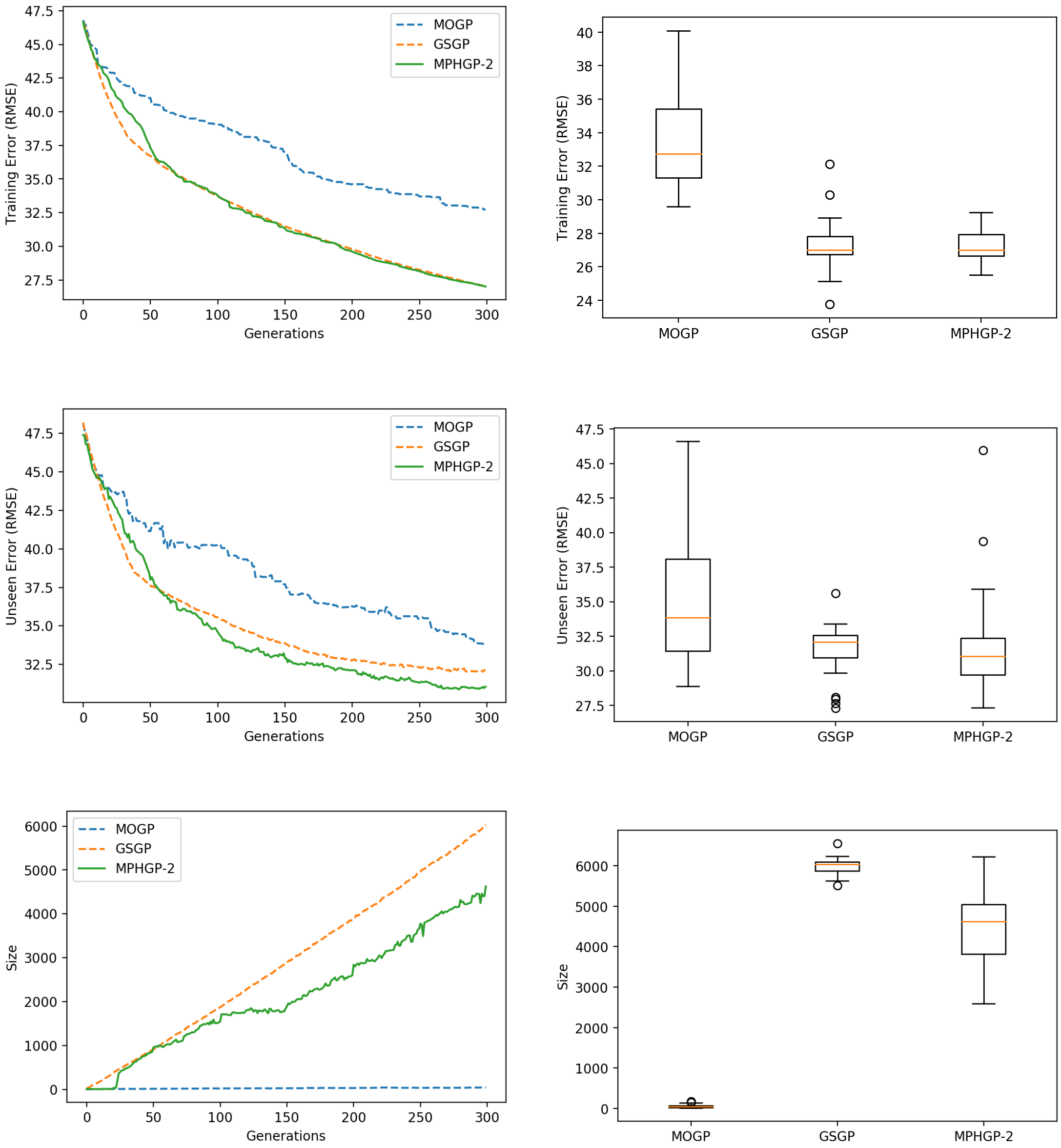


**Figure A.11.:** Bioavailability (%F) - Performance of 2-subpopulation MPHGP measured against the standalone benchmarks MOGP and GSGP. From the top, training error, unseen error and size.

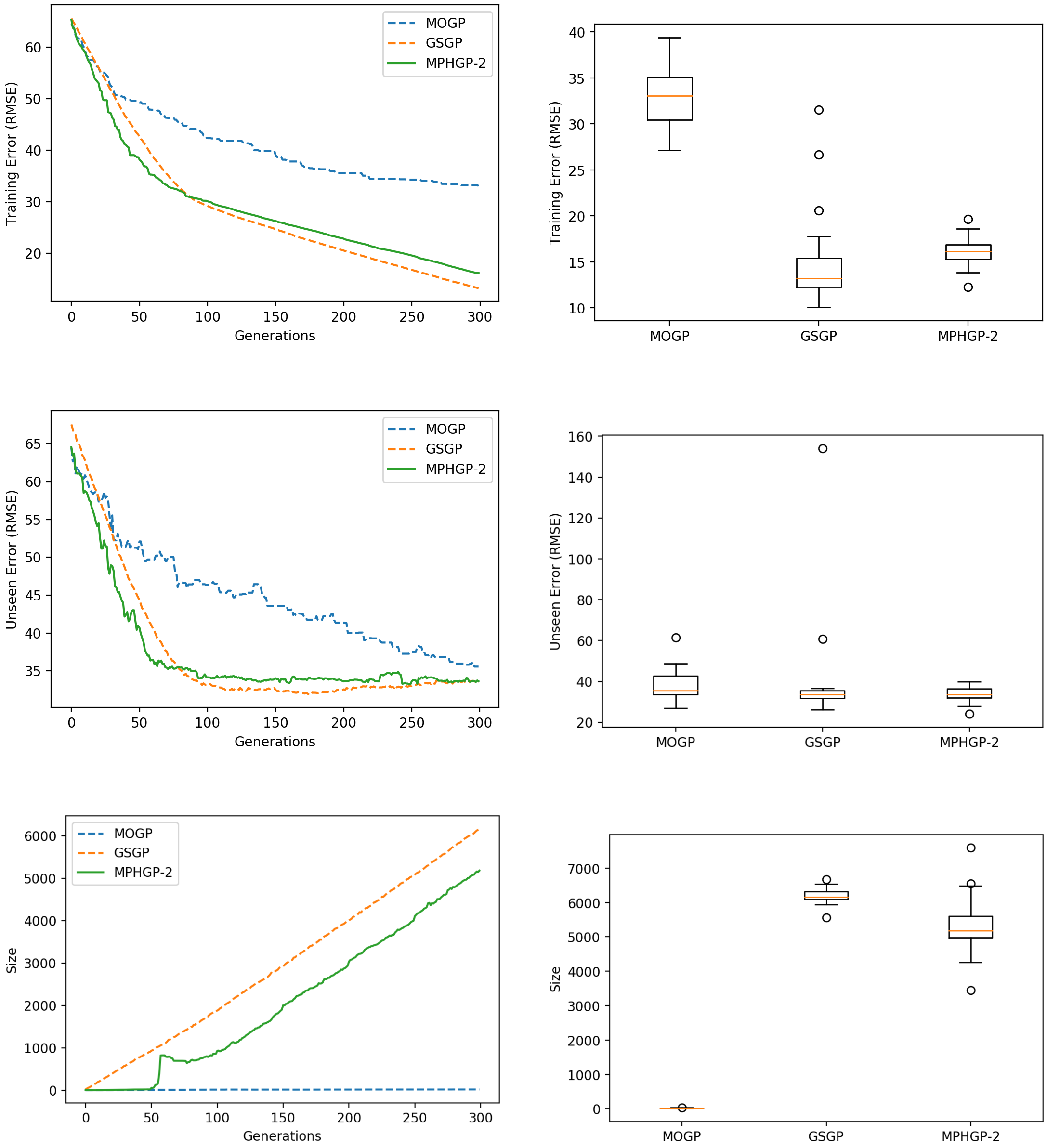


**Figure A.12.:** PPB - Performance of 2-subpopulation MPHGP measured against the standalone benchmarks MOGP and GSGP. From the top, training error, unseen error and size.

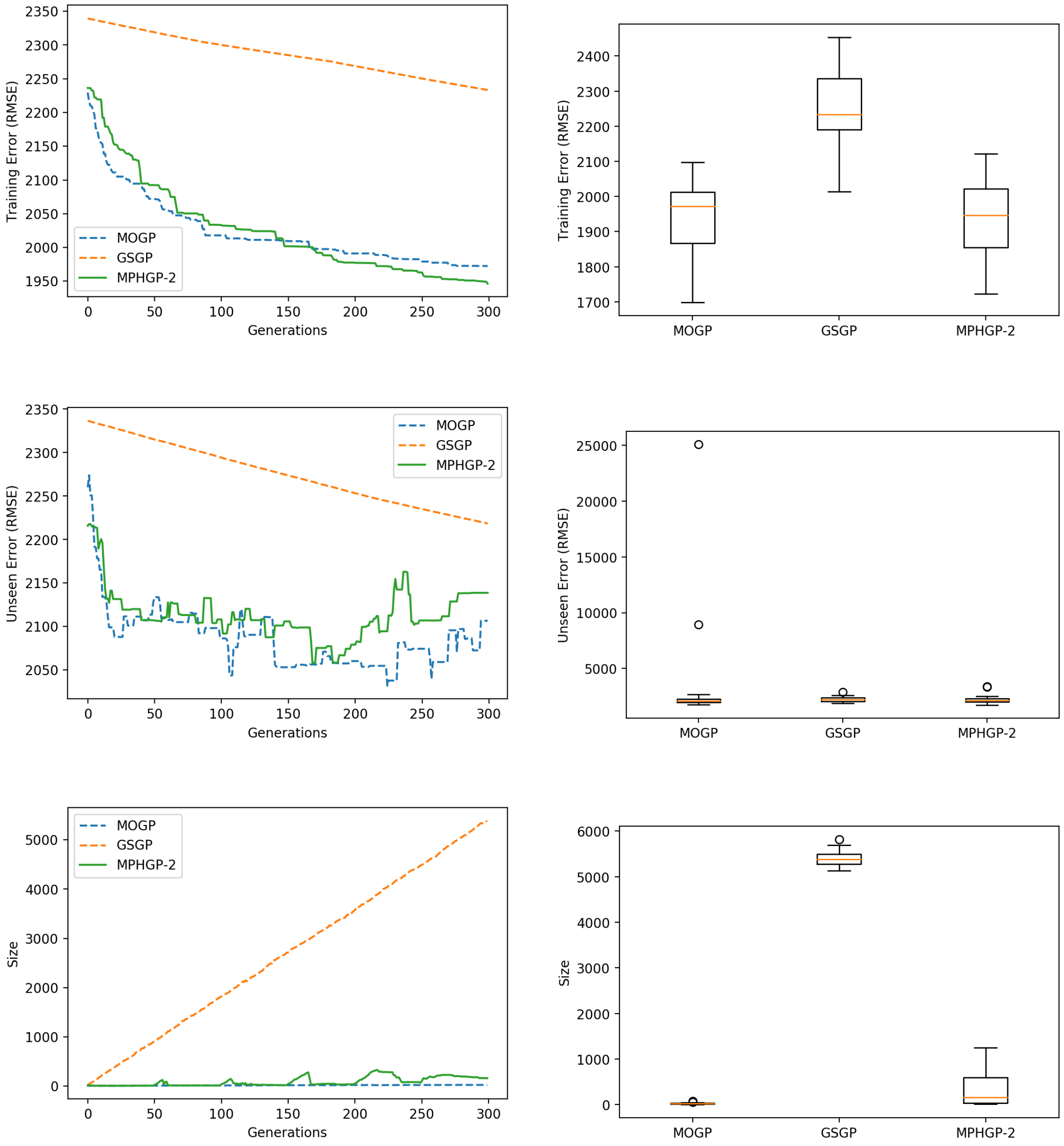


**Figure A.13.:** Toxicity (LD50) - Performance of 2-subpopulation MPHGP measured against the standalone benchmarks MOGP and GSGP. From the top, training error, unseen error and size.

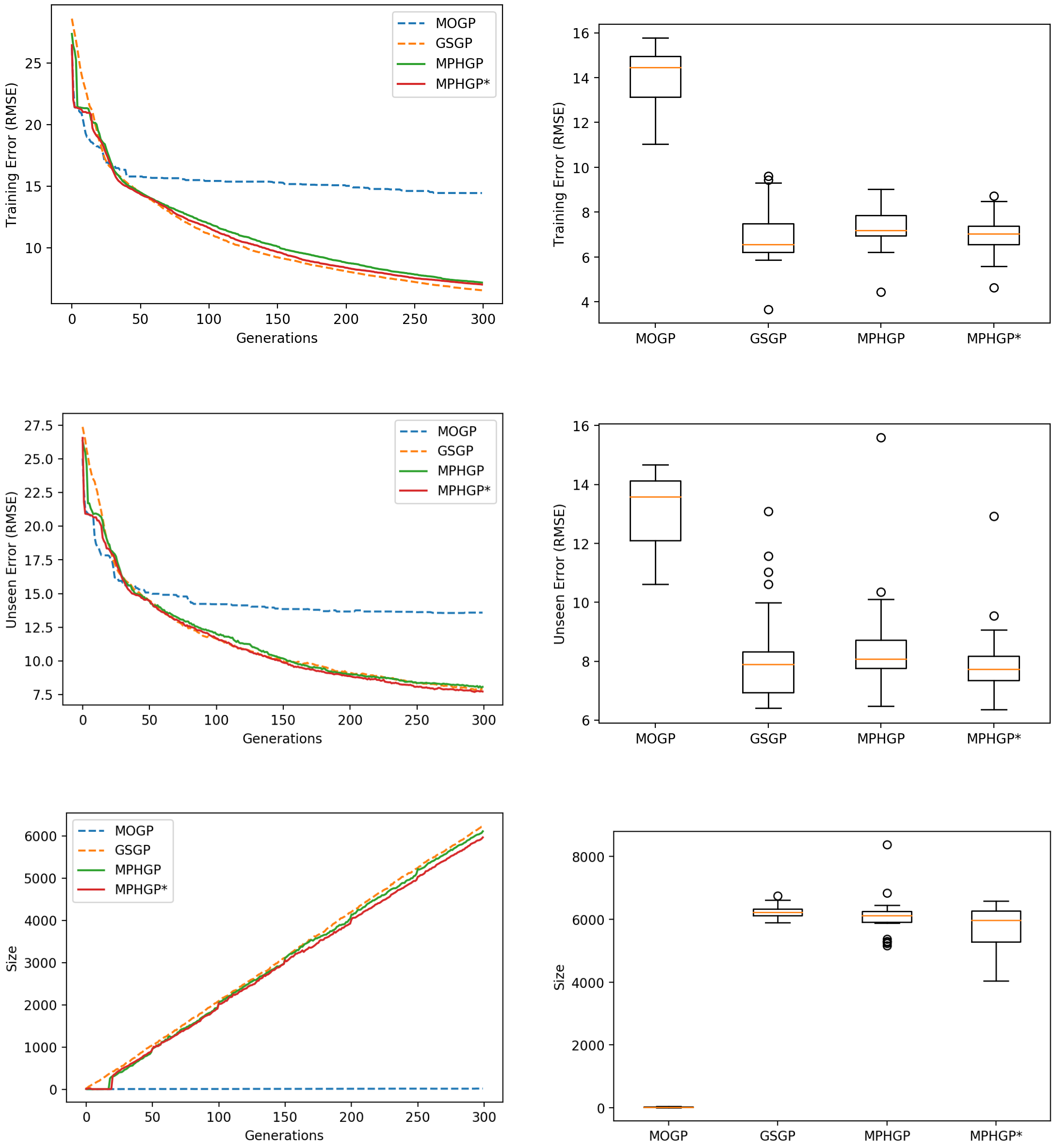


**Figure A.14.:** Concrete - Performance of 2-subpopulation MPHGP measured against the standalone benchmarks MOGP and GSGP. From the top, training error, unseen error and size.

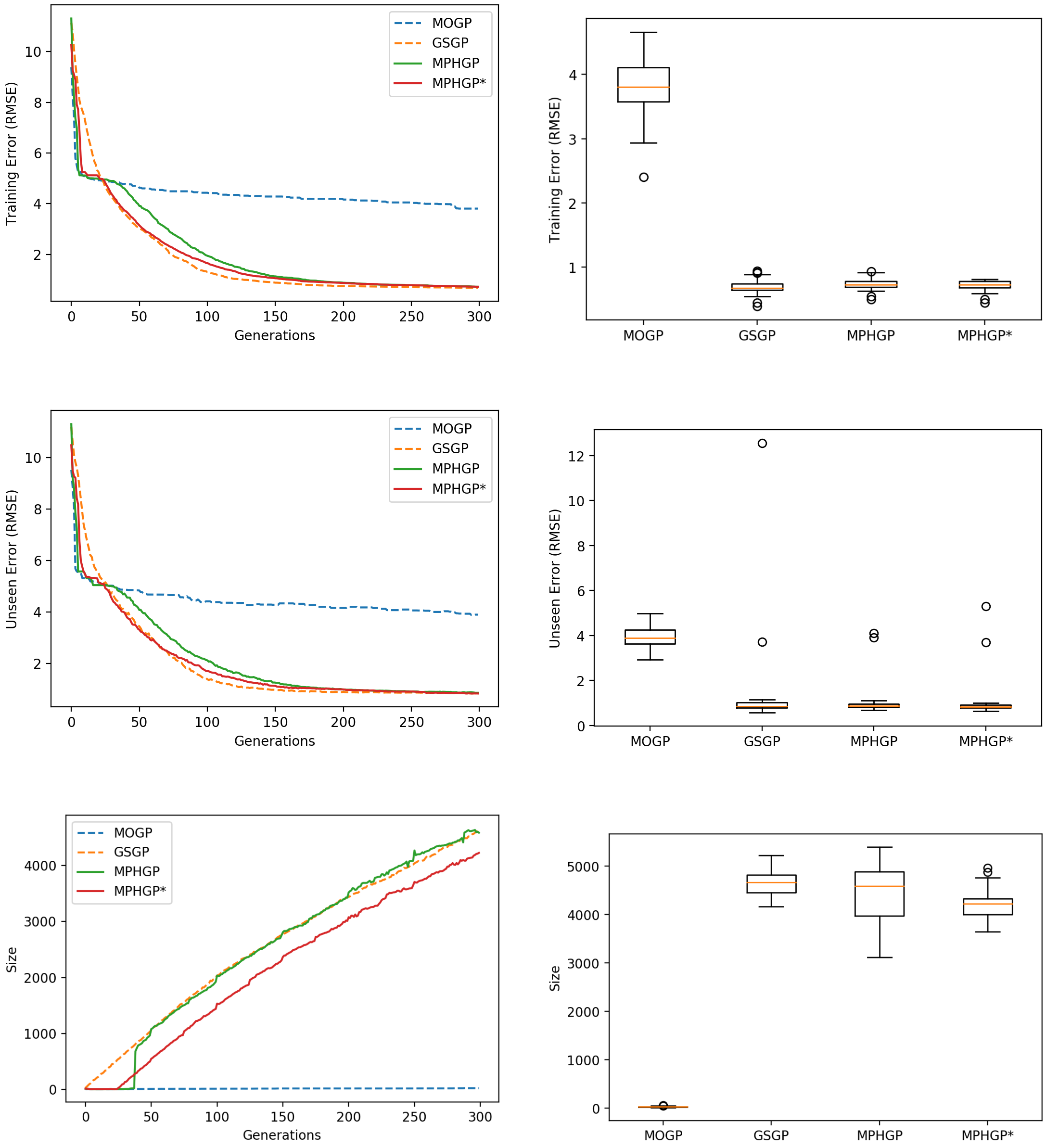


**Figure A.15.:** Energy - Performance of 2-subpopulation MPHGP measured against the standalone benchmarks MOGP and GSGP. From the top, training error, unseen error and size. MPHGP with $f = 50$ and MPHGP* with $f = 25$.

| %F | Train | Unseen | Size |
|---|---|---|---|
| MPHGP vs MOGP | 1.73E-06 | 0.00066 | 1.73E-06 |
| MPHGP vs GSGP | 0.64352 | 0.25364 | 2.13E-06 |

**Table A.26.:** Bioavailability (%F) - Rank-Sum test results in terms of $p$-values, for MPHGP-2

| PPB | Train | Unseen | Size |
|---|---|---|---|
| MPHGP vs MOGP | 1.73E-06 | 0.00385 | 1.73E-06 |
| MPHGP vs GSGP | 0.00171 | 0.18462 | 2.97E-05 |

**Table A.27.:** PPB - Rank-Sum test results in terms of $p$-values, for MPHGP-2

| LD50 | Train | Unseen | Size |
|---|---|---|---|
| MPHGP vs MOGP | 0.53044 | 0.31849 | 1.53E-05 |
| MPHGP vs GSGP | 1.73E-06 | 0.03501 | 1.73E-06 |

**Table A.28.:** Toxicity (LD50) - Rank-Sum test results in terms of $p$-values, for MPHGP-2

| Concrete | Train | Unseen | Size |
|---|---|---|---|
| MPHGP* vs MOGP | 1.73E-06 | 1.73E-06 | 1.73E-06 |
| MPHGP* vs GSGP | 0.38203 | 0.87740 | 0.00080 |

**Table A.29.:** Concrete - Rank-Sum test results in terms of $p$-values, for MPHGP*-2

| Energy | Train | Unseen | Size |
|---|---|---|---|
| MPHGP* vs MOGP | 1.73E-06 | 2.13E-06 | 1.73E-06 |
| MPHGP* vs GSGP | 0.22102 | 0.64352 | 8.47E-06 |

**Table A.30.:** Energy ($f = 25$, $r = 0.35$) - Rank-Sum test results in terms of $p$-values, for MPHGP*-2

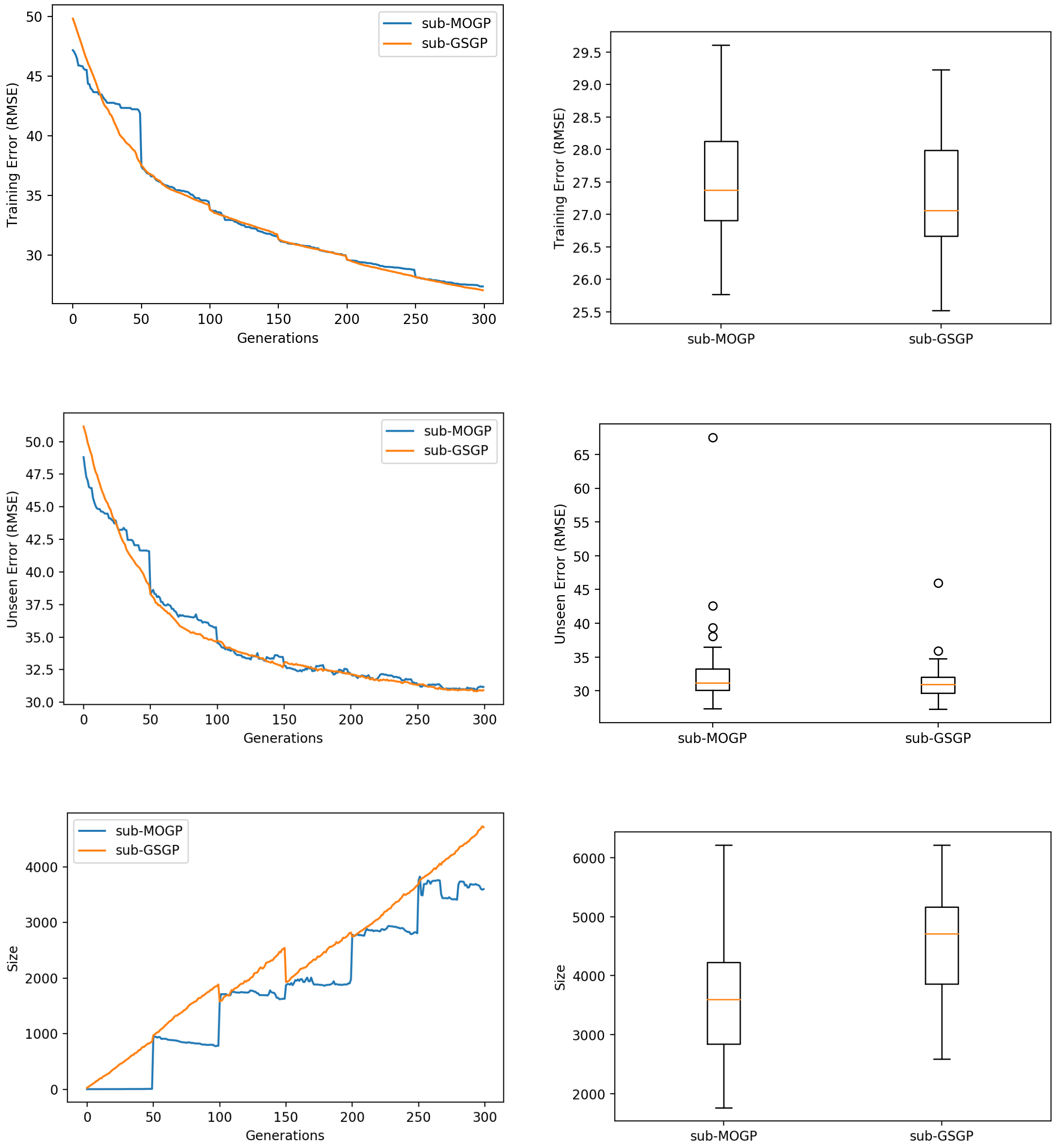


**Figure A.16.:** Bioavailability (%F) - Introspection of 2-subpopulation MPHGP.

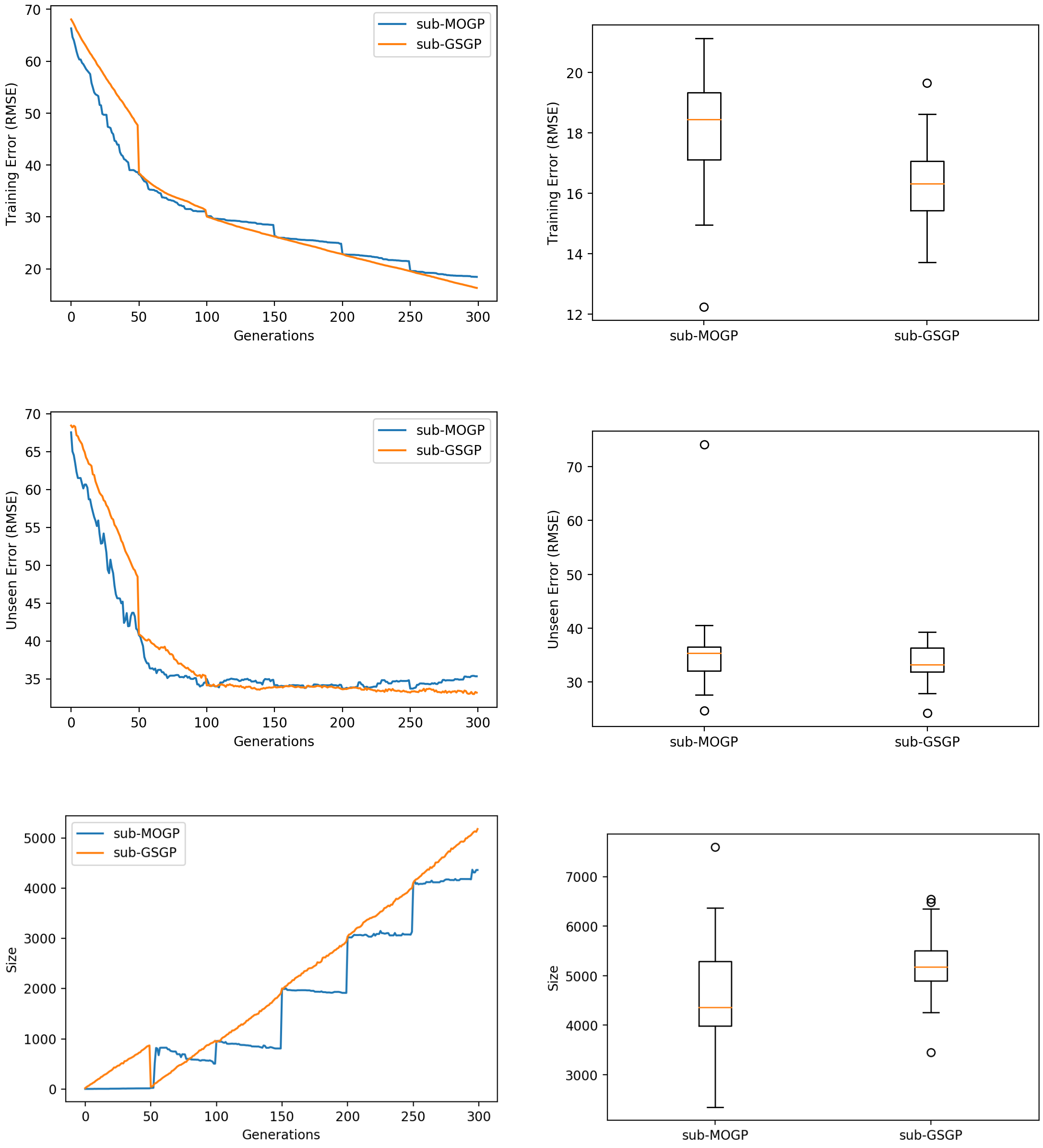


**Figure A.17.:** PPB - Introspection of 2-subpopulation MPHGP.

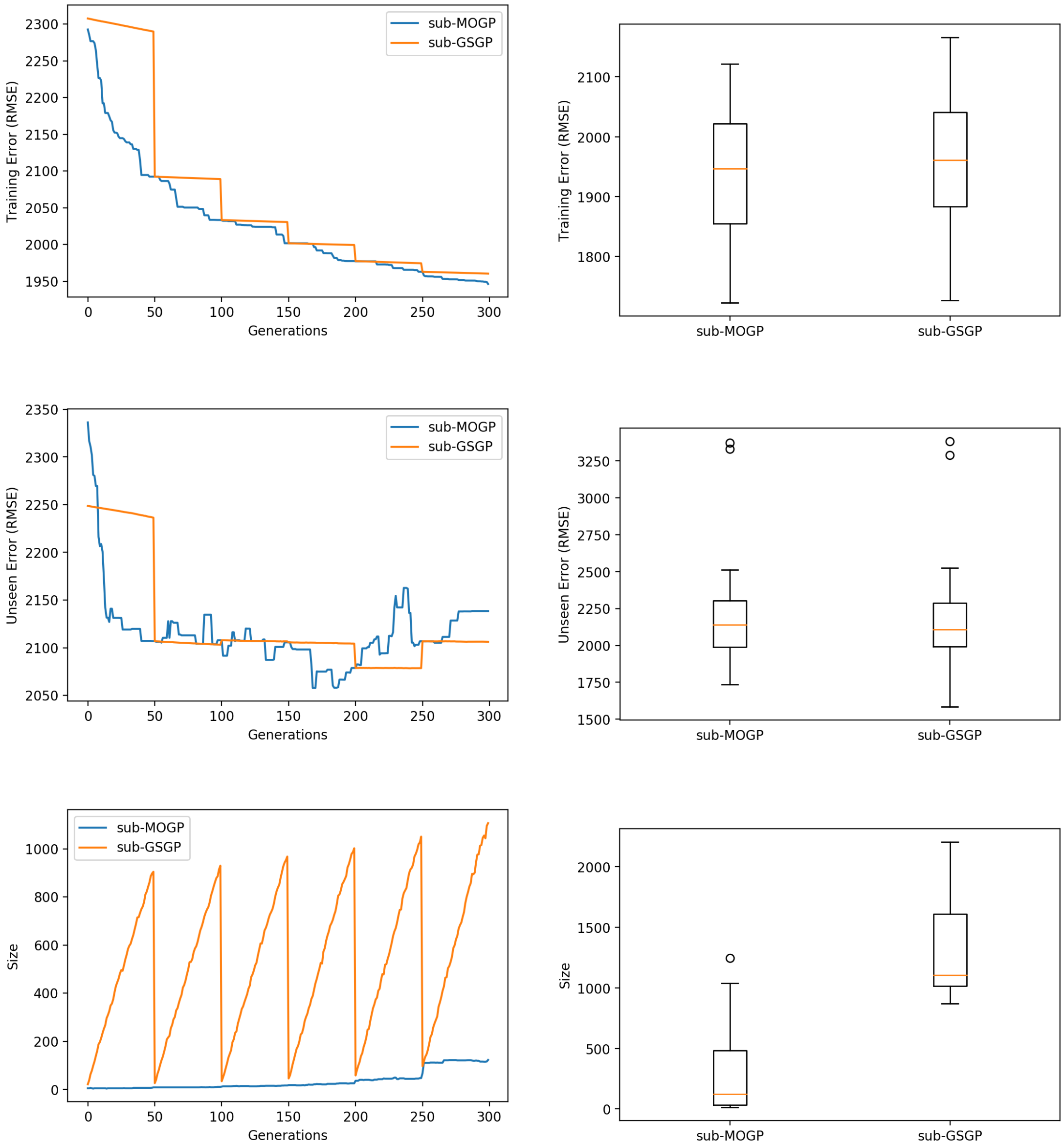


**Figure A.18.:** Toxicity (LD50) - Introspection of 2-subpopulation MPHGP.

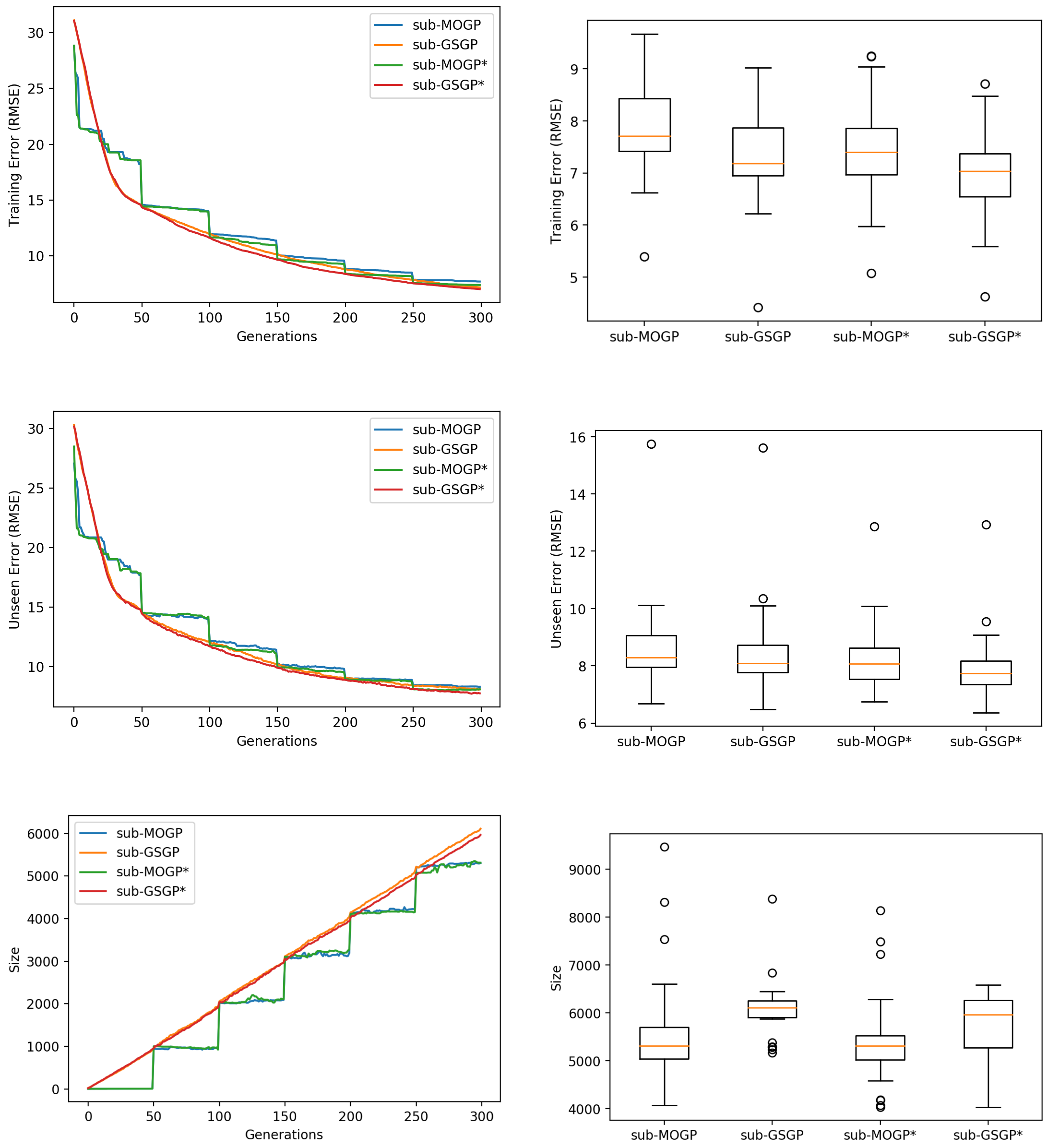


**Figure A.19.:** Concrete - Introspection of 2-subpopulation MPHGP and MPHGP*.

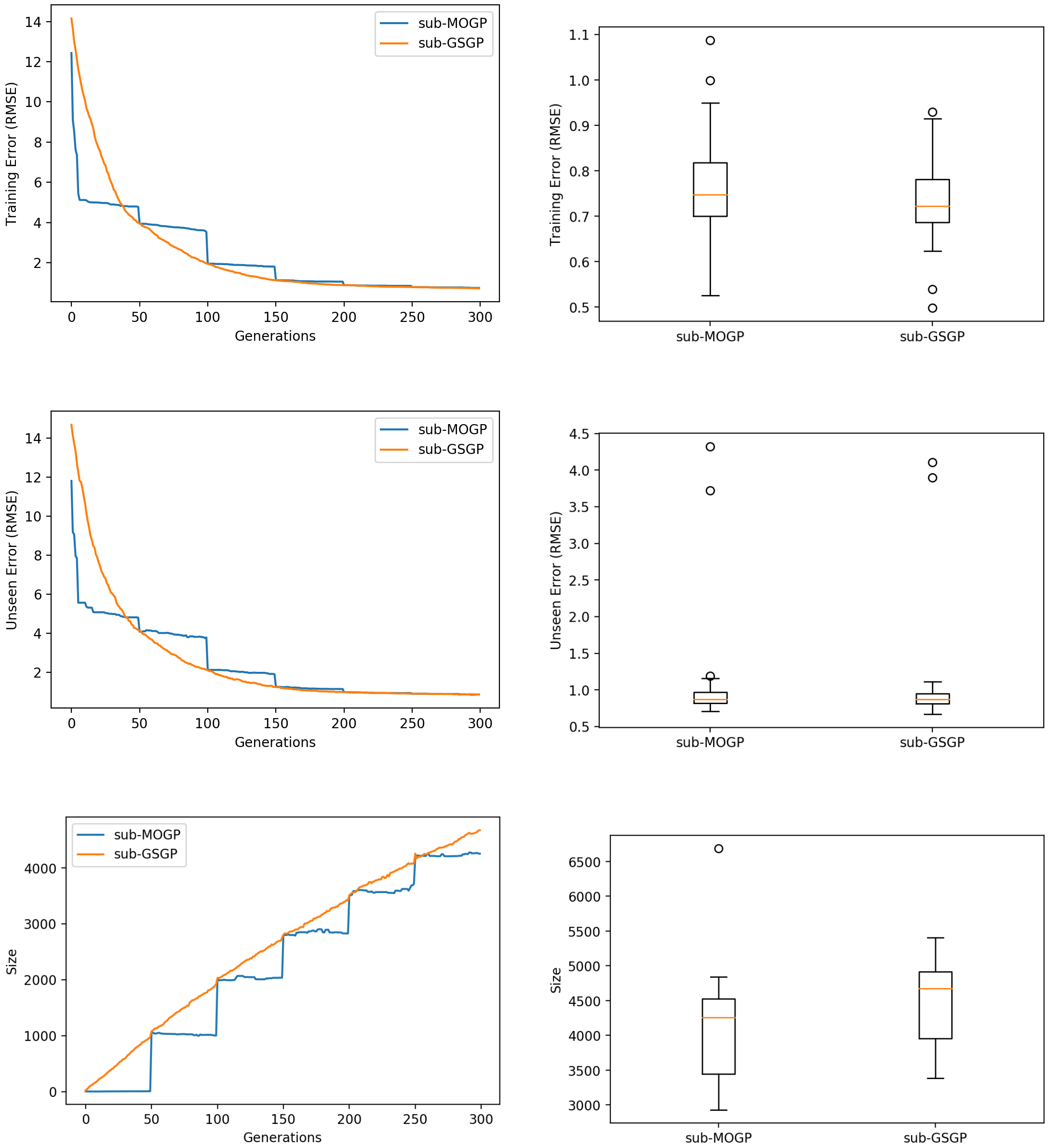


**Figure A.20.:** Energy - Introspection of 2-subpopulation MPHGP. Note that $f = 50$

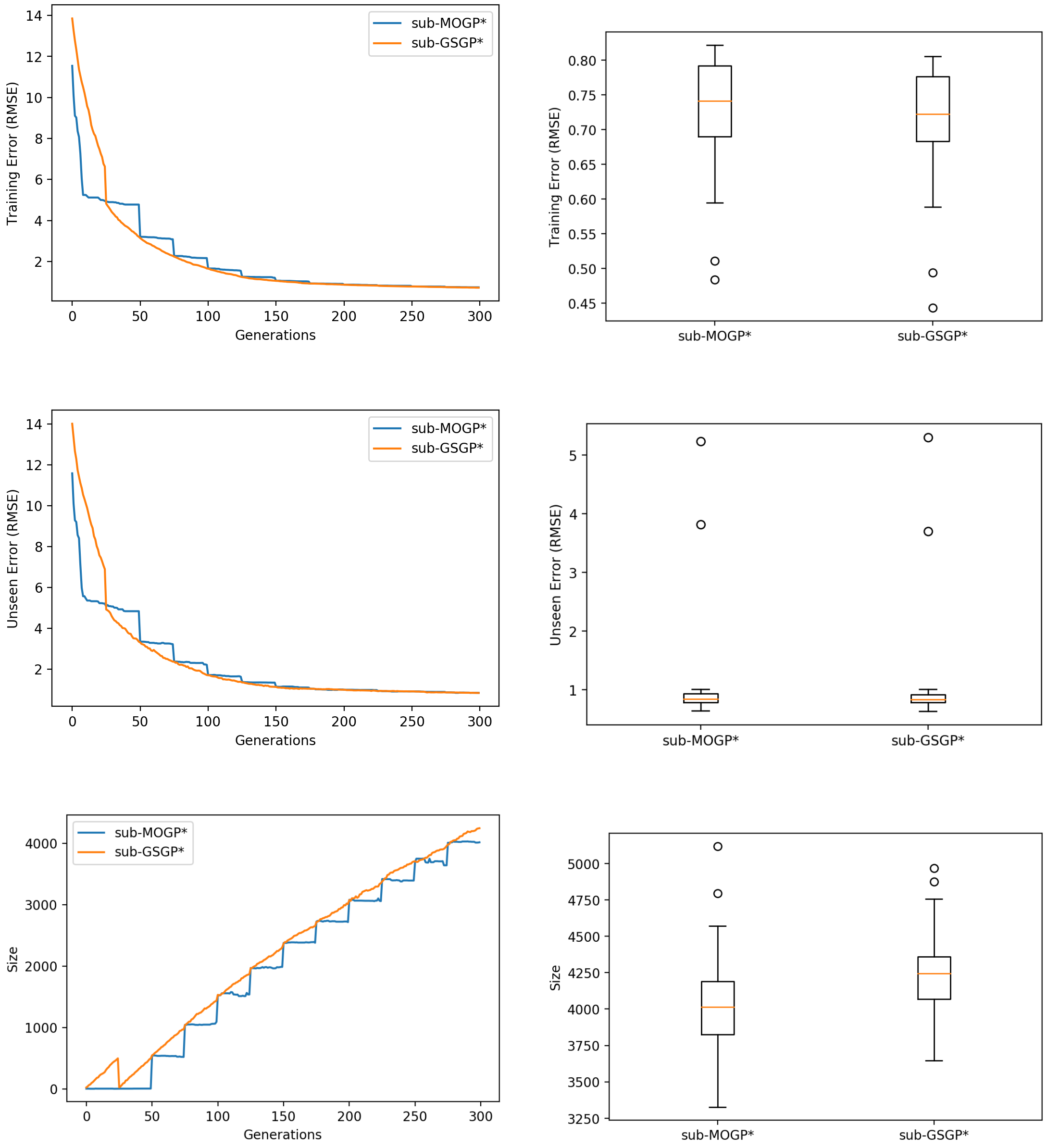


**Figure A.21.:** Energy - Introspection of 2-subpopulation MPHGP*. Note that $f = 25$

## A.4 Increasing Number of Subpopulations

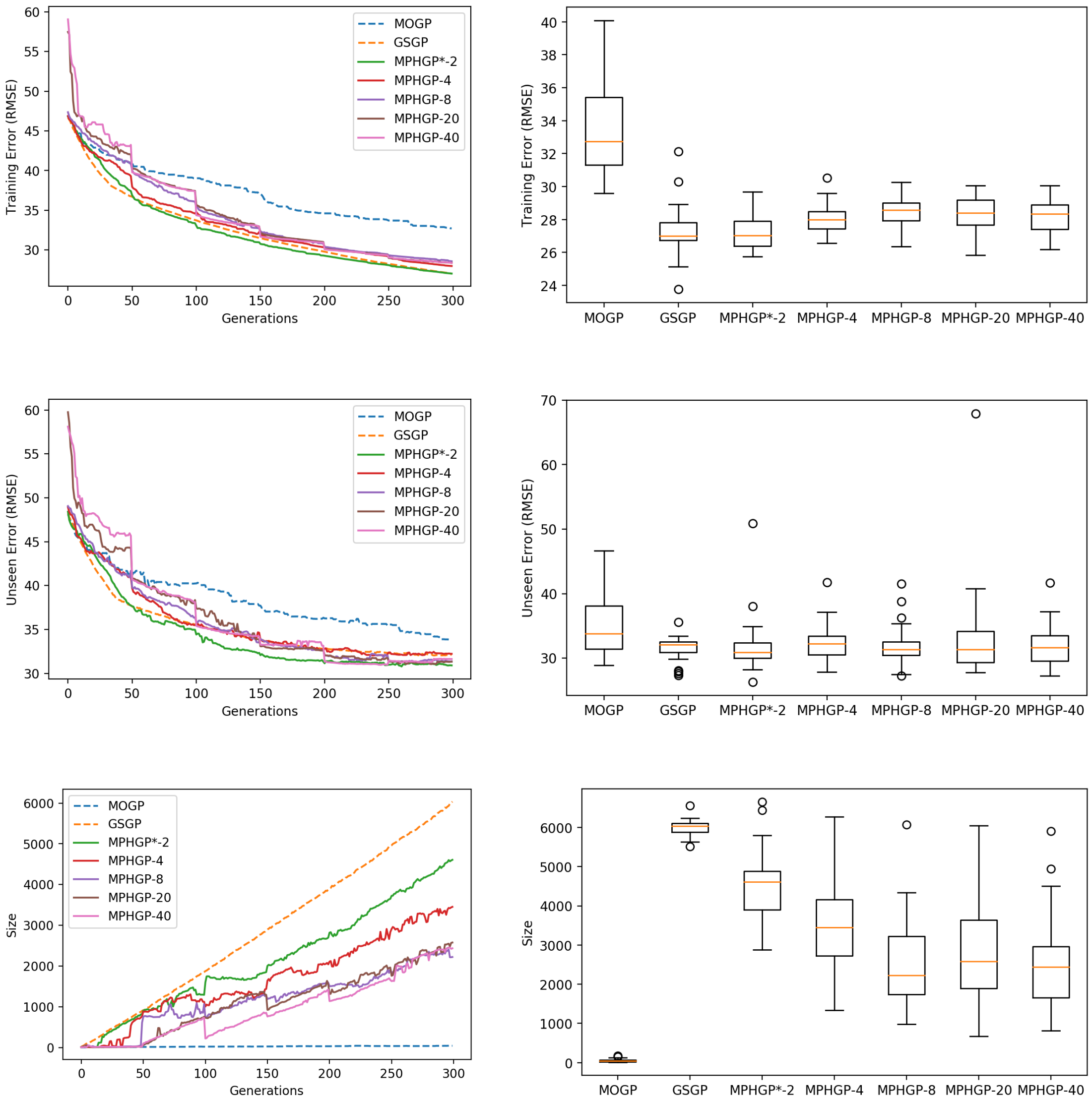


**Figure A.22.:** Bioavailability (%F) - Increasing number of subpopulations of MPHGP.

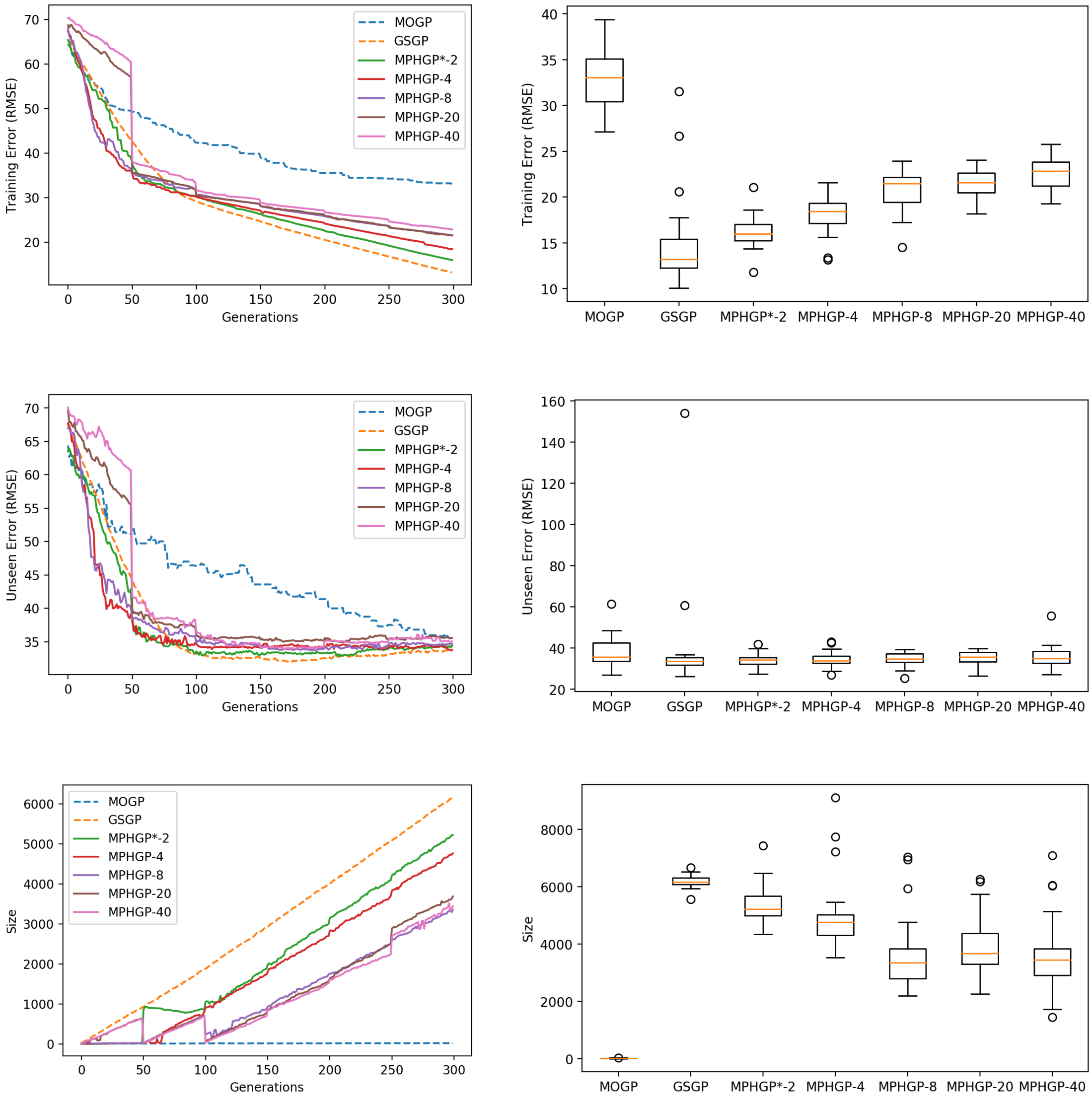


**Figure A.23.:** PPB - Increasing number of subpopulations of MPHGP.

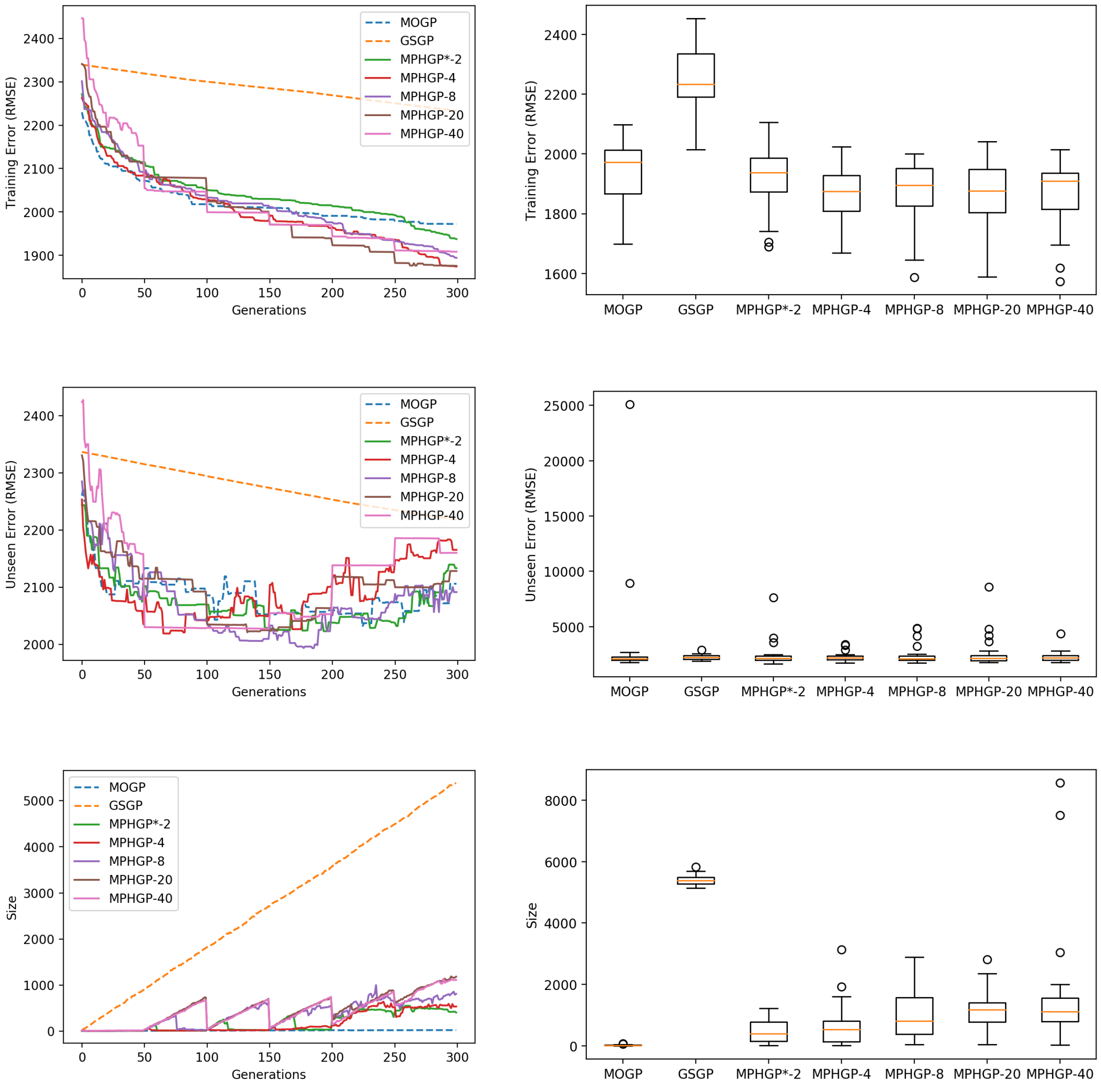


**Figure A.24.:** Toxicity (LD50) - Increasing number of subpopulations of MPHGP.

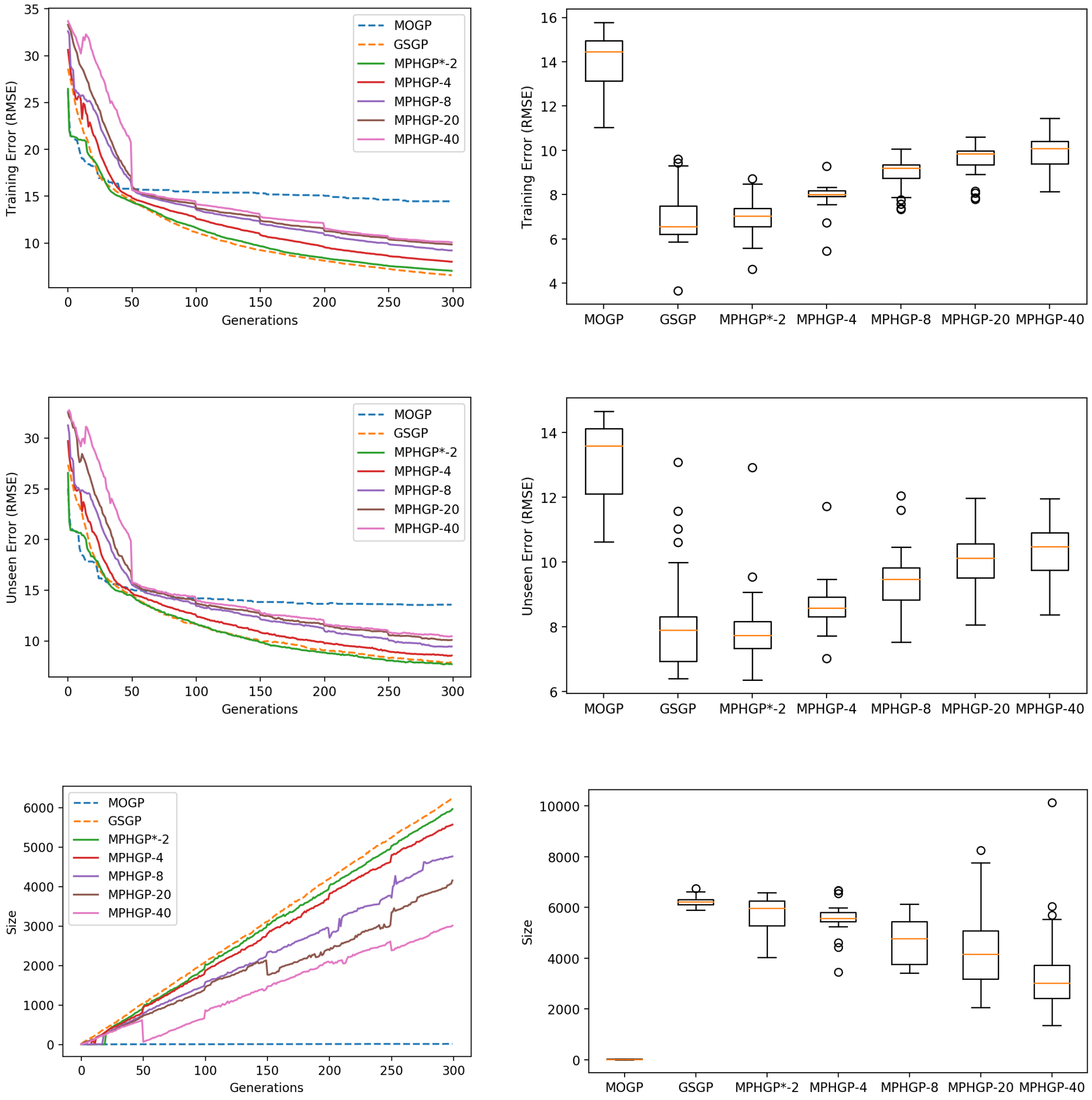


**Figure A.25.:** Concrete - Increasing number of subpopulations of MPHGP.

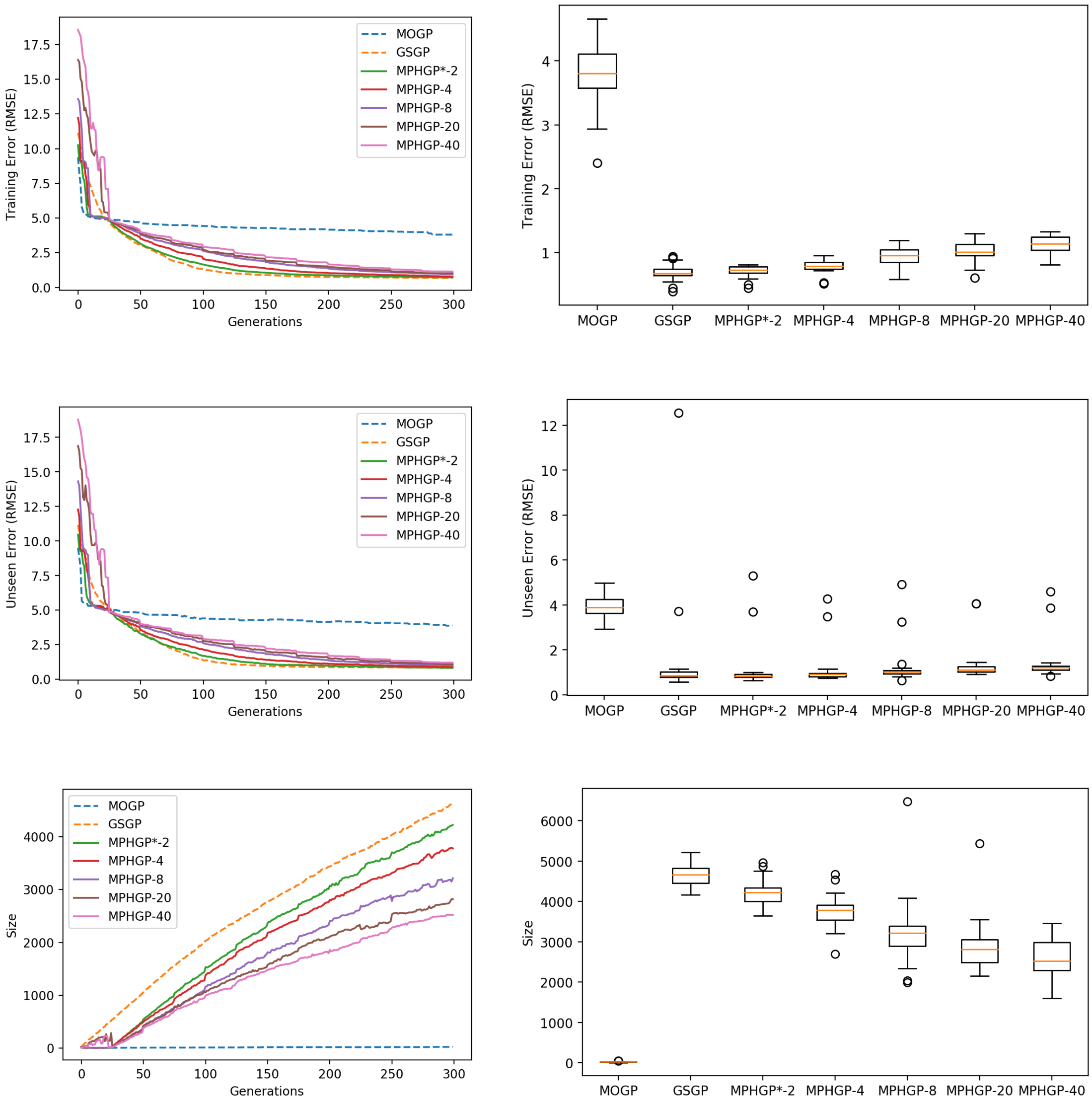


**Figure A.26.:** Energy - Increasing number of subpopulations of MPHGP.

| $ns$ | 2 | 4 | 8 | 20 | 40 |
|---|---|---|---|---|---|
| 2 | - | 0.15286 | 0.49080 | 0.46528 | 0.86121 |
| 4 | 0.00014 | - | 0.18462 | 0.61431 | 0.37094 |
| 8 | 0.00003 | 0.05984 | - | 0.29894 | 0.97539 |
| 20 | 0.00007 | 0.10201 | 0.46528 | - | 0.61431 |
| 40 | 0.00057 | 0.18462 | 0.55774 | 0.39333 | - |

**Table A.31.:** Bioavailability (%F) - Wilcoxon Rank-Sum tests on training and unseen errors for an increasing number of subpopulations. Below diagonal lie the $p$-values for tests on training error and above for unseen error. Migration frequency $f = 50$.

| $ns$ | 2 | 4 | 8 | 20 | 40 |
|---|---|---|---|---|---|
| 2 | - | 0.26230 | 0.03327 | 0.00277 | 0.02703 |
| 4 | 1.80E-05 | - | 0.73433 | 0.11093 | 0.22102 |
| 8 | 1.92E-06 | 1.49E-05 | - | 0.22888 | 0.36004 |
| 20 | 1.73E-06 | 5.75E-06 | 0.15286 | - | 0.87740 |
| 40 | 1.73E-06 | 1.73E-06 | 1.24E-05 | 0.00773 | - |

**Table A.32.:** PPB - Wilcoxon Rank-Sum tests on training and unseen errors for an increasing number of subpopulations. Below diagonal lie the $p$-values for tests on training error and above for unseen error. Migration frequency $f = 50$.

| $ns$ | 2 | 4 | 8 | 20 | 40 |
|---|---|---|---|---|---|
| 2 | - | 0.36004 | 0.84508 | 0.73433 | 0.32857 |
| 4 | 5.31E-05 | - | 0.27116 | 0.64352 | 0.44052 |
| 8 | 4.07E-05 | 0.82901 | - | 0.28021 | 0.74987 |
| 20 | 6.89E-05 | 0.30861 | 0.50383 | - | 0.90993 |
| 40 | 0.00015 | 0.47795 | 0.55774 | 0.57165 | - |

**Table A.33.:** Toxicity (LD50) - Wilcoxon Rank-Sum tests on training and unseen errors for an increasing number of subpopulations. Below diagonal lie the $p$-values for tests on training error and above for unseen error. Migration frequency $f = 50$.

| $ns$ | 2 | 4 | 8 | 20 | 40 |
|---|---|---|---|---|---|
| 2 | - | 0.00049 | 8.47E-06 | 3.18E-06 | 1.36E-05 |
| 4 | 2.84E-05 | - | 0.00049 | 8.47E-06 | 1.02E-05 |
| 8 | 5.75E-06 | 1.13E-05 | - | 0.01108 | 0.00258 |
| 20 | 1.73E-06 | 2.13E-06 | 0.00096 | - | 0.12044 |
| 40 | 1.73E-06 | 1.73E-06 | 0.00011 | 0.03160 | - |

**Table A.34.:** Concrete - Wilcoxon Rank-Sum tests on training and unseen errors for an increasing number of subpopulations. Below diagonal lie the $p$-values for tests on training error and above for unseen error. Migration frequency $f = 50$.

| $ns$ | 2 | 4 | 8 | 20 | 40 |
|---|---|---|---|---|---|
| 2 | - | 0.27116 | 0.00072 | 3.72E-05 | 3.11E-05 |
| 4 | 0.00045 | - | 0.00277 | 2.84E-05 | 2.13E-06 |
| 8 | 1.92E-06 | 1.49E-05 | - | 0.02183 | 0.00196 |
| 20 | 1.73E-06 | 1.73E-06 | 0.02431 | - | 0.09777 |
| 40 | 1.73E-06 | 1.73E-06 | 3.72E-05 | 0.00822 | - |

**Table A.35.:** Energy - Wilcoxon Rank-Sum tests on training and unseen errors for an increasing number of subpopulations. Below diagonal lie the $p$-values for tests on training error and above for unseen error. Migration frequency $f = 25$.

## A.5 Running Times

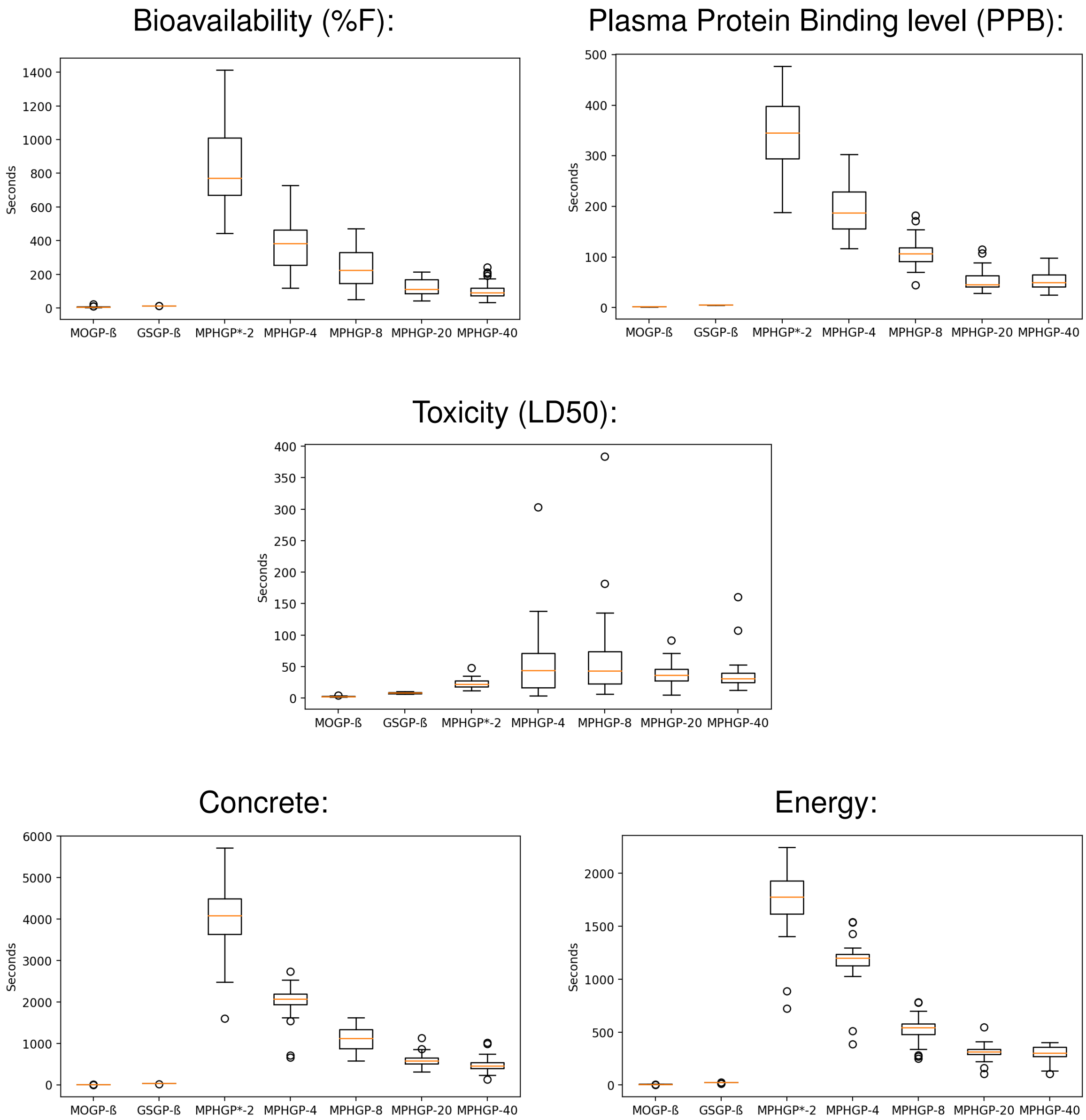


**Figure A.27.:** Median running time over 30 independent runs. Notes: (a) MOGP-ß and GSGP-ß are the single-population benchmarks of MOGP and GSGP without the cosine function; (b) MPHGP*-2 is the special MPHGP with two subpopulations with $f = 5$ and $r = 0.5$ (thus, 100 individuals) - this is an extremely worse scenario in terms of speed; (c) MPHGP-4 to MPHGP-40 represent the base MPHGP with a number of subpopulations corresponding to $\{4, 8, 20, 40\}$ with the number of migrants specified by 2.3 and $f = 50$ except for the Energy dataset where $f = 25$.

| Algorithm | %F | PPB | LD50 | Concrete | Energy |
|---|---|---|---|---|---|
| MOGP | 0:00:05 | 0:00:02 | 0:00:03 | 0:00:09 | 0:00:07 |
| GSGP | 0:00:12 | 0:00:05 | 0:00:09 | 0:00:39 | 0:00:27 |
| MPHGP*-2 | 0:12:51 | 0:05:46 | 0:00:22 | 1:08:07 | 0:29:36 |
| MPHGP-4 | 0:06:24 | 0:03:07 | 0:00:44 | 0:34:37 | 0:19:59 |
| -8 | 0:03:45 | 0:01:46 | 0:00:43 | 0:18:45 | 0:09:04 |
| -20 | 0:01:50 | 0:00:45 | 0:00:36 | 0:09:40 | 0:05:12 |
| -40 | 0:01:31 | 0:00:50 | 0:00:31 | 0:07:38 | 0:05:00 |

**Table A.36.:** Median running time [h:mm:ss] with increasing number of subpopulations.

| %F | MOGP-ß | GSGP-ß | MPHGP*-2 | MPHGP-4 | -8 | -20 | -40 |
|---|---|---|---|---|---|---|---|
| MOGP-ß | - | 3.11E-05 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 |
| GSGP-ß | 1.73E-06 | - | 1.80E-05 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 |
| MPHGP*-2 | 1.73E-06 | 1.73E-06 | - | 0.00042 | 5.75E-06 | 9.32E-06 | 1.13E-05 |
| MPHGP-4 | 1.73E-06 | 1.73E-06 | 2.35E-06 | - | 0.00984 | 2.88E-06 | 0.00927 |
| -8 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 0.00241 | - | 3.41E-05 | 4.86E-05 |
| -20 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 0.02849 | 0.51705 | - | 0.67328 |
| -40 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 2.35E-06 | 0.86121 | 0.09777 | - |

**Table A.37.:** Bioavailability (%F) - Statistical significance of impact of number of subpopulations on running times and size. The $p$-values pertain to the Wilcoxon Rank-Sum test and significance at 5% is highlighted with light grey. Below the diagonal the Rank-Sum test is performed on the samples of results of running times; above the diagonal, of size.

| PPB | MOGP-ß | GSGP-ß | MPHGP*-2 | MPHGP-4 | -8 | -20 | -40 |
|---|---|---|---|---|---|---|---|
| MOGP-ß | - | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 |
| GSGP-ß | 1.73E-06 | - | 0.00211 | 2.88E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 |
| MPHGP*-2 | 1.73E-06 | 1.73E-06 | - | 0.00031 | 4.29E-06 | 6.98E-06 | 1.92E-06 |
| MPHGP-4 | 1.73E-06 | 1.73E-06 | 2.60E-06 | - | 0.00042 | 1.73E-06 | 0.00039 |
| -8 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.92E-06 | - | 5.22E-06 | 2.35E-06 |
| -20 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 0.00873 | 0.17791 | - | 0.15886 |
| -40 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 0.81302 | 0.86121 | - |

**Table A.38.:** PPB - Statistical significance of impact of number of subpopulations on running times and size. The $p$-values pertain to the Wilcoxon Rank-Sum test and significance at 5% is highlighted with light grey. Below the diagonal the Rank-Sum test is performed on the samples of results of running times; above the diagonal, of size.

| LD50 | MOGP-ß | GSGP-ß | MPHGP*-2 | MPHGP-4 | -8 | -20 | -40 |
|---|---|---|---|---|---|---|---|
| MOGP-ß | - | 1.73E-06 | 1.73E-06 | 2.56E-06 | 1.92E-06 | 1.73E-06 | 1.92E-06 |
| GSGP-ß | 1.73E-06 | - | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 2.35E-06 |
| MPHGP*-2 | 1.73E-06 | 1.73E-06 | - | 0.04949 | 0.00049 | 1.24E-05 | 7.69E-06 |
| MPHGP-4 | 1.73E-06 | 8.47E-06 | 0.00499 | - | 0.06871 | 0.36004 | 0.00241 |
| -8 | 1.73E-06 | 3.18E-06 | 0.00019 | 0.34935 | - | 0.14704 | 0.02183 |
| -20 | 1.73E-06 | 1.92E-06 | 2.60E-05 | 0.01319 | 0.40483 | - | 0.51705 |
| -40 | 1.73E-06 | 1.73E-06 | 0.00039 | 0.31849 | 0.29894 | 0.41653 | - |

**Table A.39.:** Toxicity (LD50) - Statistical significance of impact of number of subpopulations on running times and size. The $p$-values pertain to the Wilcoxon Rank-Sum test and significance at 5% is highlighted with light grey. Below the diagonal the Rank-Sum test is performed on the samples of results of running times; above the diagonal, of size.

| Concrete | MOGP-ß | GSGP-ß | MPHGP*-2 | MPHGP-4 | -8 | -20 | -40 |
|---|---|---|---|---|---|---|---|
| MOGP-ß | - | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 |
| GSGP-ß | 1.73E-06 | - | 0.00053 | 1.92E-06 | 1.73E-06 | 2.35E-06 | 3.18E-06 |
| MPHGP*-2 | 1.73E-06 | 1.73E-06 | - | 5.03E-05 | 1.73E-06 | 1.02E-05 | 8.07E-06 |
| MPHGP-4 | 1.73E-06 | 1.73E-06 | 1.73E-06 | - | 0.00015 | 1.73E-06 | 5.31E-05 |
| -8 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 8.47E-06 | - | 4.73E-06 | 2.13E-06 |
| -20 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 0.00015 | 0.14139 | - | 0.00773 |
| -40 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 0.00062 | 0.00642 | - |

**Table A.40.:** Concrete - Statistical significance of impact of number of subpopulations on running times and size. The $p$-values pertain to the Wilcoxon Rank-Sum test and significance at 5% is highlighted with light grey. Below the diagonal the Rank-Sum test is performed on the samples of results of running times; above the diagonal, of size.

| Energy | MOGP-ß | GSGP-ß | MPHGP*-2 | MPHGP-4 | -8 | -20 | -40 |
|---|---|---|---|---|---|---|---|
| MOGP-ß | - | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 |
| GSGP-ß | 1.73E-06 | - | 4.07E-05 | 1.73E-06 | 1.92E-06 | 1.92E-06 | 1.73E-06 |
| MPHGP*-2 | 1.73E-06 | 1.73E-06 | - | 0.00031 | 2.60E-05 | 8.47E-06 | 1.73E-06 |
| MPHGP-4 | 1.73E-06 | 1.73E-06 | 1.73E-06 | - | 0.00019 | 1.73E-06 | 1.73E-06 |
| -8 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | - | 1.64E-05 | 2.60E-06 |
| -20 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 2.60E-05 | 0.00143 | - | 0.12044 |
| -40 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 1.73E-06 | 0.00017 | 0.94261 | - |

**Table A.41.:** Energy - Statistical significance of impact of number of subpopulations on running times and size. The $p$-values pertain to the Wilcoxon Rank-Sum test and significance at 5% is highlighted with light grey. Below the diagonal the Rank-Sum test is performed on the samples of results of running times; above the diagonal, of size.

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