Evolving Multi-Objective Evolutionary Algorithms using Multi-Objective Genetic Programming

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Hannes Wyss
(U2708061)

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Preface

This Dissertation is dedicated to my wife Clíodhna Ní Aodáin, who had her own storm to weather and still had time to bring me a fresh cup of really hot tea. I would also like to thank my business associate Zeno Davatz whose equanimity I can only aspire to, and my tutor Malcolm Jenner for his concise criticism and his patience with my penchant for open-sourced word processors. All my gratitude goes to my parents, my sister and my brother, whose never-ending support has kept me afloat.

Table of Contents

List of Figures

List of Tables

Abstract

Many real-world optimization problems present decision-makers with multiple conflicting objectives. Such Multi-Objective Optimization problems are preferably solved by providing the decision-maker with a maximally diverse selection of optimized solutions. Since Evolutionary Algorithms – due to their population paradigm – already work on several solutions in parallel, their ability to optimize multiple objectives is an inherent property and many successful Multi-Objective Evolutionary Algorithms have been described. In Genetic Programming, the concept of evolutionary search is used to search for algorithms. Owing to their common ancestry in evolutionary computation, the techniques employed in Multi-Objective Evolutionary Algorithms are largely applicable to Genetic Programming.

The search for good Multi-Objective Evolutionary Algorithms is itself a multi-objective problem: such an algorithm is said to be “good” if it finds both maximally optimized and maximally distributed solutions. Based on this assumption, the presented dissertation examines whether it is possible to evolve Multi-Objective Evolutionary Algorithms by applying Multi-Objective Evolutionary techniques to Genetic Programming. In particular, the following three questions are examined:

- Can Genetic Programming find a good Multi-Objective Evolutionary Algorithm by pure recombination of known genetic operators and selection methods?
- Can Genetic Programming define new genetic operators or selection methods, if given appropriate building blocks, and are they of similar quality as methods taken from the literature?

- How well do the best of these automatically generated Multi-Objective Evolutionary Algorithms perform in more complex test problems, when compared to known good algorithms?

To support this new process, an existing classification system of dominance relations is extended and two finer-grained dominance relations are introduced: “distribution-comparable” and “convergence-comparable” are able to completely and exclusively classify so-called incomparable approximation sets.

Experiments investigating the recombination of high-level genetic operators from the literature appear to support the initial assumption, although statistical analysis of the collected data yields mostly inconclusive results. Subsequent exploration of new selection operators evolved from lower-level functions are successful: the Triple Tournament selection operator is the first genetic operator programmed by means of natural selection. This and other resulting algorithms, while unable to outperform NSGA-II, highlight the importance of underlying parameters and the dangers of over-specialization in complex Genetic Programming environments.

Chapter 1 Introduction

From the second half of the twentieth century onwards, computer scientists have investigated the idea of artificial intelligence. If computing machinery was able to relieve us from tedious repetition, why should it not also assist us in solving more complex problems? Two prominent concepts of the field, machine learning and evolutionary computation, were first envisioned by Alan Turing (Turing, 1950) in his seminal article "Computing Machinery and Intelligence":

> Instead of trying to produce a programme to simulate the adult mind, why not rather try to produce one which simulates the child's? If this were then subjected to an appropriate course of education one would obtain the adult brain. [...]
>
> We have thus divided our problem into two parts. The child-programme and the education process. These two remain very closely connected. We cannot expect to find a good child-machine at the first attempt. One must experiment with teaching one such machine and see how well it learns. One can then try another and see if it is better or worse. There is an obvious connection between this process and evolution, by the identifications
>
> | | |
> |---|---|
> | Structure of the child machine | = Hereditary material |
> | Changes " " | = Mutations |
> | Natural selection | = Judgment of the experimenter |

Half a century later, both parts of Turing's original problem have found many competent solutions. In some instances, two paradigms have been successfully combined. Particularly in the field of neuroevolution (where evolutionary algorithms are used to configure an Artificial Neural Network) investigators have found promising results (Gruau and Whitley, 1993; Yao, 1999; Pardoe et al., 2005). This thesis aims to do the same for Multi-Objective Evolutionary Algorithms and Genetic Programming.

1.1 Multi-Objective Evolutionary Optimization

The ancestral line of *Genetic Programming* can be traced back to R. Friedberg's article "A Learning Machine" (Friedberg, 1958), in which he describes the iterative creation of a program that solves a simple bit-moving problem. The lineage of *Evolutionary Optimization* – the search for optimal solutions modelled after Darwinian evolutionary theory – comes from ideas first investigated by Hollstien (1971), Holland (1975) and particularly De Jong (1975). Conjoined by the field of Multi-Objective Optimization, Genetic Programming and Evolutionary Optimization form the foundation of the present thesis.

1.1.1 Multi-Objective Optimization

Optimization is the search for a set of parameters that describe an optimal solution when translated by an objective function; this is usually expressed as the minimization or maximization of the objective function. It is helpful to regard this process as a mapping from parameter space into solution space, where n parameters define the n-dimensional parameter space, and m objective functions define the m-dimensional solution space. Figure 1 shows an example of such a mapping, with shaded areas marking the feasible search-space – those parts of the parameter and solution spaces for which a meaningful mapping exists. The border-segment of the feasible solution space marked by a solid line contains all optimal solutions for the case of minimization.

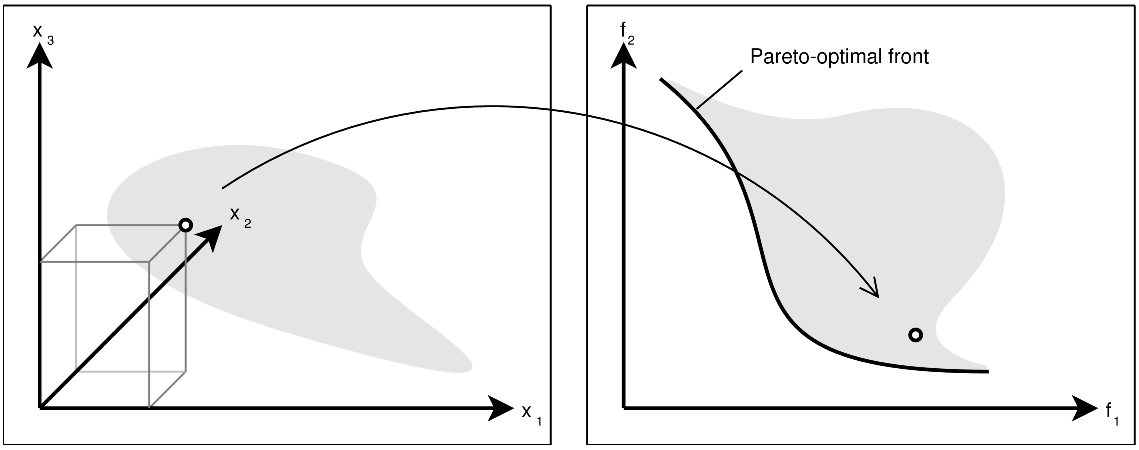

Figure 1: Mapping from a 3-dimensional parameter-space into a 2-dimensional solution-space

In many real-world optimization problems, multiple objectives need to be optimized in order to find a satisfactory solution. An optimization problem in which two or more objective functions share at least one parameter is called a Multi-Objective Optimization problem. In interesting cases there are two or more conflicting and often incommensurable objectives; this leads to so-called trade-off situations in which each objective can only be improved at the cost of degradation in one or more other objectives. Due to the non-linear nature of Multi-Objective Optimization problems, deceptive local trade-off solutions may exist. Such a local trade-off solution is called a *local optimum*. Its counterpart, the global optimum, is also called *Pareto-optimal solution*.

The field of Multi-Objective Optimization seeks to assist a (human) *decision-maker* in choosing an appropriate solution (Coello Coello, 2000; Deb, 2001). A typical classification of methods for multi-objective decision making (Hwang and Masud, 1979) describes four possible points of influence when the decision-maker's preferences may enter the formal decision-making process:

1. No point of influence (automatic search without intervention from the decision-maker)
2. Before the search (a priori approach)
3. During the search (progressive approach)
4. After the search (a posteriori approach)

Since the decision-maker cannot usually be expected to have *a priori* insight in the exact trade-off among objective functions, it is generally considered desirable to use the *a posteriori* approach and present the decision-maker with a selection of promising solutions – an *approximation set* – which takes into account such trade-off behaviour.

The relation between two of these promising solutions is captured in the concept of Pareto-nondomination: a solution x_1 is said to *dominate* another solution x_2 (also written $x_1 \preceq x_2$) if the following conditions are both satisfied:

1. x_1 is no worse than x_2 in all objectives;
2. x_1 is better than x_2 in at least one of the objectives.

If either of the two conditions are not satisfied, then x_1 does not dominate x_2.

Non-domination does not permit any assertions about the reversal of the relation: simply because $x_1$does not dominate x_2, it does not necessarily follow that x_2 dominates x_1. On the other hand, if x_1 dominates x_2, we can conversely say that x_2 does not dominate x_1. If neither solution dominates the other, the two are non-dominated to each other. The subset of all solutions within the feasible solution space $x^* \in S^* : S^* \subseteq S$ which are not dominated by any other solution $x \in S$ is called the Pareto-optimal set or Pareto-optimal front. All members of the Pareto-optimal set are thus by definition non-dominated to each other.

1.1.2 Evolutionary Algorithms

Evolutionary Algorithms leverage concepts found in Darwinian evolutionary theory to model efficient search behaviour. Iterating over a number of *generations*, a *population* of individual approximations is subjected to crossover and mutation operators, fitness evaluation and reproduction.

A Fitness function reflects the quality of a set of parameters with respect to the objectives of the search. Individual solutions are encoded into a *genome* (usually in binary form or as a so-called real-value genome) and subjected to genetic operators at the beginning of each generation. The mutation operator randomly modifies parts of the genome, while the crossover operator swaps parts of two individuals' genomes. The resulting modified genome is then used as an input to the fitness function. If the resulting fitness is good, this heightens the probability of an individual's inclusion in the next generation by a reproduction operator. The entire process is repeated in subsequent generations until an exit condition is reached, usually a predefined minimal fitness level or a maximum number of generations.

1.1.3 Evolutionary Algorithms in Multi-Objective Optimization

One of the defining properties of Evolutionary Algorithms is the fact that they are population based and therefore operate on multiple solutions in parallel. On an intuitive level this matches naturally with the goal of finding multiple Pareto-optimal solutions. However, it has been shown that it is not straightforward to exploit this connection; Evolutionary Algorithms have the tendency to converge towards a single solution within the feasible solution space, whereas the desired result encompasses a maximally distributed subset of the entire Pareto-optimal set (Deb, 2001).

Coello Coello (2005) describes three classes of Multi-Objective Evolutionary Algorithms (MOEAs):

1. Aggregating functions reduce the multi-objective problem to a single objective problem by aggregating all objective functions into one, for example with the use of a weight or bias vector. Since such a vector must be defined before any fitness-evaluation can take place, aggregating functions fall into the class of *a priori* approaches to multi-objective decision making.
2. Population-based approaches leverage the population of an Evolutionary Algorithm to obtain diverse solutions, without making use of the concept of Pareto domination.

3. Pareto-based approaches explicitly use Pareto domination as a fitness criterion. They can be grouped into two generations: the first generation uses fitness sharing and niching combined with Pareto ranking to overcome the difficulties posed by the point-convergence behaviour. The introduction of e litism marks the beginning of the second generation. Elitism was first described in De Jong (1975) and its application to MOEAs was suggested by Rudolph (1996). In elitism, an archive population of non-dominated solutions is used to prevent the loss of promising solutions due to the stochastic nature of selection and reproduction operators.

1.1.4 Quality Characteristics in Multi-Objective Optimization

An often-mentioned distinguishing feature of Multi-Objective Optimization is the fact that the quality of an obtained approximation set is determined by two independent properties: closeness to the Pareto-optimal front (*convergence*) and the *diversity* of the obtained approximations along the same (Deb, 2001). The latter can be further divided into the criteria of *distribution* and *extent* (Figure 2), ideally approaching uniform distribution and an extent which spreads over the entire range of possible values for all parameters (ibid.; Zitzler et al., 2000). In other words: the search for a good Multi-Objective Optimization Algorithm exhibits properties of a multi-objective problem.

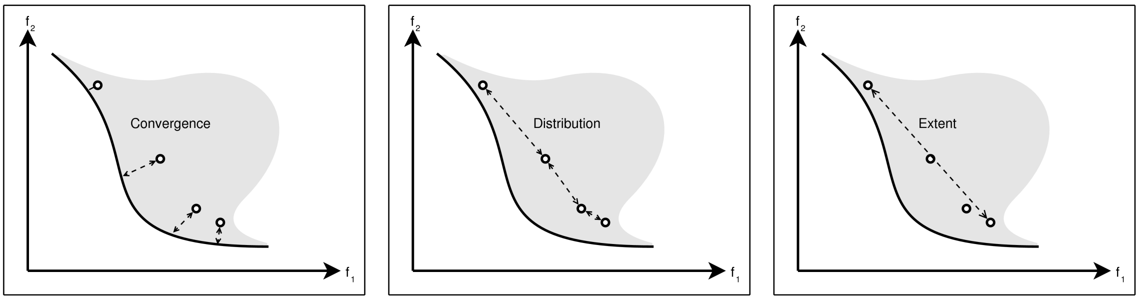

Figure 2: Quality characteristics in Multi-Objective Optimization

1.1.5 Genetic Programming

The related field of Genetic Programming (GP) is another type of evolutionary search. Here, instead of binary or real-value parameters, the genome consists of an executable program (syntax tree, linear or graph-based structures). GP can be seen as a generalization of traditional Evolutionary Algorithms: the latter usually search for optimal parameter-configurations for a given evaluation function specific to the problem domain. The former can additionally search for evaluation functions, given a set of terminals and operations specific to the problem domain.

Due to GP's close relation to traditional Evolutionary Algorithms, many concepts found in MOEA research are applicable in GP. Rodriguez-Vazquez et al. (1997) explored the area of Multi-Objective Genetic Programming; others have investigated the utility of the concept of Pareto dominance in dealing with the problem of "code bloat" (De Jong et al., 2001; Ekárt and Németh, 2001; De Jong and Pollack, 2003). In a somewhat less obvious way the concepts of GP should be applicable to the search for new MOEAs: since the search for a good Multi-Objective Optimization Algorithm is itself a multi-objective problem; and since GP is designed to evolve algorithms, and MOEA-concepts are applicable within GP; it follows that it should be feasible to search for a Multi-Objective Evolutionary Algorithm using Multi-Objective Genetic Programming.

1.2 Searching for non-dominated Multi-Objective Evolutionary Algorithms

The aim of the presented research is to investigate how Multi-Objective Genetic Programming (MOGP) can be used in the search for new MOEAs. Borrowing from Turing, one could say it attempts to teach MOEA child machines to learn, employing MOGP as a substitute teacher. The curriculum: MOEAs and evolutionary computation in general are well-researched fields; there are many genetic operators (crossover, mutation, fitness evaluation, selection and reproduction) to choose from the literature, which can then be utilized as (high-level) building-blocks in an MOGP system. Additionally, lower-level functions can be extracted from them and used to search new genetic operators.

Besides defining a framework for the generation of MOEAs within an MOGP system and proposing a selection of such high- and lower-level building blocks, the introduction of a classification for formally incomparable approximation sets is another contribution to knowledge by this thesis. Furthermore, it presents insights into the idiosyncrasies of such nested evolutions and provides researchers with statistical data concerning the trade-off behaviour between convergence and diversity. Practitioners may find the same information helpful in selecting an MOEA for their specific problem domain.

1.3 Overview of the Dissertation

This dissertation attempts to fulfil its aims in three phases. Based on related research, a framework for the evolutionary generation of Multi-Objective Evolutionary Algorithms (MOEAs) is first defined, including test problems and a combination of performance metrics. In a second experimental part, it shows that the concepts of Genetic Programming (GP) are indeed applicable to the domain of MOEAs: firstly by exploring combinations of known good genetic operators, and secondly by searching for new selection operators using a number of lower-level functions extracted from the same.

Third, the collected data and its analysis yield insights into the performance of various genetic operators and selection mechanisms. Three interesting automatically produced combinations of lower-level functions are presented in detail and the most promising of them is quantitatively compared to an established MOEA.

1.4 Summary

From the second half of the 20th century, computer scientists have sought ways to teach machines to learn. In the presented thesis, two areas within the field of machine learning are of special interest: Multi-Objective Evolutionary Algorithms (MOEA), and Genetic Programming (GP). The area of MOEAs poses many problems to the researcher, namely the trade-off between convergence and diversity. GP profits from results found in MOEA research, and may in turn present us with ways to tackle some of MOEAs' foremost problems. By teaching MOEA child machines to learn with the aid of a GP teacher, this thesis aims to explore some of these paths.

Chapter 2 Literature Review

2.1 Introduction

This dissertation aims to draw together the two research fields of Multi-Objective Evolutionary Algorithms (MOEAs) and Genetic Programming (GP). The literature review concentrates on those aspects of both fields that are necessary or beneficial prerequisites for the empirical steps towards that aim. In the case of GP, our substitute teacher, we need an overview of the concept and its applicability to the problem domain, along with an indication of the greatest pitfalls to be avoided. In the case of MOEAs, which play the role of child machines, we look at what there is to learn for them, and how to test and rate their progress.

2.2 Genetic Programming

2.2.1 Inception and theory

First described by John R. Koza (1990), GP provides a framework for the automatic generation of computer programs using evolutionary algorithms. Unlike traditional evolutionary algorithms, which usually operate on parameter-vectors, GP manipulates program structures. Subsequent research has theoretically validated key concepts, including convergence proofs for both linear and tree-based GP (Langdon and Poli, 2002). It has also been demonstrated empirically that GP can be a valid tool in finding new solutions to complex problems in many domains (Koza et al., 1999).

2.2.2 Code-bloat

One problem often observed in GP experiments is the so-called *code-bloat*: During the course of a GP run, the average size of the individuals in a GP-population will grow uncontrollably, leading in extreme cases to stagnation – no further evolution is possible.

Code-bloat is closely associated with so-called *introns*, arbitrarily large occurrences of superfluous code that do not alter the result produced by an individual (Banzhaf et al. 1998). It has been shown empirically that genetic operators work most efficiently on dense program structures with few introns; these findings were reinforced and explained through theoretical analysis (Greene, 2005). Classic approaches in dealing with code bloat include defining an upper limit for program size, and linearly degrading individual fitness as program size grows. Unfortunately, the former requires a confident estimate of the program size needed for a satisfactory solution and thus does not scale well, whereas with the latter approach, good solutions may be lost due to the resulting indiscriminate selection pressure.

2.2.3 Multi-Objective Genetic Programming

A promising approach to dealing with code-bloat is explored in De Jong et al. (2001), Bleuler et al. (2001) and De Jong and Pollack (2003): it is generally an implicit goal in GP to obtain small candidate solutions with as few introns as possible. In the Multi-Objective GP approach (MOGP) that goal is made explicit. Various Pareto-domination-based algorithms can then be used to address this newly defined multi-objective problem. To preclude the problem of premature convergence, a crowding metric can be employed as a third objective.

2.2.4 Necessary Preparations for a GP-System

Before a GP-System can be run, the following five preparatory steps need to be taken (Koza, 1994):

1. Determine the set of terminals
2. Determine the set of primitive functions

3. Define the fitness measure

4. Choose the parameters for controlling the run

5. Define a method for designating a result and termination criteria.

In the experiments conducted in the course of this study, the first three of these come from the domain of MOEAs. The following section provides background on the possible choices.

2.3 Multi-Objective Evolutionary Optimization

In order to define a valid fitness measure for the GP-System, a deeper look at performance comparison of MOEAs is needed: in the context of this thesis, each GP-experiment will yield an approximation set of individual solutions P, of which each element $Q \in P$ is itself an evolutionary algorithm and, after fitness evaluation, an associate approximation set. The fitness of Q should reflect how well it approximates the Pareto-optimal set of any given multi-objective problem. In the last several years much thought and research has gone into establishing methods that allow an objective comparison of MOEAs. Efforts in this field can be grouped into two distinct areas: performance metrics and test problems

2.3.1 Performance metrics

The set of solutions Q found by an MOEA is called the *approximation set*. While it is theoretically possible for Q to be a subset of the Pareto-optimal set S^*, this is usually not the case. Performance Metrics provide an unbiased way to measure how well an MOEA can approximate the Pareto-optimal front. The adequacy of a set of solutions is determined by both its closeness (*convergence)* to the Pareto-optimal front and its diversity (or *distribution*) along the same (Deb, 2001; Bosman and Thierens, 2003).

Zitzler et al. (2000) name the *extent* (or spread) as a separate third objective. In order to obtain quantitative expressions of these objectives, many performance metrics have been defined:

- An early metric measuring the quality of distribution of the solutions in an approximation set is the Spacing Metric (Schott, 1995). It essentially depicts the standard deviation from the mean distance between neighbouring members of the approximation set and thus does not take into account the extent of the approximation set.
- Fonseca and Fleming (1996) describe the Attainment Surface Metric. The attainment surface is the boundary which separates all points in the solution space that are dominated by at least one result-vector from the ones that are not. If multiple runs of an MOEA are considered, the $n\%$-attainment surface encompasses all points that are likely to be dominated in at least $n\%$ of all runs. The main limitation of this approach, as stated by the investigators themselves, is that probability estimates for attainment can only be made for single points and not for the entire surface.
- The Generational Distance metric (Van Veldhuizen and Lamont, 1998) measures the average distance between an approximation set Q and the Pareto optimal set S^*. For each of the $|Q|$ members x_i of the approximation set, the nearest member x_j^* of the Pareto optimal set is identified and their Euclidean distance d_i (the length of a straight line in solution space from x_i to x_j^*) is computed. The Generational

Distance is defined as the arithmetic average of these values:

$$GD = \frac{\sqrt{\sum_{i=1}^{|Q|} d_i^2}}{|Q|}$$

- The Hypervolume Metric first described by Zitzler and Thiele (1998b) is derived from the volume of the union of all hypercubes formed with the elements of the approximation set and a reference point W. It corresponds to the size (the hypervolume) of that part of the solution space which comprises all points dominated by at least one member of the approximation set.
- The Set Coverage Metric suggested ibid. calculates the proportion of solutions in an approximation set Q_1 which are strongly dominated (or covered) by any member of another approximation Q_2.
- The Error Ratio (Van Veldhuizen, 1999) is defined as the proportion of solutions in an approximation set which are not part of the Pareto-optimal set:

  $$E = \frac{\sum_{i=1}^{|Q|} e_i}{|Q|}$$

  where $|Q|$ is the number of individuals in Q, $e_i = 1$ if the solution i is part of the Pareto optimal set and $e_i = 0$ otherwise.
- The Maximum Pareto Front Error (ibid.) determines a maximum error band with respect to the Pareto optimal front, which encompasses all members of an approximation set. Similar to the Generational Distance, for each of the members of the approximation set the nearest member of the Pareto optimal is identified and their Euclidean distance calculated. The greatest of these values is the Maximum Pareto Front Error.

- The Maximum Spread Metric defined by Zitzler (1999) measures the diagonal of that hypercube which encompasses all solutions in the approximation set; this hypercube is identified by the extreme values found in the approximation set with respect to each objective function.

- As mentioned above, one problem associated with the Spacing Metric is the fact that it carries no information about the obtained range of solutions. Whether the solutions spread over a wide range or are concentrated in one small area of the Pareto optimal front, an approximation set will have perfect spacing as long as the solutions are distributed evenly. To alleviate this problem, the Spread Metric was suggested by Deb et al. (2000). For each objective m, the distance d_m^e between the champion solution in the Pareto optimal set and the corresponding closest member of the approximation set Q is taken. The sum of these is then used as follows:

  $$\Delta = \frac{\sum_{m=1}^{M} d_m^e + \sum_{i=1}^{|Q|} |d_i - \overline{d}|}{\sum_{m=1}^{M} d_m^e + |Q|\overline{d}}$$

  where $d_i$is the shortest distance (e.g. the Euclidean distance, others are allowed also) between a member x_i of the approximation set and any other member and $\overline{d}$ is the mean value of all of these distances.

- A recent Performance Metric concerned with distribution quality was suggested by Farhang-Mehr and Azarm (2002a). To calculate the Entropy Metric, an m-dimensional approximation set is first mapped into an $(m-1)$-dimensional space with the aid of a procedure known as the Gram-Schmidt orthogonalization. The Density function of the resulting density-hypersurface can then be calculated with the aid of an influence function – a decreasing function of the distance to a point in the density-hypersurface (e.g. a Gaussian function). Finally the Entropy Metric is found by calculating the flatness of the Density function.

- A shortcoming of the Generational Distance metric is the fact that an approximation set consisting of one single good individual has a smaller (i.e. better) Generational Distance value than another approximation set which finds slightly worse solutions all along the Pareto optimal front. In other words, the distribution of the approximation set is not taken into account. By including this information, the Reverse Generational Distance described by Bosman and Thierens (2003) alleviates this problem. It is defined as the average Euclidean distance of each member of the Pareto optimal set to the closest member of the approximation set. Although Bosman and Thierens define the Reverse Generational Distance for continuous problems as a line integration over the entire Pareto optimal front, they suggest using a uniformly sampled set of solutions for most practical test applications.
- Similar to the Entropy Metric, the Sparsity Measure (Deb et al., 2005) maps solutions into a suitable hyperplane. Each projected solution is then given a surrounding hyper-cube with a side-length defined by a parameter d. The total hyper-volume covered by all hyper-cubes created in this way, normalized by dividing with the total hyper-volume that could be covered if none of the hyper-cubes would overlap, is the resulting Sparsity Measure.

In the late 1990s, theoretical investigations have shown that most of the above Performance Metrics are inadequate for the comparison of MOEAs. Hansen and Jaszkiewicz (1998) lay the theoretical foundations for the comparison of approximation sets by defining a set of outperformance relations. They recognized the main difficulty with this approach to be that the majority of theoretically possible approximation sets are in fact incomparable by the said outperformance relations. On this base, they then proceeded to propose a range of comparison operators. To deal with the problem of incomparability, comparison operators based on utility functions and other quantitative comparison methods were proposed. Unfortunately all of these are only weakly compatible with the outperformance relations. Knowles and Corne (2002) expanded on this work to put known metrics in the context of the outperformance relations. According to their results, the usefulness of most metrics must be severely doubted.

Building on the work by Hansen and Jaszkiewicz (1998), Zitzler et al. (2002) gave a general proof of the incompleteness of unary performance metrics: there is no unary performance metric from which it can be induced that one approximation set is better than another. In the general case, not even a finite combination of unary performance metrics is sufficient. It can be shown that there is no comparison method possible which is both compatible (a sufficient condition for a binary relation) and complete (a necessary condition for a binary relation) in respect with a binary relation stronger than *A is not worse than B*.

These findings reinforce the point made earlier, that the search for good MOEAs is itself a multi-objective problem. A useful comparison of MOEAs can only be made with the aid of at least two independent Performance Metrics.

2.3.2 Test design

The second aspect of Performance assessment is the design of appropriate test problems. A considerable amount of research has gone into defining scalable test problems that can be tuned to the various difficulties that an MOEA must overcome in order to find the Pareto optimal set. Deb (1999) identifies eight difficulties that an

MOEA faces. Four of those act against convergence of an MOEA towards the Pareto-optimal front:

1. Multimodality: multi-modal problems may exhibit a very large number of local optima, causing an MOEA to stagnate: if the variations introduced by mutation and crossover are too small to overcome the attraction of a local optimum, they may be rejected even though they lie closer to the global optimum.
2. Deception: a deceptive attractor may be favoured by a majority of the search space and thus disturb the direction of search. This difficulty is similar to multimodality, but instead of many small deceptions it poses few widespread ones.
3. Isolated optimum: some problems exhibit a very flat fitness landscape, divulging next to no information about the location of the optimum; the search process stagnates due to lack of direction.
4. Collateral noise: problems with excessive variation in the solution space can lead to misleading fitness evaluations; good building blocks for one objective may be ignored if the solution performs poorly for other objectives.

Three more difficulties oppose diversity of the solutions:

1. Shape of the Pareto-optimal front: if the fitness of a solution is proportional to the number of solutions it dominates, convex regions of the Pareto-optimal front favour solutions close to the centre of the region, while non-convex regions tend to converge towards extreme solutions.
2. Discontinuous Pareto-optimal front: due to the stochastic nature of MOEAs, some sub-regions of an approximation set may not survive a generation. If the

Pareto-optimal front is not continuous, there may be no possibility to repopulate such an extinct sub-region.

3. Non-uniform distribution of solutions along the Pareto-optimal front: If the density of solutions along the Pareto-optimal front is not uniform, MOEAs may naturally converge towards the denser regions.

The last difficulty is the incorporation of constraints, which may oppose both convergence towards the Pareto-optimal front and diversity of solutions by rendering high-fitness solutions infeasible.

After his rigorous analysis, Deb (ibid.) proceeds to define a generic two-objective problem, for which the amount of difficulty caused by the above points can be finely tuned, and which may be extended to an arbitrary number of objectives:

$$\text{Minimize} f_1(x) = f_1(x_1, x_2, ..., x_m)$$
$$\text{Minimize} f_2(x) = g(x_{m+1}, ..., x_N) h(f_1, g)$$

A critique of Deb's construction principles, along with a collection of different test problems, can be found in the doctoral dissertation submitted by Van Veldhuizen (1999). Building on Deb's work, Zitzler et al. (2000) designed one test problem for each of the six distinct difficulties identified by Deb, four of which are used in the present research and explained in detail below. Test problems with more than two objectives were presented in Deb et al. (2002).

2.3.3 Algorithms and Genetic Operators

The terminal and primitive function set that are employed in the experimental phase of this research project are assembled from distinct elements of MOEAs described in literature. The first investigation in Evolutionary Multi-Objective Optimization was undertaken in J. D. Schaffer's doctoral dissertation (1984). Schaffer's Vector Evaluated

Genetic Algorithm (VEGA) divides the population into equal parts, optimizing each subpopulation for one single objective. Obviously this approach strongly favours those solutions which are specialized for one single objective. It was assumed that the application of a crossover operator would result in other solutions along the Pareto-optimal front. However, inherent high selection pressure leads to convergence towards individual champion solutions.

In his textbook on Genetic Algorithms, Goldberg (1989) suggested the use of a non-dominated sorting procedure, thus introducing the concept of Pareto optimality into the field of MOEAs. Nearly a decade after Schaffer's VEGA, Horn and Nafpliotis, and Fonseca and Fleming independently followed Goldberg's suggestion. In Fonseca and Fleming (1993), an individual's fitness is determined according to its rank, which is defined as the number of other solutions in a generation which dominate it (the rank is then augmented by one, to avoid zero-values). The described Multi-Objective Genetic Algorithm (MOGA) also employs a niche sharing technique, scaling the individual fitness within each rank according to their niche count. The niche count is equivalent to the number of solutions that lie within a solution-space hypercube with a predefined side-length σ_{share}. The obvious drawback to this technique is that σ_{share} needs to be defined in advance, which requires *a priori* insights on the shape of the solution space and may be a difficult choice depending on the problem domain.

Another approach is described in Horn and Nafpliotis (1993). The Niched Pareto Genetic Algorithm (NPGA) introduces a way to enhance diversity within a population of solution vectors: NPGA uses a tournament selection operator based on Pareto dominance. Whenever there is a tie, i.e. no solution dominates the other, selection is performed according to which solution has the lower niche count.

Yet another application of Pareto dominance and niching is presented in form of the Non-dominated Sorting Genetic Algorithm (NSGA) (Srinivas and Deb, 1994). There are two main differences to Horn and Nafpliotis' NPGA: NSGA uses non-dominated sorting as opposed to Pareto domination tournaments and performs the niching calculation within the resulting Pareto fronts. Also, NSGA performs the niche counts in parameter space, as opposed to solution space. Srinivas and Deb suggest that this will prevent the danger of differing decision-variable configurations cancelling each other out if they result in similar result-vectors.

In a series of papers, Günter Rudolph was able to provide a formal proof for the convergence of an MOEA towards the Pareto-optimal set in finite time (Rudolph, 1996; Rudolph, 1998; Rudolph, 2001a; Rudolph, 2001b). Key to the successful proof is the introduction of an elite archive (first described in De Jong, 1975), which guarantees that the best found solutions can not be lost due to the application of genetic operators. Although it was later shown in Hanne (1999) that elite archives of a finite size may suffer from partial deterioration, the proof still holds for elite archives of infinite size.

The Strength Pareto Evolutionary Algorithm (SPEA), described in Zitzler and Thiele (1998a), incorporates an elitist strategy (here the concept was taken from Ishibuchi and Murata, 1996), a newly introduced strength fitness measure which was applied in a tournament selection scheme, and finally the average linkage clustering method, a parameter-less replacement for the niche count described earlier. Comparison with other MOEAs showed however that SPEA suffers from three main weaknesses: the coarse fitness assignment gives identical fitness to all candidate solutions that are dominated by the same members of the elite archive – in the extreme case where the elite archive contains only one member, all members of the population are assigned the same fitness. Furthermore, SPEA employs its clustering algorithm only with regard to the elite archive and thus fails to effectively preserve diversity in the search population. Finally, using clustering to reduce the elite archive size may result in loss of outer solutions. In Zitzler et al. (2001), the authors addressed these issues with the description of SPEA2. Here, the calculation of strength as well as clustering includes the entire population, whereas SPEA only considered members of the elite archive.

Another important example of an elitist MOEA is the successor to NSGA, the Elitist Non-dominated Sorting Genetic Algorithm (NSGA-II). It aims to address several problems identified with MOEAs, namely their high computational complexity, the lack of conservation of good solutions and the guesswork associated with the definition of a niche size or sharing parameter. The first issue is kept in check by a consequent focus on efficiency of the utilised algorithms, in particular the sorting of candidate solutions into Pareto fronts. The introduction of an elite archive as suggested and implemented in several other sources addresses the second point. Thirdly, diversity is ensured using the newly introduced crowding distance, which measures the average side-length of the largest cuboid enclosing each candidate solution alone (Deb et al., 2000). Since outer solutions have no nearest neighbour on one side, they are assigned an infinite cuboid and consequentially always selected for the next generation.

The concept of elitism has its limitation: as mentioned, Hanne (1999) showed that even elitist Pareto-based MOEAs may encounter partial deterioration over the course of two or more generations, if the elite set is limited in size. To solve this problem of partial deterioration and answer to the lack of formal proof of convergence for an MOEA that ensures diversity, Laumanns et al. (2001) introduced the concept of ϵ-dominance. In order to guarantee convergence, their algorithm needs to work on two levels. On a coarse level, finding an ϵ-approximate set can be achieved by only replacing a solution from the elite archive if it is ϵ-dominated (in other words if it is dominated by more than a small value ϵ). Once an algorithm has found an approximation within ϵ-vicinity, this coarse-level strategy obviously prevents an algorithm from finding the true Pareto-optimal set; a second, finer level is needed: If a solution dominates an elite solution by less than ϵ, but lies within the coarse-level box with side-lengths ϵ, it may be replaced – thus maintaining the possibility of definitive convergence.

There are a number of Multi-Objective Algorithms inspired by MOEAs which depart from the classic model of evolution and its operators, either by adding additional local search algorithms or by completely replacing the genetic operators. The inclusion of these lies outside of the scope of this thesis. Three are mentioned here in order to establish what lies beyond the fence.

The Entropy-based Multi-Objective Genetic Algorithm (E-MOGA) developed by Farhang Mehr and Azarm (2002b) adds a local search component based on the ideal gas model. A multi-objective optimizer built on the principles of Particle-Swarm Optimization is presented by Hu and Eberhart (2002). Hernández-Díaz et al. (2006) suggested an MOEA based on differential evolution combined with a local search using recent research on Rough Sets.

2.4 Research question

The presented research draws together the two existing fields of MOEAs and GP. It explores the concept of utilizing GP in the search for an MOEA with good convergence and distribution characteristics. Based on the reviewed literature, in particular taking in account the breadth of applications of GP and the well-researched fundamentals of MOEAs, I pose the following two Hypotheses:

1. It is feasible for a (Multi-Objective) Genetic Programming Algorithm to find an MOEA that has similar or better convergence and distribution properties than

known “good” MOEAs if the search is performed using High-Level building-blocks – such as Selection-, Crossover- and Mutation-Operators described in the literature.

2. It is very improbable that an MOGP System can find new genetic operators and selection mechanisms, although it is possible to build a GP-System that searches for such operators.

2.5 Summary

The current body of knowledge relevant to the proposed project is roughly divided in two areas. The first area is concerned with Genetic Programming, a form of Evolutionary Computation which manipulates programs instead of configurations. Researchers have discussed problems related to the uncontrollable growth of GP individuals, which can be alleviated by allowing multiple objectives, and making a small program size one of them. Among the five preparatory steps for a GP experiment, three (in the context of this research project) fall into the domain of Multi-Objective Evolutionary algorithms. First, a fitness measure for GP must be chosen from one of the many MOEA-performance metrics. There is however some uncertainty concerning the theoretic validity of the available metrics and more thought needs to go into the validation of any selection. For both the second and third steps – selection of terminal and primitive function sets – high-level operators can be chosen from a wealth of MOEAs. Building on this foundation, the hypothesis is posed, that the attempted nested evolution can yield useful results.

Chapter 3 Research Methods

3.1 Introduction

In pursuit of answers to the research question defined in the preceding chapter, controlled experiments will be conducted to explore the following partial questions:

- Can GP find a good MOEA by pure recombination of known genetic operators and selection methods?
- Can GP define new selection methods, if given appropriate building blocks, and are they of similar quality as methods taken from the literature?
- How well do the best of these automatically generated MOEAs perform in more complex test problems, when compared to known good MOEAs?

These experiments are based on a Multi-Objective Genetic Programming system, running an implementation of NSGA-II. But which are the objectives? As has been discussed in the literature review, minimization of program size has been successfully employed to control code-bloat and figure as an objective throughout the experiments. To determine the rest of the objectives the following needs to be done: a Performance Metric or a combination thereof needs to be selected with care; this then needs to be applied to one or more test functions. The combination of these will result in a number of measurements that will serve as the remaining objective functions.

3.2 The Open BEAGLE Framework

In order to run the proposed experiments, a framework for Evolutionary Computation is needed. The concomitant requirements include support for both Multi-Objective Evolutionary Algorithms and Genetic Programming, high computational efficiency, and provisions for the comprehensive collection of data. Additionally, ease of configuration and code reuse are criteria towards the selection of a framework. The selected Open BEAGLE Framework (Gagné and Parizeau, 2006) includes all of these features; its GP implementation is tree-based and provides genetic operators that can perform mutation and crossover safely on populations with multiple data types.

3.3 NSGA-II

The Open BEAGLE Framework provides an implementation of NSGA-II, as described in Deb et al. (2000). First, an initial population of tree-based genomes is generated, the individual fitness evaluated and non-dominated solutions are inserted into an unbounded elite archive. A temporary population twice the size of the parent population is then generated by combining the parent population with an offspring population generated by applying five GP-operators:

- The crossover operator exchanges sub-trees between two individuals. In contrast to the mutation operators which all result in only one offspring, here two offspring solutions are copied to the temporary population.
- The standard mutation operator replaces a sub-tree with a newly generated one.
- The shrink mutation operator deletes a sub-tree from a solution.
- The swap mutation operator replaces a node in the tree with another one from the set of primitives
- The sub-tree swap mutation operator exchanges two sub-trees within an individual

The resulting temporary population is then sorted into non-dominated fronts: first, all individuals that are not dominated by any others are identified, and removed from the population. The same is done for the remaining individuals recursively, until there are no individuals left and the population is completely sorted.

The selection procedure starts with the first non-dominated front. If it is smaller than the configured population size, all members are copied into the next generation; the same is then done with the next non-dominated front. This step is repeated until the population is full. If there are superfluous members in the last included non-dominated front, those members are selected which have the greatest crowding distance: for each candidate individual, the two nearest neighbours in the non-dominated front are found for each objective. These form a cuboid, the average side-length of which is the crowding distance.

Finally, the elite archive is updated, considering only individuals in the first non-dominated front.

3.4 Tree depth instead of program size

In the tree-like genome employed throughout the experiments, program size can be seen as equivalent to the number of nodes in a tree. Preliminary experiments showed however, that this leads to an unfair advantage inversely proportional to the number of arguments of an operator. Using the depth of the tree instead provides a similar pressure against code-bloat and did not exhibit such a bias; this configuration was therefore used in the remainder of the experiments.

3.5 Selection of a Performance Metric: the Reverse Generational Distance

The usefulness of performance metrics for the comparison of approximation sets has been severely doubted. Great care must therefore be taken in choosing such metrics and the validation of that choice.

3.5.1 Dominance Relations

In preparation of their investigation into performance metrics, Zitzler et al. (2002) define a set of dominance relations used to assess the utility of a performance metric:

In a n-dimensional solution space S we define the two arbitrary approximation vectors x^1 and x^2: $x^1 = (x_1^1, ..., x_n^1), x^2 = (x_1^2, ..., x_n^2) \in S$. The following relations are then defined:

- x^1 *strictly dominates* x^2, or $x^1 \succ\succ x^2$, if $x^1$is better than x^2 in all objectives
- x^1 *dominates* x^2, or $x^1 \succ x^2$, if $x^1$is better than x^2 in at least one objective, and not worse in any objective
- x^1 *weakly dominates* x^2, or $x^1 \succeq x^2$, if $x^1$is not worse than x^2 in any objective
- x^1 and x^2 are *incomparable*, or $x^1||x^2$, if neither objective vector weakly dominates the other

The formal definition of an approximation set is then given as follows; a set $A \subseteq S$ is called an approximation set, if each of its members is incomparable (or non-dominated) to all other members: $\forall x^1, x^2 \in A : x^1 = x^2 \vee x^1||x^2$. The set of all approximation sets is called Ω.

After these definitions, the objective-vector relations are used to define relations between two approximation sets $A_1, A_2 \in \Omega$:

- A_1 *strictly dominates* A_2, or $A_1 \succ\succ A_2$, if every objective vector in A_2 is strictly dominated by at least one objective vector in A_1
- A_1 *dominates* A_2, or $A_1 \succ A_2$, if every objective vector in A_2 is dominated by at least one objective vector in A_1

- A_1 *weakly dominates* A_2, or $A_1 \succeq A_2$, if every objective vector in A_2 is weakly dominated by at least one objective vector in A_1
- A_1 is *better* than A_2, or $A_1 \rhd A_2$, if $A_1 \succeq A_2$ and $A_1 \neq A_2$
- A_1 and A_2 are *incomparable*, or $A_1||A_2$, if neither approximation set weakly dominates the other

Finally, Zitzler et al. define the concepts of compatibility and completeness for a vector of unary quality indicators $I = (I_1, I_2, ..., I_k)$ and a corresponding binary relation, together with the previously defined binary relations between approximation sets. A quality-indicator-relation is *compatible* with an approximation-set-relation if the former implies the latter (for example, if $I(A_1) > I(A_2) \Rightarrow A_1 \succ A_1$, then $I(A)$ is $\succ$-compatible). On the other hand, a quality-indicator-relation is *complete* in respect to an approximation-set-relation if the former follows from the latter (in other words, if $A_1 \succ A_1 \Rightarrow I(A_1) > I(A_2)$, then $I(A)$ is $\succ$-complete).

For the performed experiments, in particular for the fitness evaluation of automatically generated MOEAs and two objectives, we are ideally looking for a $\rhd$-complete quality indicator – if A_1 is *better* than A_2, the value returned by the chosen metric for A_1 must be greater (or smaller in the case of minimization) than the corresponding value for A_2. With respect to compatibility, Zitzler et al. (2002) have shown that it is theoretically impossible to create a unary quality indicator that is both $\rhd$-complete and $\rhd$-compatible. Fortunately it turns out that we are not interested in $\rhd$-compatibility: such a quality indicator would be too coarse for the intended use, since we need to be able to meaningfully compare approximation sets that are incomparable according to Zitzler et al.'s classification.

3.5.2 Grades of comparability

I therefore propose the following informal classification for incomparable approximation sets:

- Distribution-comparable: let A_1 and A_2 be two approximation sets such that $A_1 \neq A_2 \wedge A_1 \cup A2 \in \Omega$, in other words the union of A_1 and A_2 is itself a different, larger approximation set (and all its elements are non-dominated to each other). In this case that approximation set is preferable which has the better overall distribution. Note that in this class it is still possible to have comparison-draws for different approximation sets, for example two sets that both include a dense cluster of solutions in different locations along the Pareto optimal front. However the author sees no reason why such a comparison should not yield identical quality indicator values, since without preference-input from the decision maker none can be said to be preferable to the other.
- Convergence-comparable: let A_1 and A_2 be two approximation sets and A_1^1, A_1^2, A_2^1, A_2^2 four subsets of A_1 and A_2, with $A_1 = A_1^1 \cup A_1^2$, $A_2 = A_2^1 \cup A_2^2$ and $A_1^1 \succeq A_2^1 \wedge A_2^2 \succeq A_1^2$. Here, most known convergence-based unary quality indicators will provide a result that favours the approximation set which has the greater proportion of good solutions. However, draws are possible, and it is easy to construe situations where such a quality indicator will favour an approximation set with a few perfect and many bad solutions over one with consistently good solutions. To alleviate this last problem, the standard deviation of a convergence-based metric can be used instead. This is an arbitrary choice to emphasize good overall convergence over a few champion solutions – in the real-world case, where a decision-maker chooses one solution from the obtained approximation set, it is

important to minimize the probability of the chosen solution being an outlier far from the Pareto-optimal front; favouring approximation sets with uniform convergence properties therefore raises the confidence in any chosen solution.

3.5.3 Reverse Generational Distance

As stated above, we are looking for a $\rhd$-complete quality indicator, which – instead of also being $\rhd$-compatible – yields finer-grained information about the convergence and distribution qualities of incomparable approximation sets. The Reverse Generational Distance (RGD) – described in greater detail in the literature review – suggested by Bosman and Thierens (2003) is such an indicator. It is chosen because it includes information about the spread and distribution along the Pareto optimal front as well as convergence towards the Pareto optimal front. One problem associated with this metric is however that it requires careful definition of a uniform and sufficiently large set $S^*$of members of the Pareto optimal front. If S^* is smaller than the approximation set Q, some members of Q will be ignored in the fitness calculation. The RGD denotes the average closeness of an approximation set to the Pareto optimal front. As suggested above, the standard deviation from this metric will serve to favour individuals with good uniform convergence.

3.6 Test Problems

The inclusion of two separate Performance metrics into the objectives of our experiment poses a problem: to prevent building an MOEA specialised for one single problem, at least two test problems must be included in the GP-objectives. The combination of these with two Performance measurements, together with the above mentioned minimization of program size, results in a minimum of 5 objectives. In this scenario only the most basic test problems can be incorporated. This is a problem for two reasons: on one hand the presentation of results is difficult for more than 3 objectives. On the other hand it has been observed that too many objectives may lead to stagnation of convergence (Coello Coello, 2005). For those two reasons the decision was taken to combine the performance measurements of all test problems. This leaves us free to explore four test problems defined by Zitzler et al. (2000). All of these follow the construction principle for two-objective problems defined by Deb (1999):

$$\begin{aligned}&\text{Minimize} f_1(x) = f_1(x_1, x_2, ..., x_m)\\&\text{Minimize} f_2(x) = g(x_{m+1}, ..., x_N)h(f_1, g)\end{aligned}$$

- The simplest problem, ZDT1, is a 30-variable problem with a continuous convex Pareto optimal front:

  $$ZDT1 : \begin{cases} f_1(x) & = x_1, \\ g(x) & = 1 + \frac{9}{n-1}\sum_{i=2}^{n} x_i, \\ h(f_1, g) & = 1 - \sqrt{f_1/g}, \\ n & = 30. \end{cases}$$

  The Pareto optimal front is found for $0 \leq x_1 \leq 1$ and $x_i = 0$ for $i = (2, 3, ..., 30)$. The set of Pareto optimal solutions S^* needed for the RGD-Metric can thus be formed from uniform subdivisions of the value-range of x_1.

- ZDT2 complements ZDT1 in that it is the non-convex counterpart:

  $$ZDT2 : \begin{cases} f_1(x) & = x_1, \\ g(x) & = 1 + \frac{9}{n-1}\sum_{i=2}^{n} x_i, \\ h(f_1, g) & = 1 - (f_1/g)^2, \\ n & = 30. \end{cases}$$

  The calculations of the Pareto optimal front and of S^* are as in ZDT1.

- ZDT3 exercises the difficulty of a discontinuous Pareto optimal front:

$$ZDT3: \begin{cases} f_1(x) & = x_1, \\ g(x) & = 1 + \frac{9}{n-1}\sum_{i=2}^{n} x_i, \\ h(f_1, g) & = 1 - \sqrt{f_1/g} - (f_1/g)sin(10\pi f_1), \\ n & = 30. \end{cases}$$

Here, S^* can be formed with relative ease by travelling along uniform subdivisions of the value-range of x_1 in increasing order, and selecting each point that results in a new optimum for f_2. Like in the other test problems, the remaining optimal parameters are $x_i = 0$ for $i = (2, 3, ..., 30)$.

- ZDT4 has many local Pareto optimal fronts, making convergence difficult

$$ZDT4: \begin{cases} f_1(x) & = x_1, \\ g(x) & = 1 + 10(n-1) + \sum_{i=2}^{n}(x_i^2 - 10cos(4\pi x_i)), \\ h(f_1, g) & = 1 - \sqrt{f_1/g}, \\ n & = 10. \end{cases}$$

The calculations of the Pareto optimal front and of P^* are as in ZDT1.

3.7 Wilcoxon rank-sum test

The result of the data collection phase is a number of populations (and in particular their elite archive) of tree-like genomes, assembled from predefined building blocks. For each building block we can examine how it contributes to either objective by taking two samples: one containing the elite archive, the other comprised of all individuals of the elite archive that contain the specified building block. The distributions of the two samples can now be compared with respect to each objective. Since the elite archive is the result of an evolutionary process, we must assume that the distribution of either sample is non-normal; therefore we do not have sufficient information about the parameters of the samples' probability distributions to employ a parametric test like Student's t-test. The Wilcoxon rank-sum test is used instead – a non-parametric test that can compare the medians of two independent samples (Rinne, 2003; R Development Core Team, 2006).

To determine whether an operator contributes to good convergence properties, all individuals of an elite set that contain the operator in question are selected into the first statistical sample X of size n_x. The second sample Y comprises the entire elite set with n_y individuals. The null-hypothesis H_0 assumes that the distributions of X and Y are identical, while the alternative hypothesis H_1 states that X is stochastically smaller than Y. The individuals in the two samples are now ranked according to their performance measurements, and the sum W_n of the ranks of the individuals in X is calculated (ties are resolved by averaging the respective ranks). H_0 is rejected with confidence α if $W_n \leq w_{n_x;n_y;\alpha}$. The critical value $w_{n_x;n_y;\alpha}$ can be taken from statistical tables. This use of the Wilcoxon rank-sum test depends on the assumption that X and Y can be regarded as independent samples.

3.8 Summary

The presented research concentrates on controlled experiments in the overlapping domains of GP and MOEAs. The foundation for the experiments is provided by the Open BEAGLE framework, with an NSGA-II algorithm as the main loop. The first objective in this MOGP is the minimization of tree depth. By using the Reverse Generational Distance metric in conjunction with its Standard Deviation as the second and third objectives, an arbitrary choice is made to emphasise uniform convergence over a few champion solutions. This choice is justified by two newly introduced classes of incomparable approximation sets: distribution-comparable and convergence-comparable approximation sets. It also leads to the necessity of a priori knowledge of many points in the Pareto Optimal set. In order to avoid too many objectives, the fitness measurements are averaged between all four performed test problems. The resulting populations are then analysed using the Wilcoxon rank-sum test.

Chapter 4 Data Collection

4.1 Introduction

There are a wealth of diverse components described in literature, of which many combinations can be made into a working Multi-Objective Evolutionary Algorithm (MOEA). Putting the framework developed in the previous chapter into practice, the first experiment defines the function and terminal sets for high-level operators and explores the question whether there is an ideal combination, and whether we already know it. The second experiment searches for a new selection operator using lower-level functions. Appendix B, submitted on a separate CD, contains the developed source code and collected data.

4.2 Experiment 1: High-level Operators

A Multi-Objective GP-System built on the base of NSGA-II forms the core of this experiment. The objectives comprise the minimization of tree depth (in order to preclude code-bloat), and a combination of the Reverse Generational Distance (Bosman and Thierens, 2003) and its standard deviation taken on single runs of four test problems ZDT1-4 (Zitzler et al., 2000).

4.2.1 Function set

The utilized function set consists of evolutionary operators from the literature. In order to ensure a representative sample of subjects, the predefined functions span the range from Schaffer's Vector Evaluated Genetic Algorithm (VEGA) to SPEA2. Each MOEA described in the Literature Review was disassembled into building blocks, which can be grouped into functional families. The collection of all these building blocks make up the function set (Table 1). A tree genome then corresponds to the operations executed in the course of one generation, with fitness evaluation performed at the end of each generation.

Functional Family	***Operator***	***Origin***
Selection Strategies	Vector Based Fitness Selection	Schaffer, 1984
	Tournament Selection	Deb, 2001
	Pareto Ranking Selection	Fonseca and Fleming, 1993
	Non-Dominated Sorting Selection	Srinivas and Deb, 1994
	Pareto Tournament Selection	Horn and Nafpliotis, 1993
	Strength Pareto Selection	Zitzler et al., 2001
Fitness Modifiers	Sharing in Parameter Space	Srinivas and Deb, 1994
	Sharing in solution space	Horn and Nafpliotis, 1993
	Dynamic Sharing in solution space	Horn et al., 1994
	Crowding	Deb et al., 2001
	Density	
Crossover Operators	Naïve Crossover	Deb, 2001
	Blend Crossover	
	Simulated Binary Crossover	
Mutation Operators	Random Mutation	
	Normally Distributed Mutation	
Elite Selection Strategies	Unbounded Elite Archive	De Jong, 1975
	Truncated Elite Archive	Zitzler et al., 2001
	ϵ-Domination Elite Archive	Laumanns et al., 2001

Table 1: Function Set

4.2.2 Terminal set

One of the often-cited drawbacks of MOEAs is the fact that their performance often depends on configuration variables such as crossover probability. For the purposes of this study, such configuration variables are defined as terminals in the GP-Algorithm, in the form of randomized probability values and upper limits to elite archive size. The only other terminal is that of the population: each individual starts with a copy of the same initial population, which is randomly generated for each generation to avoid creating a bias towards one specific initial population.

4.2.3 Configuration and preliminary analysis

Over the course of 60 generations of the above Genetic Programming system, a population of 100 individuals was evolved. Each individual is itself a Genetic Algorithm, which evolves 60 individuals (each consisting of 30 real-value parameters) over the course of 60 generations. The resulting final population includes an elite archive of 67 non-dominated individuals, visualizations of which hint towards the existence of a trade-off surface (Figures 3 and 4).

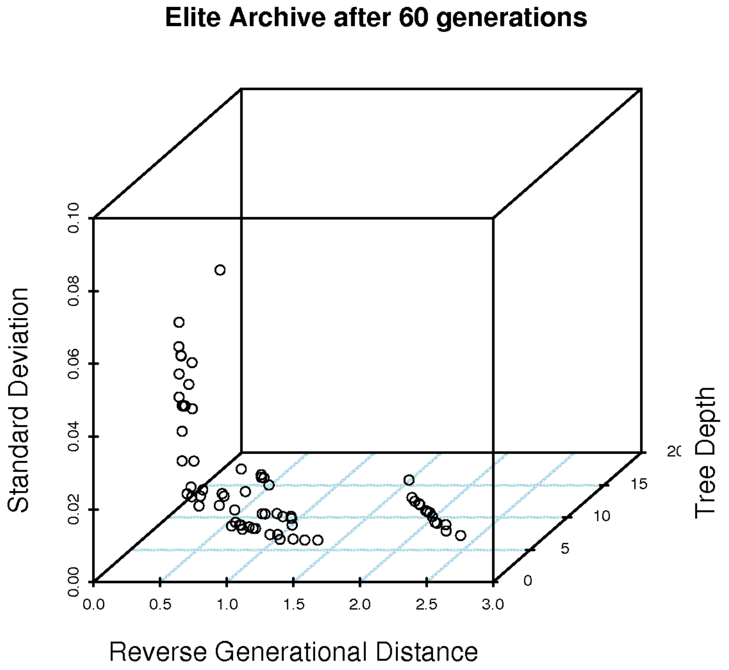

Figure 3: Elite archive of 67 individuals (60 generations per individual, 3d-scatterplot)

Preliminary analysis reveals a surprising result: none of the three elite selection strategies are present in the final population, having disappeared from the population after few generations (Table 2). Due to the importance of elite selection to formal convergence proofs (Rudolph, 1996) such a result is not expected; it also stands in contradiction to empirical investigations into the usefulness of Elite Selection (Parks and Miller, 1998; Zitzler and Thiele, 1998; Deb et al., 2000). Yet this behaviour was even intensified if each individual was run over the course of 300 generations; Unbounded, ϵ-Domination and Truncated Elite Archive were last observed in generations 2, 4 and 6 respectively in that case. Running each individual for 30 or only 15 generations (Figures 5 and 6) on the other hand consistently lead to the expected good performance throughout all generations of individuals which include an elite archive.

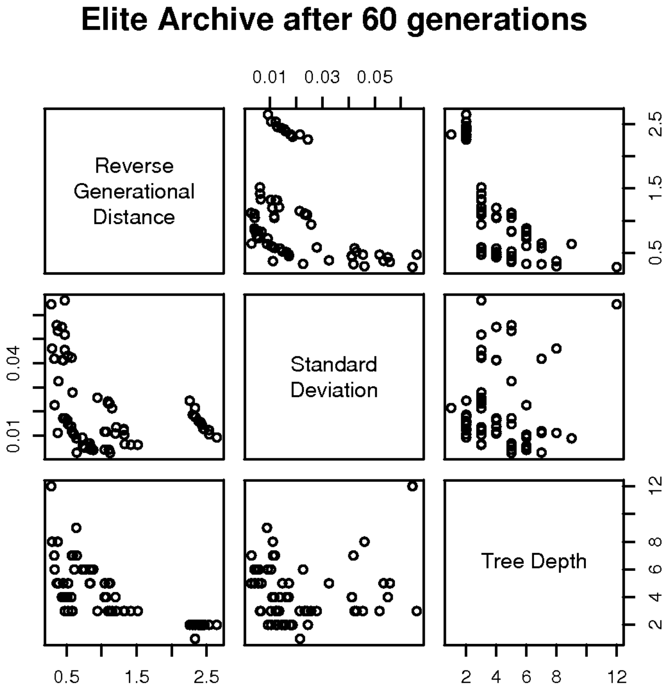

Figure 4: Elite archive of 67 individuals (60 generations per individual, plot matrix)

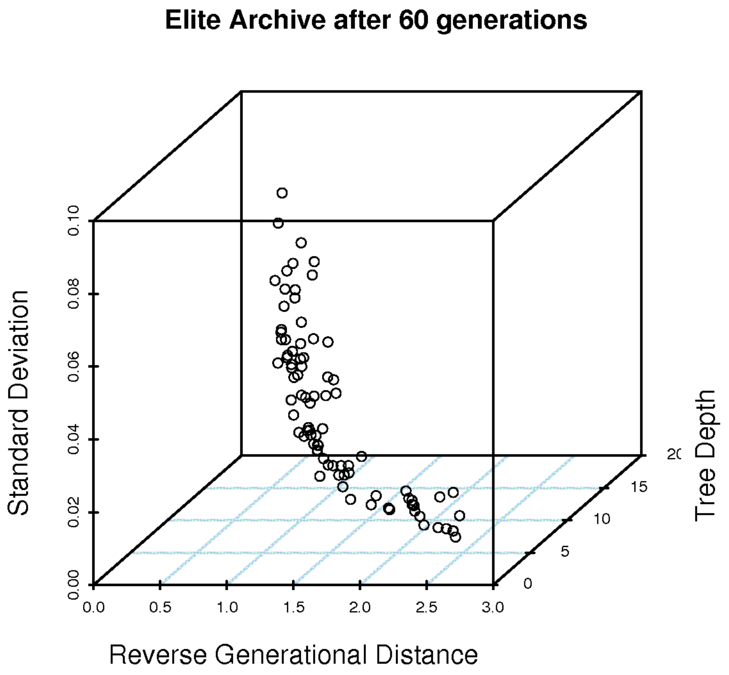

Figure 5: Elite archive of 87 individuals (15 generations per individual, 3d-scatterplot)

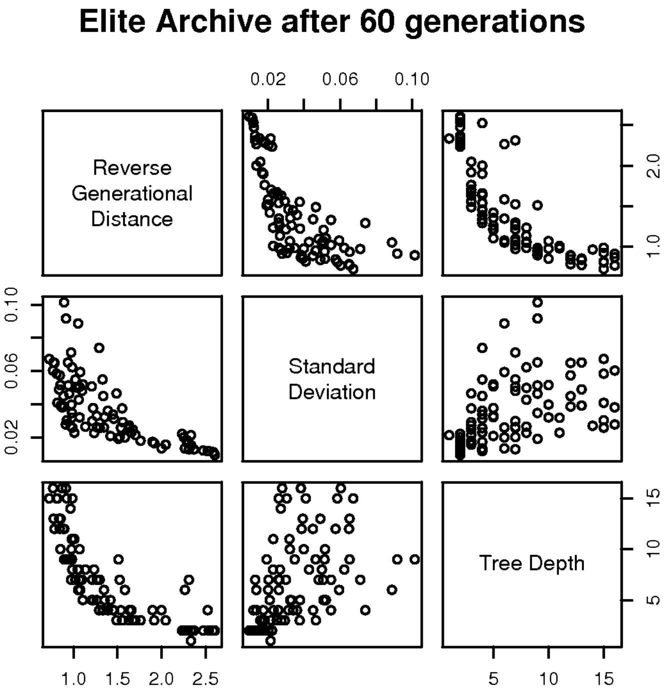

Figure 6: Elite archive of 87 individuals (15 generations per individual, plot matrix)

Operator	***Generation***
Truncated Elite Archive	5
ϵ-Domination Elite Archive	7
Unbounded Elite Archive	16

Table 2: Last occurrence of Elite Selection Strategies in individuals with 60 generations

A possible explanation for the observed pattern is, that although the inclusion of an elite archive is beneficial for an MOEA, it competes with the disadvantage of introducing an additional depth-level into the individual's genome. As the number of allowed generations increases, an individual has ample time to find good solutions – the relative importance of the elite archive decreases and is not enough to counterbalance the disadvantage in the objective of program size.

4.3 Experiment 2: Lower-level Selection

4.3.1 Function set

The selection strategies and fitness modifiers included in the function set in Table 1 are themselves built upon similar building blocks. A variation of the initial setting is therefore to replace the former with a selection of the latter in the primitive set and let the GP-System search for new combinations of these. These lower-level building blocks are used in combination with a Skeleton Selection Strategy to enable GP to explore that search space (Table 3).

4.3.2 Terminal set

Initially, no alterations were made to the terminal set. Early results showed however, that a randomized configuration variable (denoting the size-limit of the Truncated Elite Archive) in combination with the newly introduced Skeleton Selection Strategy led to a highly deceptive local optimum: an individual that includes such a combination has a small depth-level, resulting in high pressure against the intended lower-level exploration – which is not possible without additional depth-levels. After the removal of that terminal, the Genetic Programming algorithm was able to overcome this local optimum.

4.3.3 Configuration and preliminary analysis

As before, a population of 100 individuals is evolved over the course of 60 generations. Individuals are allowed to run for 15, 30 (Figures 7 and 8) and 60 generations. While populations in which individuals run for 15 generations repeatedly stagnate, both 30- and 60-generation individuals result in interesting trade-off surfaces.

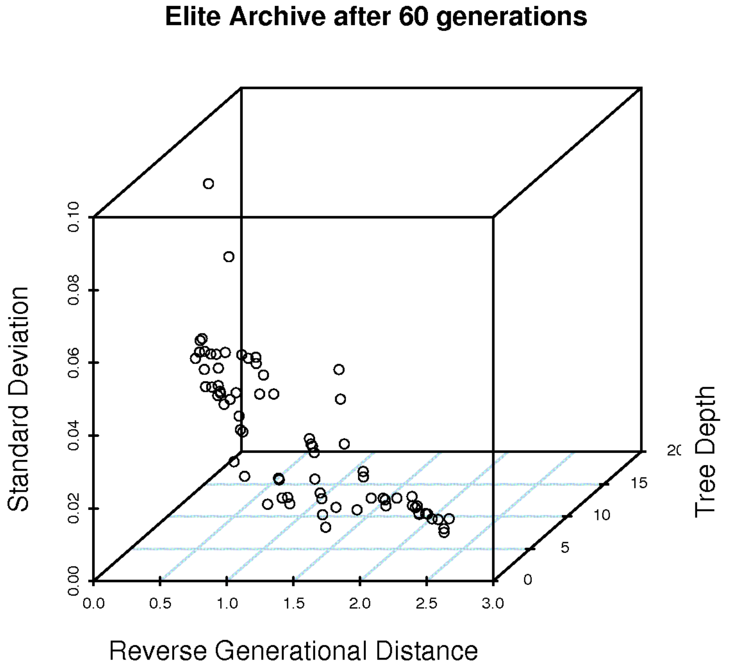

Figure 7: Elite archive of 73 individuals (30 generations per individual, 3d-scatterplot)

Lower-Level Operator	***Description***
Skeleton Selection Strategy	Creates a new population by calling its subtree once for each individual; updating the new population with an individual from the previous population at the position returned by the subtree.
Random Individual	Returns the position of a random Individual in the current population.
Select Lesser	Selects from two positions of Individuals in the current population that one, for which a subtree of metric calculations returns the lesser value.
Select Greater	Selects from two positions of Individuals in the current population that one, for which a subtree of metric calculations returns the greater value.
Least Objective Distance	Calculates the Euclidean distance in solution space between an individual and all others in the current population, and returns the least of these.
Average Objective Distance	Calculates the Euclidean distance in solution space between an individual and all others in the current population, and returns the arithmetic average of these.
Greatest Objective Distance	Calculates the Euclidean distance in solution space between an individual and all others in the current population, and returns the greatest of these.
Least Parameter Distance	Calculates the Euclidean distance in parameter space between an individual and all others in the current population, and returns the least of these.
Average Parameter Distance	Calculates the Euclidean distance in parameter space between an individual and all others in the current population, and returns the arithmetic average of these.
Greatest Parameter Distance	Calculates the Euclidean distance in parameter space between an individual and all others in the current population, and returns the greatest of these.
Dominator Count	Counts the number of individuals in the current population that dominate an individual. Equivalent to Pareto ranking.
Dominated Count	Counts the number of individuals in the current population that are dominated by an individual.
Add	Arithmetic operations. These are used to combine metrics.
Subtract	
Multiply	
Divide	
Absolute	
Sine	
Cosine	

Table 3: Lower-level building-blocks

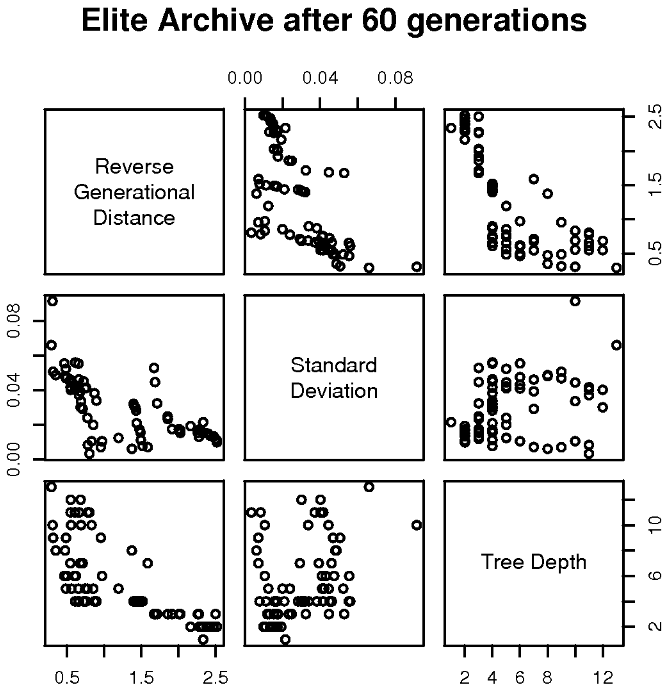

Figure 8: Elite archive of 73 individuals (30 generations per individual, plot matrix)

4.4 Summary

Controlled experiments were conducted first to explore possible recombinations of known good genetic operators. An interesting preliminary result is the fact that Elite selection strategies disappear from the population when individual solutions are run for a sufficient number of generations. Preliminary runs of a subsequent experiment exploring the combination of lower-level functions into a new selection operator displayed a similar idiosyncrasy: two unrelated primitives (the newly introduced Skeleton Selection Strategy and a randomized configuration variable) formed a highly deceptive local optimum. The removal of the latter helped circumvent that problem.

Chapter 5 Results

5.1 Introduction

The results of the two previous experiments need to be treated differently. The findings of the first experiment are grouped by functional families. In each family, a one-sided Wilcoxon rank-sum test is used to compare the distribution of solutions with each operator. For each sample of individuals, the null-hypothesis (H_0) states that the distribution of the samples is the same. The alternative hypothesis H_1 asserts that the distribution of one sample is statistically smaller than the other.

In the second experiment, promising solutions are of interest. Some sub-trees appear in multiple good solutions. These are presented in detail and potential reasons for their success are given. Finally, testing the validity of the results, one of the resulting champion solutions is run against NSGA-II.

5.2 Performance of high-level genetic operators

A first glance at the development of the Reverse Generational Distance over the course of 60 generations shows that there is indeed convergence towards a good MOEA. Both the best (Figure 9) and the average values (Figure 10) improve continuously. As is to be expected, performance of the best individual of each experiment appears to coincide with the number of generations it is allowed to run – champion solutions that ran for 60 generations perform better than champions that ran for only 15 generations. Of particular interest is an exception to this rule: one champion running for 30 generations outperforms all but the best 60-generation individual. A closer look (Figure 12) reveals the nature of this individual's advantage: repetition. By including no less than 5 selection- and 4 elite archiving operators, this individual has learned not to find an ideal combination of operators, but to run good combinations multiple times; a strategy tantamount to running for more generations. This characteristic is typical for all individuals that yield a good Reverse Generational Distance.

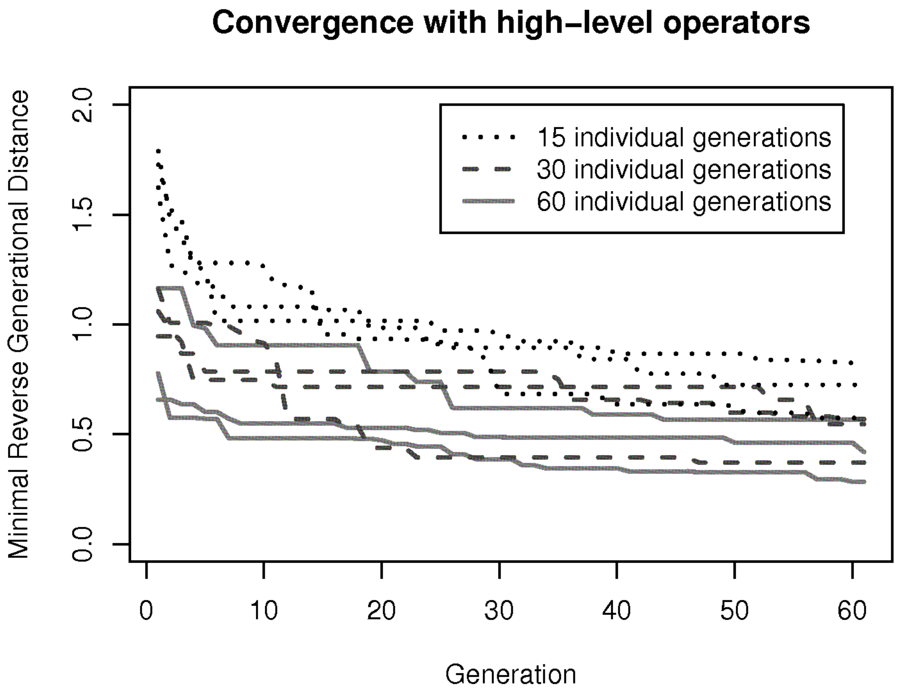

Figure 9: Convergence with high-level operators: best individuals

The same behaviour is also observed with respect to standard deviation from the Reverse Generational Distance (Figures 11 and): the most uniform approximation set was found by an individual containing 8 selection- and 2 elite archive operators.

Another interesting observation is the fact that the average performance with respect to uniformity seems to deteriorate at least when individuals are run for few generations. This may be due to a biased search space, or to the amplification of stochastic noise as individual trees grow in depth.

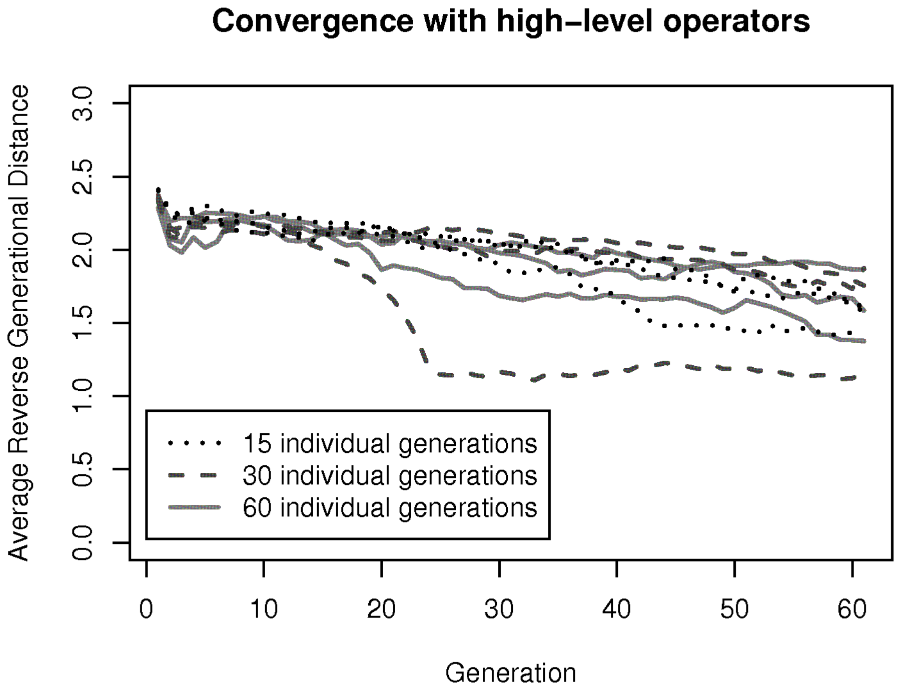

Figure 10: Convergence with high-level operators: average performance

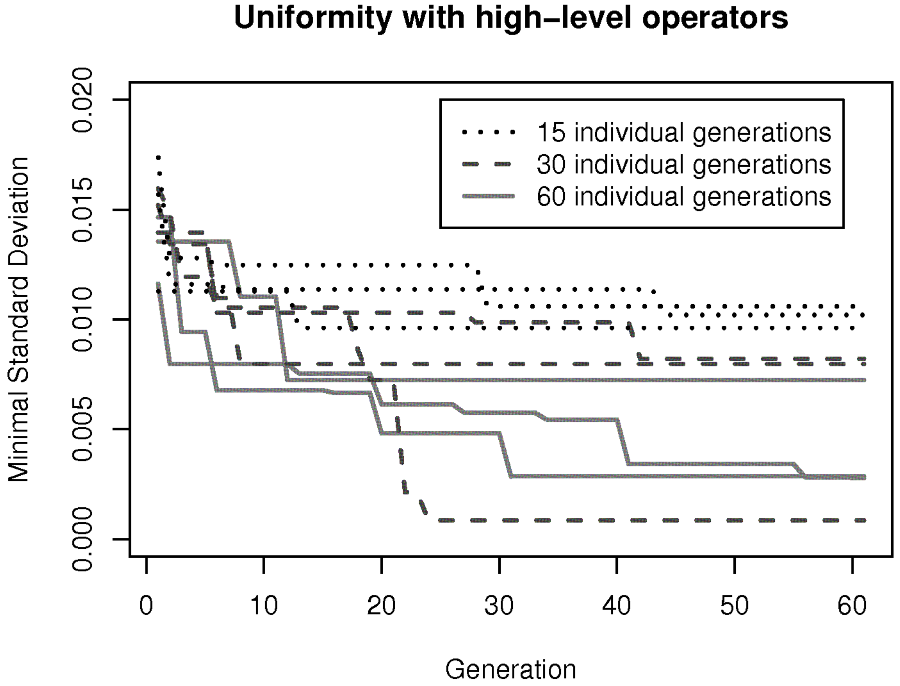

Figure 11: Uniformity with high-level operators: best individuals

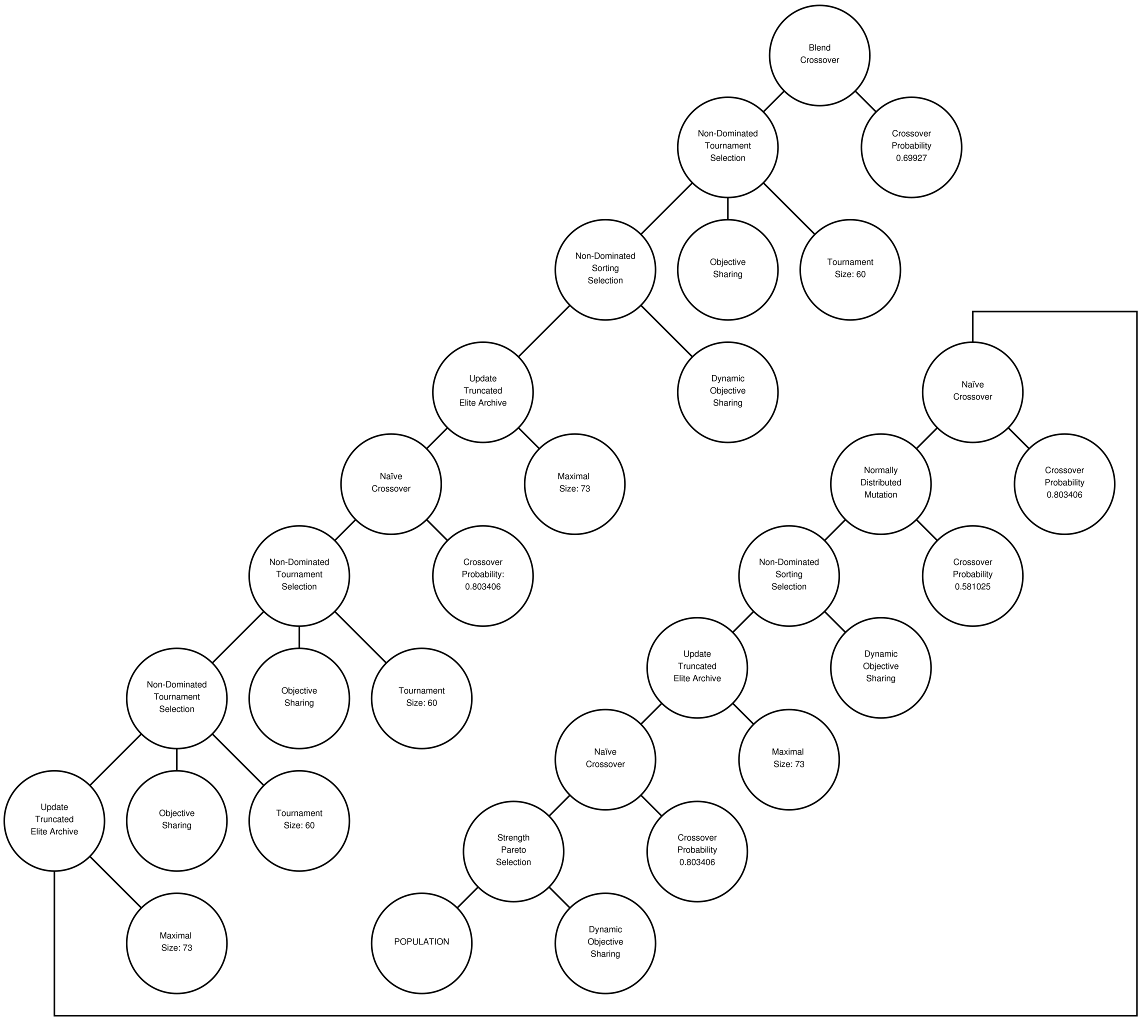
Blend Crossover
Non-Dominated Tournament Selection
Crossover Probability 0.69927
Non-Dominated Sorting Selection
Objective Sharing
Tournament Size: 60
Update Truncated Elite Archive
Dynamic Objective Sharing
Naïve Crossover
Naïve Crossover
Maximal Size: 73
Normally Distributed Mutation
Crossover Probability 0.803406
Non-Dominated Tournament Selection
Crossover Probability: 0.803406
Non-Dominated Sorting Selection
Crossover Probability 0.581025
Non-Dominated Tournament Selection
Objective Sharing
Tournament Size: 60
Update Truncated Elite Archive
Dynamic Objective Sharing
Naïve Crossover
Maximal Size: 73
Update Truncated Elite Archive
Objective Sharing
Tournament Size: 60
Strength Pareto Selection
Crossover Probability 0.803406
Maximal Size: 73
POPULATION
Dynamic Objective Sharing

Figure 12: High-level operators – Champion solution (30 generations per individual)

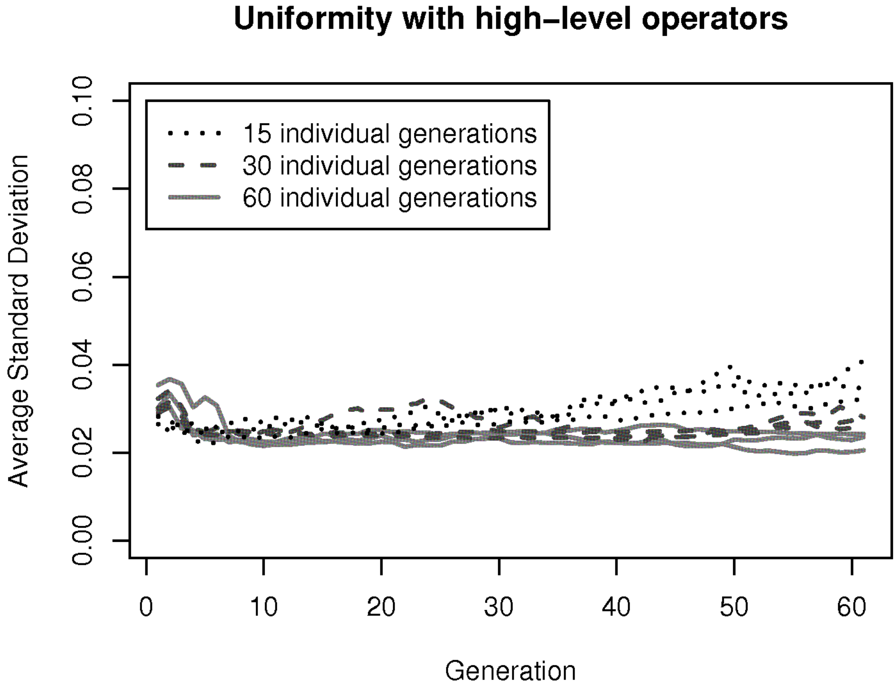

Figure 13: Uniformity with high-level operators: average performance

5.2.1 Selection strategies

Over the course of nine evolutions, each of the six predefined selection strategies was present in at least one final population. In the case of the Vector Evaluated Selection strategy, it was exactly one individual (running for 15 generations) that survived – not enough to perform a Wilcoxon rank-sum test. The simple Tournament Selection operator was never found to contribute towards a good Reverse Generational Distance; in fact, reversing H_1 to state that the RGD of individuals that contain this operator is stochastically larger than that of all individuals allows us to reject H_0 with $p = 0.0128$, or 95% confidence, in the single case where this operator survived for 60 generations.

The remaining four selection strategies were all found to contribute towards a good Reverse Generational Distance in most evolutions. This is not surprising, since the population usually also contains individuals that have no selection operator whatsoever – naturally such an individual will not converge any more than a repeated creation of random parameters. However, there are exceptions. Table 4 shows the probability for H_0 in the one-sided Wilcoxon rank-sum test for each evolution where a selection strategy is present. Where H_0 can be rejected with 95% or even 99% confidence, the upper bound of the confidence interval is given.

Further than that, no reproducible and significant hierarchy could be found; the Strength Pareto selection operator is the only one present in all final populations, which leads to the assumption that individuals containing it should perform consistently better than other selection strategies. Pairwise statistical comparison does not confirm that assumption. In fact when present in the final population, each of the three other Selection Strategies seems to perform clearly better than Strength Pareto in two instances – but worse in the two remaining direct comparisons (Table 5).

Operator	***Generations***	***$p(H_0)$***	***Upper bound of Confidence-Interval***	
			95%	***99%***
Vector Based Fitness Selection	60	n.a.		
	30	n.a.		
	15	n.a.		
Tournament Selection	60	n.a.		
	30	n.a.		
	15	0.9884		
Pareto Ranking Selection (MOGA)	60	n.a.		
	30	0.00004765	-0.1501292	-0.1035766
	15	0.001519	-0.0752172	-0.03141257
		0.00907	-0.05044163	-0.00005892
Non-Dominated Sorting Selection (NSGA)	60	0.5144		
		0.008316	-0.05630598	-0.00001663
	30	0.02828	-0.01502464	
		0.0001033	-0.2311525	-0.1134760
	15	0.0001091	-0.1151989	-0.07498298
Pareto Tournament Selection (NPGA)	60	0.9494		
	30	0.03405	-0.008254402	
		0.005159	-0.07647441	-0.007964649
	15	0.9907		
Strength Pareto Selection (SPEA)	60	0.001462	-0.09015276	-0.03478430
		0.0003927	-0.1176485	-0.06775838
		0.004583	-0.06728554	-0.005463645
	30	0.923		
		0.007582	-0.07611457	-0.000006352
		0.01879	-0.01524798	
	15	0.0007644	-0.08778878	-0.04510627
		0.01804	-0.0229707	
		0.02950	-0.007866534	

Table 4: Selection strategies – Wilcoxon rank-sum tests for the RGD-Metric, tested against the entire sample

H_1	***Generations***	***$p(H_0)$***		
MOGA < NSGA	60	MOGA not present	MOGA not present	Both not present
	30	0.02975	Both not present	1.0
	15	NSGA not present	0.4872	Both not present
MOGA < NPGA	60	both not present	MOGA not present	Both not present
	30	0.02881	Both not present	0.7857
	15	0.000000143	NPGA not present	Both not present
MOGA < SPEA	60	MOGA not present	MOGA not present	MOGA not present
	30	0.00001207	Both not present	0.6216
	15	0.6784	0.08438	MOGA not present
NSGA < MOGA	60	MOGA not present	MOGA not present	Both not present
	30	0.9707	Both not present	0.1
	15	0.6784	0.5192	Both not present
NSGA < NPGA	60	NPGA not present	0.00004059	Both not present
	30	0.477	NPGA not present	0.01258
	15	NSGA not present	NPGA not present	Both not present
NSGA < SPEA	60	0.9996	0.8829	NSGA not present
	30	0.004173	NSGA not present	0.0006698
	15	NSGA not present	0.01376	NSGA not present
NPGA < MOGA	60	Both not present	MOGA not present	Both not present
	30	0.9716	Both not present	0.2857
	15	1.0	NPGA not present	Both not present
NPGA < NSGA	60	NPGA not present	1.0	Both not present
	30	0.5256	Both not present	0.9894
	15	NSGA not present	NPGA not present	Both not present
NPGA < SPEA	60	NPGA not present	1.0	NPGA not present
	30	0.006313	NPGA not present	0.07677
	15	1.0	NPGA not present	NPGA not present
SPEA < MOGA	60	MOGA not present	MOGA not present	MOGA not present
	30	1.0	MOGA not present	0.4054
	15	0.3250	0.9173	MOGA not present
SPEA < NSGA	60	0.0003787	0.1191	NSGA not present
	30	0.996	NSGA not present	0.9994
	15	NSGA not present	0.9864	NSGA not present
SPEA < NPGA	60	NPGA not present	0.000001103	NPGA not present
	30	0.994	NPGA not present	0.9264
	15	0.000000164	NPGA not present	NPGA not present

Table 5: Selection strategies – pairwise Wilcoxon rank-sum tests between operators

Operator	***Generations***	***p(H$_0$)***	***Upper bound of Confidence-Interval***	
			95%	***99%***
Vector Based Fitness Selection	60	n.a.		
	30	n.a.		
	15	n.a.		
Tournament Selection	60	n.a.		
	30	n.a.		
	15	0.01280	-0.003846905	
Pareto Ranking Selection (MOGA)	60	n.a.		
	30	0.973		
	15	0.9981		
		0.9926		
Non-Dominated Sorting Selection (NSGA)	60	0.0006776	-0.004810987	-0.002274547
		0.2722		
	30	0.02935	-0.0004309259	
		0.998		
	15	0.9969		
Pareto Tournament Selection (NPGA)	60	0.08092		
	30	0.03222	-0.0003296422	
		0.9858		
	15	0.003068	-0.003677512	-0.001207473
Strength Pareto Selection (SPEA)	60	0.8967		
		0.597		
		0.9084		
	30	0.698		
		0.8981		
		0.9367		
	15	0.9928		
		0.9765		
		0.9354		

Table 6: Selection strategies – Wilcoxon rank-sum tests for the standard deviation from the RGD-Metric, tested against the entire sample

With respect to uniformity, one result is interesting: individuals that contain the Strength Pareto selection strategy perform never more uniform than the rest of the population; the same holds for individuals that perform selection according to Pareto

Ranking (Table 6). Reversing H_1 to state that individuals containing these operators perform less uniform (i.e. display a greater Standard Deviation from the Reverse Generational Distance) leads to the rejection of H_0 with confidence between 55% and 99% (Table 7). Again, this is not a clear enough result to make further conclusions.

Operator	***Generations***	***p(H_0)***	***Lower bound of Confidence-Interval***	
			95%	***99%***
Pareto Ranking Selection (MOGA)	60	n.a.		
	30	0.02722	0.000575265	
	15	0.001929	0.005382293	0.002256502
		0.007624	0.004384796	0.0001187272
Strength Pareto Selection (SPEA)	60	0.1046		
		0.4055		
		0.09316		
	30	0.3055		
		0.1038		
		0.06438		
	15	0.007334	0.003676457	0.00001717084
		0.02368	0.0007337736	
		0.06516		

Table 7: Selection strategies – Wilcoxon rank-sum tests for the standard deviation from the RGD-Metric with reversed H_1, tested against the entire sample

5.2.2 Fitness modifiers

The inclusion of fitness modifiers depends on the presence of certain selection strategies in an individual. Due to this dependency, a comparison against the entire population is not meaningful. A pairwise comparison could yield meaningful results, since in such a test both samples would be subject to the same bias. However, like in the pairwise comparison of selection strategies, no conclusive result was found for convergence or uniformity.

5.2.3 Crossover operators

The results for crossover operators look much the same: performance measurements are inconsistent both with respect to convergence and uniformity (Tables 8 and 9). One interesting observation is to be made: in the performance of the Blend Crossover operator, the trade-off between convergence and uniformity becomes apparent.

Operator	***Generations***	***p(H_0)***	***Upper bound of Confidence-Interval***	
			95%	***99%***
Naïve Crossover	60	0.05145		
		0.2393		
		0.7003		
	30	0.0482	-0.00004843614	
		0.7105		
		0.9271		
	15	0.9081		
		0.005953	-0.04551753	-0.006990989
		0.03033	-0.007832787	
Blend Crossover	60	0.003842	-0.06461553	-0.01250502
		0.2199		
		0.00914	-0.04032902	-2.771684e-05
	30	0.2071		
		0.002329	-0.1104435	-0.04243788
		0.02425	-0.006809555	
	15	0.01535	-0.02294651	
		0.03882	-0.00002264148	
		0.004112	-0.04517392	-0.01178846
Simulated Binary Crossover	60	0.01024	-0.07069292	
		0.9972		
	30	0.003001	-0.1639836	-0.05685838
		0.9938		
		0.9977		
	15	0.9963		

Table 8: Crossover operators – Wilcoxon rank-sum tests for the RGD-Metric, tested against the entire sample

Although the minimal confidence lies only at 75%, we can tentatively say that the Blend Crossover operator has good convergence properties according to the Reverse Generational Distance metric. On the other hand it performs worse than other operators with respect to uniformity (Table 10). The other two crossover operators exhibit similar albeit less pronounced trade-off behaviour.

Operator	***Generations***	***$p(H_0)$***	***Upper bound of Confidence-Interval***	
			95%	***99%***
Naïve Crossover	60	0.08279		
		0.00271	-0.001596323	-0.0005149918
		0.001818	-0.004117106	-0.001392432
	30	0.1490		
		0.008219	-0.001797548	-0.00003974828
		0.003765	-0.00328261	-0.0006801973
	15	0.02886	-0.0007144907	
		0.8568		
		0.8157		
Blend Crossover	60	0.8923		
		0.9996		
		0.9942		
	30	0.6505		
		0.9977		
		0.9773		
	15	0.9818		
		0.9541		
		0.996		
Simulated Binary Crossover	60	0.01214	-0.001141311	
		0.09819		
	30	0.7985		
		0.06482		
		0.01041	-0.002060077	
	15	0.007161	-0.004876103	-0.0006350011

Table 9: Crossover operators – Wilcoxon rank-sum tests for the standard deviation from the RGD-Metric, tested against the entire sample

Operator	*Generations*	*$p(H_0)$*	*Lower bound of Confidence-Interval*	
			95%	*99%*
Blend Crossover	60	0.1090		
		0.0003604	0.004197881	0.00242686
		0.005981	0.003122627	0.0001638100
	30	0.3506		
		0.002432	0.006857041	0.001568558
		0.02321	0.0008158804	
	15	0.01847	0.001725731	
		0.04623	0.00007268932	
		0.004112	0.003416843	0.0007284367

Table 10: Blend Crossover – Wilcoxon rank-sum tests for the standard deviation from the RGD-Metric with reversed H_1, tested against the entire sample

5.2.4 Mutation operators and elite selection strategies

Similar trade-off behaviour was observed with mutation operators and elite selection strategies: while mutation operators – surprisingly – seem to hinder convergence, they appear to be beneficial to uniformity. And while elite selection strategies, where present, optimize convergence with 99% confidence (Table 11), they appear to increase the standard deviation from the Reverse Generational Distance.

Operator	*Generations*	*$p(H_0)$*	*Upper bound of Confidence-Interval*	
			95%	*99%*
Unbounded Elite Archive	60	n.a.		
	30	n.a.		
	15	0.0001119	-0.1129449	-0.07190025
Truncated Elite Archive	60	n.a.		
	30	0.007425	-0.05244089	-0.0000161888
	15	0.00001993	-0.1722501	-0.1073530
ϵ-Domination Elite Archive	60	n.a.		
	30	0.0001133	-0.2481601	-0.1371289
	15	n.a.		

Table 11: Elite archives – Wilcoxon rank-sum tests for the RGD-Metric, tested against the entire sample

5.3 Lower-level functions

Like with the high-level operators, the populations investigating lower-level functions converge towards good values for both Reverse Generational Distance (Figures 14 and 15) and the Standard Deviation thereof (Figures 16 and 17). An exception to this are individuals running for only 15 generations; these stagnate early and are unable to perform notably better than the initial random generation.

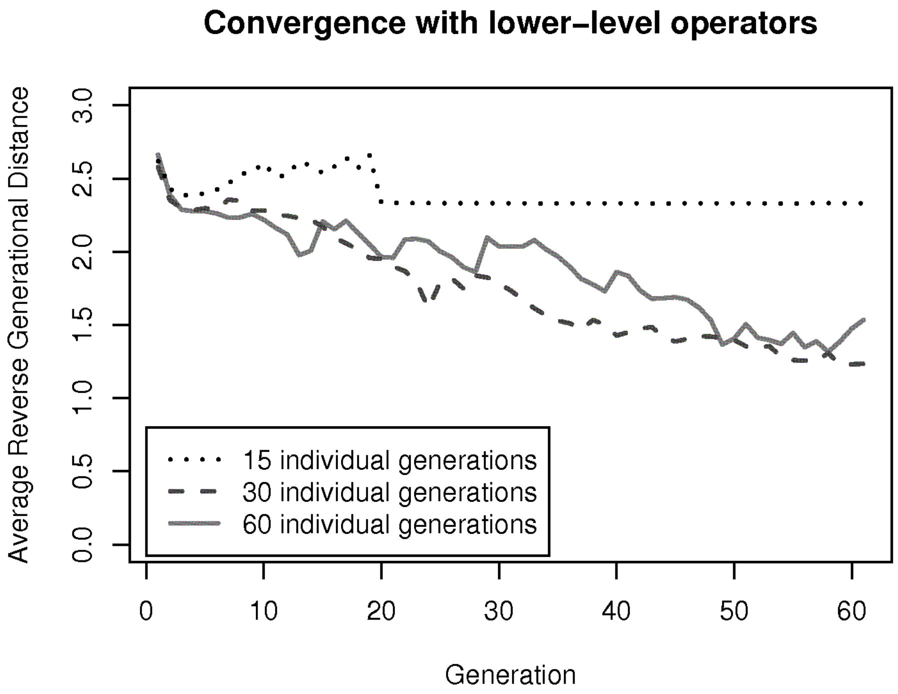

Figure 14: Convergence with lower-level operators: average performance

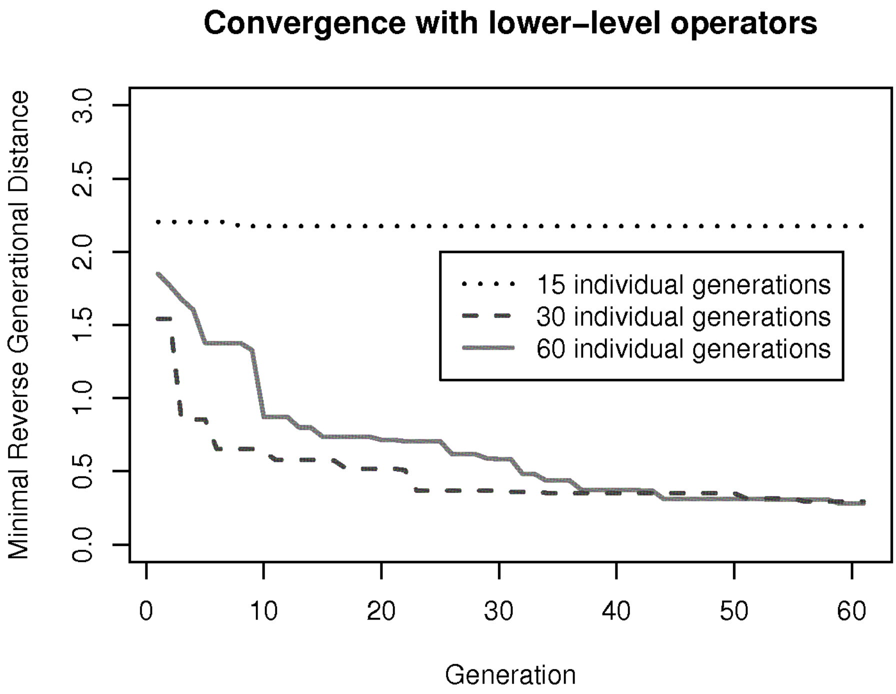

Figure 15: Convergence with lower-level operators: best individuals

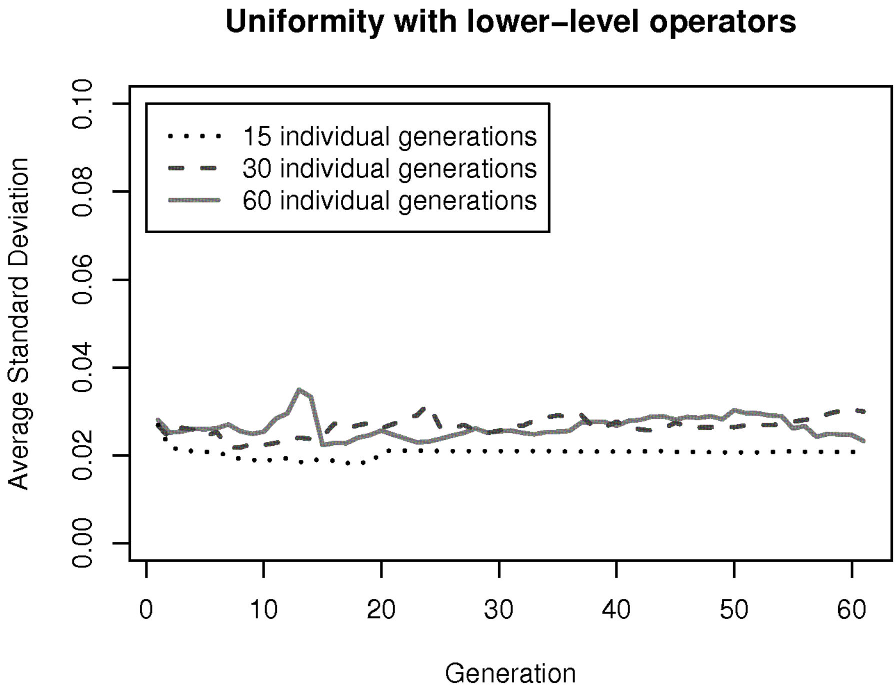

Figure 16: Uniformity with lower-level operators: average performance

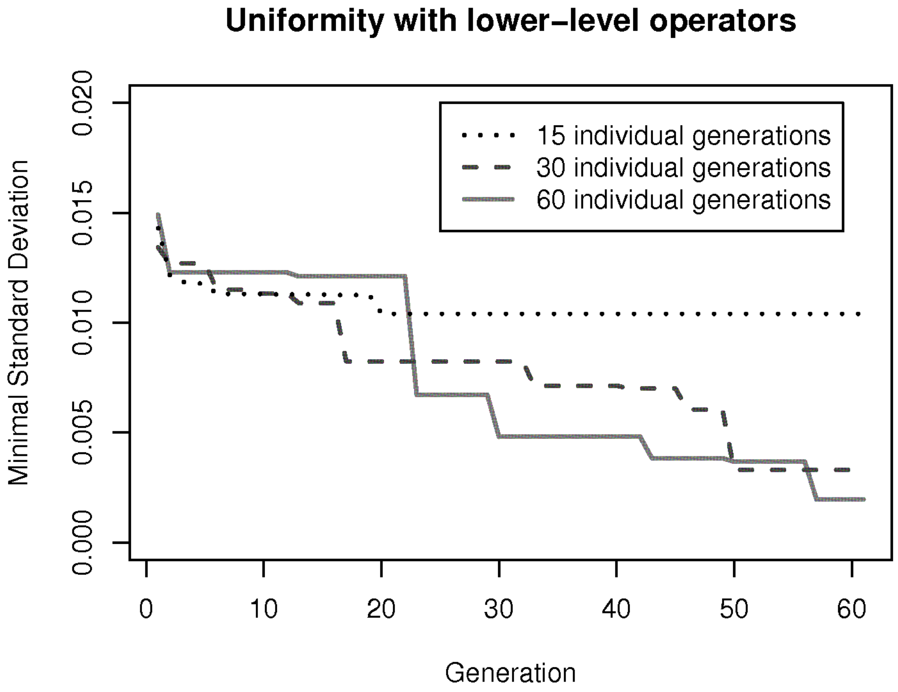

Figure 17: Uniformity with lower-level operators: best individuals

5.3.1 Interesting solutions

Similar to the earlier experiment, the champion solutions – in particular the solutions that display good convergence characteristics – owe a major part of their success to the ability to perform multiple mutation-, crossover- and selection-cycles in one generation. Nevertheless there are two sub-trees – used in champion solutions and several good individuals – that look promising:

Figure 18 shows a detail repeatedly found in an evolution where individuals ran for 30 generations. In this double tournament selection, the dominator count – the number of solutions that dominate an individual, essentially equivalent to the Pareto Ranking described in Fonseca and Fleming (1996) – plays an important role. First, two individuals are randomly drawn from the population. Of these two, that solution which is dominated by fewer other members of the population proceeds to the second tournament, where it competes against another randomly drawn individual. In this second tournament, the distance in parameter space to the furthest other individual is computed, and the dominator count is subtracted from it. That individual for which this process results in the greater number is chosen into the next generation.

In other words, this selection strategy corresponds to a tournament with 3 participants; the individual which wins the first round for its better Pareto rank is only selected, if it resides in the outer regions of the parameter space – otherwise a random individual is selected.

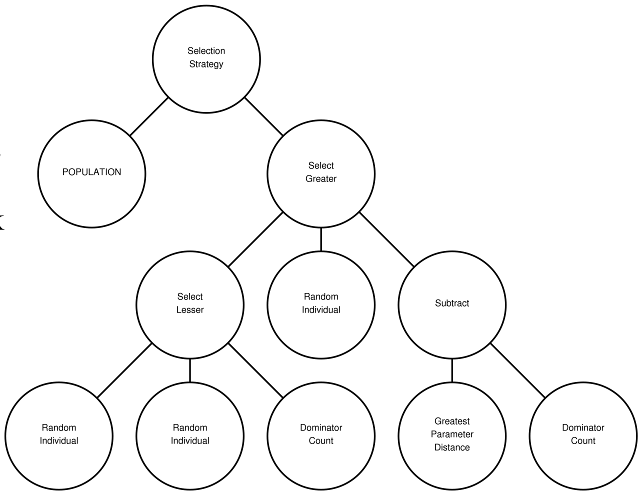

Figure 18: Double Tournament selection strategy: detail from champion solution (30 generations)

A more competent variation on this theme is found in 60-generation individuals. In the Triple Tournament Selection strategy (Figure 19), four individuals are randomly drawn from the population. Two of these are compared with respect to their dominator counts or Pareto ranks; that individual which is dominated by fewer other solutions is the winner of the first tournament. For each of the other two solutions, the average distance in parameter space to all other solutions in the population is computed. That individual which has the greater average parameter distance competes against the winner of the first tournament.

For each of these two remaining individuals, both the greatest and the least distance in parameter space to any of the other individuals in the population are computed. The product of these two values will be called "Solitude" for the remainder of this dissertation; it reflects the distribution of an approximation set (nearest neighbour) as well as its extent (multiplying by the distance to the furthest neighbour gives an advantage to individuals near the edges of each parameter-range). The raw fitness of each individual is then found by subtracting the dominator count from the Solitude-Metric. Finally, that individual which has the greater raw fitness is copied into the next generation. This procedure is roughly equivalent to selecting the individual which is dominated by fewer other solutions, and breaking a tie by choosing the individual that has the greater Solitude: in the four test problems used, where all parameters lie between 0 and 1 and good parameters are close to 0, the Solitude Metric will be greater than 1 only for few special cases that have no close neighbours. In all other cases, the individual with the smaller dominator count will be selected.

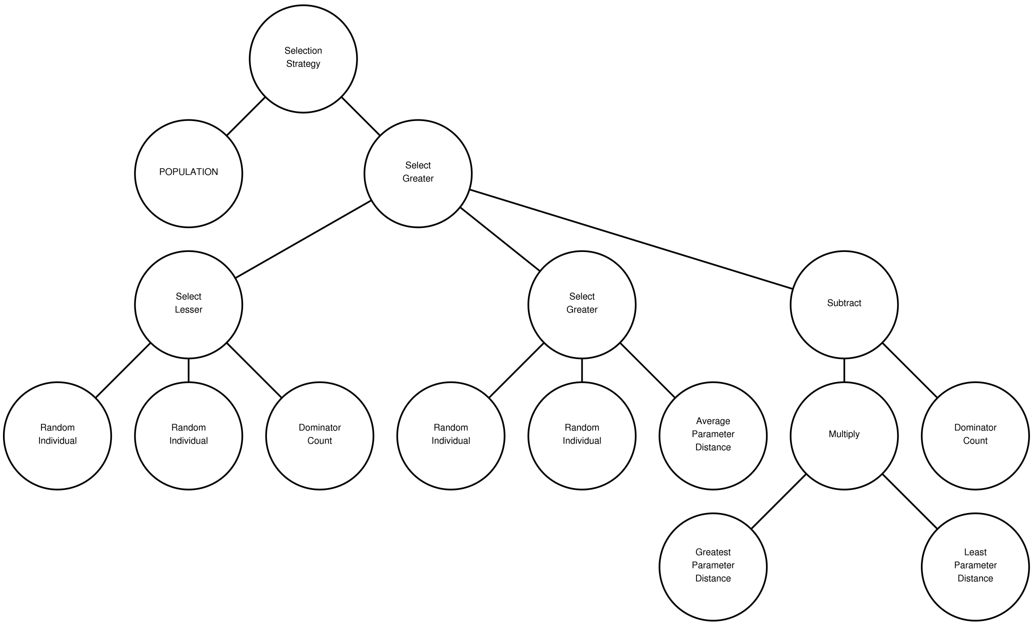

Figure 19: Triple Tournament selection strategy: detail from champion solution (60 generations per individual)

Most of the well-performing individuals achieve good convergence by applying multiple selection operators per generation. This statement does not apply to the champion solution which contains the triple tournament selection. In fact, apart from multiple crossover operators, this individual includes no repeated stages (Figure 20). It will be referred to in the remainder of this thesis as the Multiobjective Evolutionary Triple-tournament Algorithm (META).

Finally it is worth mentioning a peculiar detail: the ϵ-Domination Elite Archive was found in a number of individuals with good Reverse Generational Distance. This operator needs a parameter ϵ, which governs the distance in solution space between individuals admitted into the Elite Archive. In all of these solutions, ϵ was determined by randomly choosing an individual from the population and calculating the greatest parameter distance from this to any other individual. The fact that the distance between individuals was computed in parameter space precludes the possibility that this is a valid form of dynamic ϵ-Domination. It is more likely that in this case the GP-search has found a subtree that is optimized for the combination of employed test problems and performance metric:

All four test problems are 30-variable problems, in which $x_i = 0$ for $i = (2, 3, ..., 30)$ for the entire Pareto-optimal front. As the entire population converges and more individuals find $x_i = 0$, the greatest parameter distance of a random individual is likely to decrease. More individuals are accepted into the Elite Archive due to a smaller ϵ, which in turn reduces the Reverse Generational Distance.

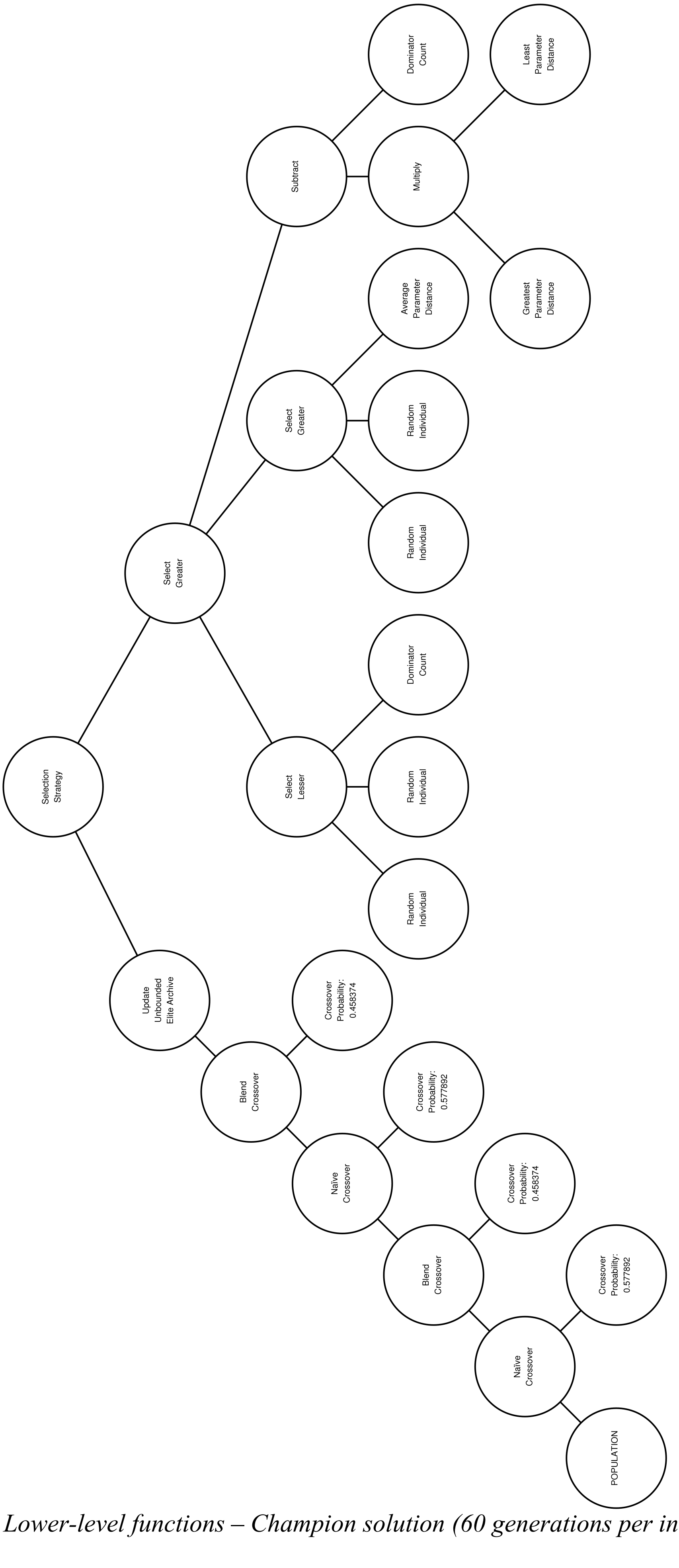

Figure 20: Lower-level functions – Champion solution (60 generations per individual)

5.4 Validation

It is apparent from the previous experiments that while it exhibits some difficulties finding a good combination of high-level operators, a Multi-Objective Genetic Programming environment can successfully find new selection operators. But how do these perform in direct comparison to a known good Multi-Objective Algorithm? To examine their quality, the obtained champion-solution and two of the details extracted from it were run against NSGA-II:

1. An implementation of the entire champion-solution, including four instances of crossover and no mutation operator (META).
2. The Triple Tournament Operator used as Selection Operator, with all other configuration-details identical to NSGA-II (Triple Tournament).
3. A variation of NSGA-II, with the Solitude metric replacing NSGA-II's crowding distance (Solitude).

These three and NSGA-II were each run over the course of 30, 60 and 100 generations, with 30 measurements taken per configuration. Appendix A contains comparative box-plots of these measurements for each configuration.

5.4.1 Results

Neither of the three tested variations is an equivalent replacement for NSGA-II. When run over the course of 100 generations, NSGA-II consistently found the best approximation sets. For 60-generation evolutions the Solitude-variant resulted in better mean values. Finally, the META-variant outperforms all other configurations after 30 generations. This is very probably the effect of forgoing the inclusion of a mutation operator: good solutions propagate quickly without the deteriorating effects of mutation. But once the best combinations of all genomes are found – and because no new genomes are introduced – the search stagnates. This also demonstrates the importance of the choices made for the MOGP System configuration: it seems that the resulting algorithms have been specialized for being run over few generations.

5.5 Summary

Experiments on the combination of high-level operators yield results consistent with literature. However, these results are only occasionally statistically significant. Nevertheless, there is evidence supporting the contribution of selection strategies, crossover operators and elite archives towards convergence. Of the tested crossover operators, Blend Crossover leans most aggressively towards convergence, and contributes least to uniformity. Surprisingly, mutation operators appear to be mainly responsible for uniform approximation sets.

The search for new selection strategies using lower-level functions yields three interesting partial trees, two of which are promising candidates. The third is evidence towards the danger of over-specialization: it is probable that its good performance has more to do with the nature of the test problems than with Multi-Objective Optimization in general.

Chapter 6 Conclusions

6.1 Project review

This project has investigated the feasibility of nesting Multi-Objective Evolutionary Algorithms (MOEAs) in Genetic Programming (GP) experiments, with the aim to search for and find new selection strategies. A number of experiments were conducted, first exploring the ability of GP to recombine high-level operators into good MOEAs, later investigating whether new operators could be found from lover-level building blocks, and finally comparing the obtained results to NSGA-II, one of the best-known algorithms in the field.

In support of these experiments, a framework for nested evolution was developed both conceptually and in an implementation based on the Open BEAGLE framework (Appendix B). While not comprehensive, it offers a broad range of high-level operators and lower-level functions for inclusion in subsequent investigations. More importantly, it provides researchers with a structural base that solves the problem of evolving iterative processes, limited for the special case of evolutionary algorithms. And finally, it is extensible in so far as building-blocks, test problems and performance metrics can be replaced with equivalent operators. Limitations include the fact that the generational structure is constant – as in most GP-Projects, the search space cannot include loop operators. Overcoming the problems of automatically nested loops and the connected halting problem are still matters of investigation with researchers examining the foundations of Genetic Programming. Consequently, the presented framework cannot model approaches that diverge from classical evolutionary algorithms.

Also prerequisite to the experiments, it was shown that the theoretical limits that govern unary performance metrics for multi-objective approximation sets can be worked around. The definition of finer-grained comparability – for those cases where two approximation sets are incomparable according to the dominance relations described by Hansen and Jaszkiewicz (1998) and Zitzler et al. (2002) – and the arbitrary choice to favour uniform approximation sets over few champion solutions, together enable two approximation sets to be compared with a simple process.

The distribution of solutions in the resulting data sets support the initial assumption that the search for MOEAs is itself a multi-objective problem: all experiments yielded elite sets with distinct trade-off surfaces that can be observed to converge towards better solutions as the GP-evolution progresses. However, the recombination of high-level operators did not yield the expected clear recommendations on which building blocks to use in which case. In-depth analysis of the obtained data showed several limitations of the chosen approach: many of the fittest solutions had solved the posed problem by repeating elements from each functional family (elite-set selection, mutation and crossover) several times per generation, thus gaining the advantage of additional generations. This resulted in many ties in the ranking process inherent to the Wilcoxon rank-sum test, which may explain the fact that few significant differences in the performance of the employed building-blocks were found. Additionally, a distinct propensity to specialize was found: the shape of both the search-space and the Pareto-optimal front defined by the employed test problems influence the generated solutions. In the four test problems employed in this study, most parameters needed to approach zero in order for the population to converge towards the Pareto-optimal front. In certain GP-individuals a specialization for this fact was found. And while it is of course desirable to find such a specialization in the MOEA-individuals depicting the approximation set, for the GP-individuals that describe how the approximation set should be found, a more general proficiency is favoured.

It also needs to be noted that the criteria determining the end of an evolution influence the results: in this study, the number of generations was fixed to a low level, due to the exceedingly high computational complexity of nested evolutionary algorithms. This has resulted in a related specialization and in what appears to be a separation of Mutation and Crossover operators – demonstrated in the validation experiments, where the absence of a Mutation operator from the Multi-objective Evolutionary Triple-Tournament Algorithm (META) leads to significantly better results after 30, but also significantly worse results after 100 generations.

In conclusion we can state that neither of the two hypotheses posed in conjunction with the research question are unquestionably supported or rejected. While no combination of high-level building blocks was found which has convergence properties similar to those of known "good" MOEAs, the insights gained into the process of nested evolution may enable successful experimental configurations in future research. Similarly, the search for new selection strategies was more successful than expected: in what is the most exciting result, two new selection strategies consisting of lower-level functions were found. One of these is the Triple Tournament Selection operator which includes the Solitude distance operator, a new and somewhat surprising method of ensuring diversity.

6.2 Future research

There are several variants of the developed framework that are worth investigating: since the objective of uniformity is secondary to that of convergence, and since the standard deviation from the Reverse Generational Distance (RGD) metric was observed to be several orders of magnitude smaller than the metric itself, it may be worth combining the two by simple addition. The expected behaviour of such a combined metric would be to select individuals with good convergence properties, while additionally favouring individuals with slightly worse but significantly more uniform convergence.

The optimization of program size remains an interesting quandary. In the context of evolving MOEAs from high-level building blocks, it may be a valid strategy to limit the program size to the number of identified functional families. In addition to removing one of the objectives from the multi-objective problem, that approach would also significantly reduce the search space by limiting the number of possible operator-combinations.

Many more building-blocks would be possible. Of particular interest are lower-level functions that provide a form of introspection into the state of the evolution: a generation counter, the average fitness-improvement from the previous generation, or other internal information, could be used to influence the relative probability of mutation and crossover. Can an evolutionary process find such a relation?

Results from this study suggest that – at least for the test problems employed – crossover is most efficient for short evolutions, whereas mutation is more important in evolutions over many generations. It seems likely that there are at least two phases in an evolution, in which a population reacts differently to the operations it is subjected to. The identification of such phases (for lack of a better example: early, middle and late), and the role of each genetic operator in these, seem a topic worth exploring, both for the single- and the multi-objective case. Also of interest is the precise role that the number of generations per individual plays in the nested evolutionary system.

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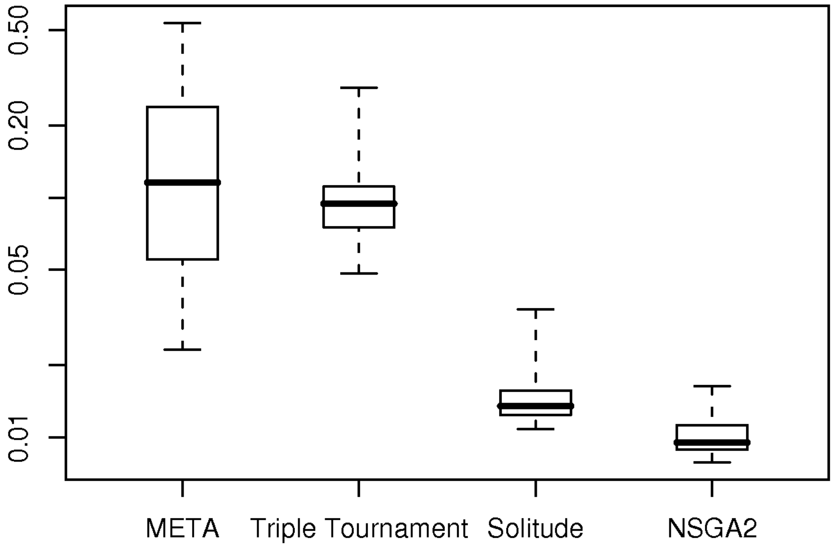
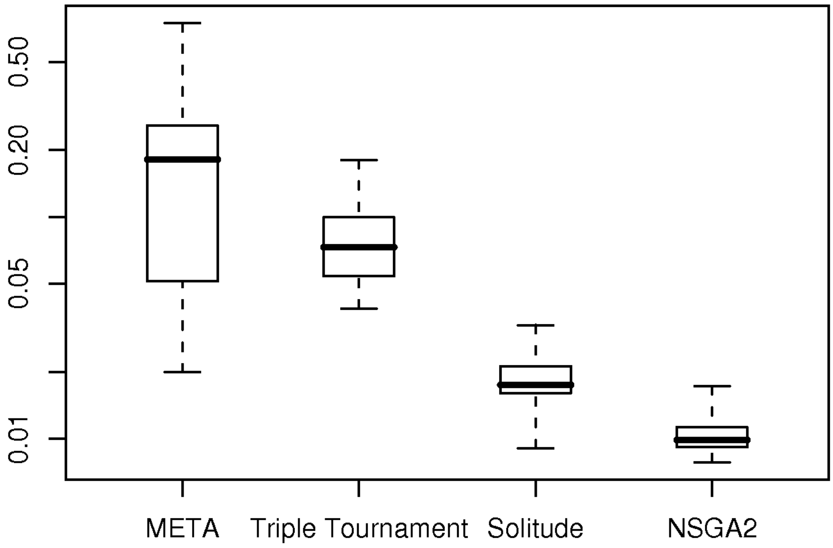
Index

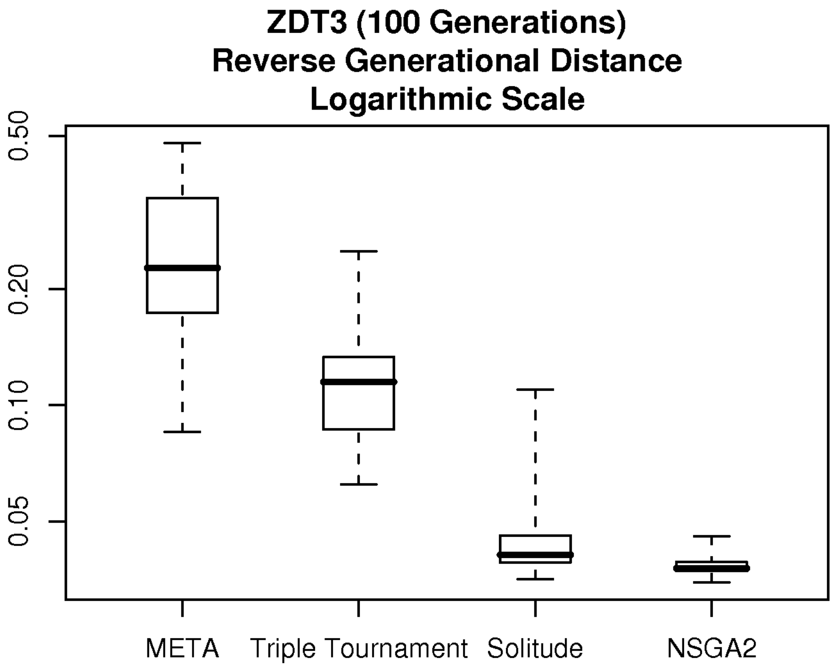
Appendix A

ZDT1 (100 Generations)
Reverse Generational Distance
Logarithmic Scale



ZDT2 (100 Generations)
Reverse Generational Distance
Logarithmic Scale




ZDT3 (100 Generations)
Reverse Generational Distance
Logarithmic Scale
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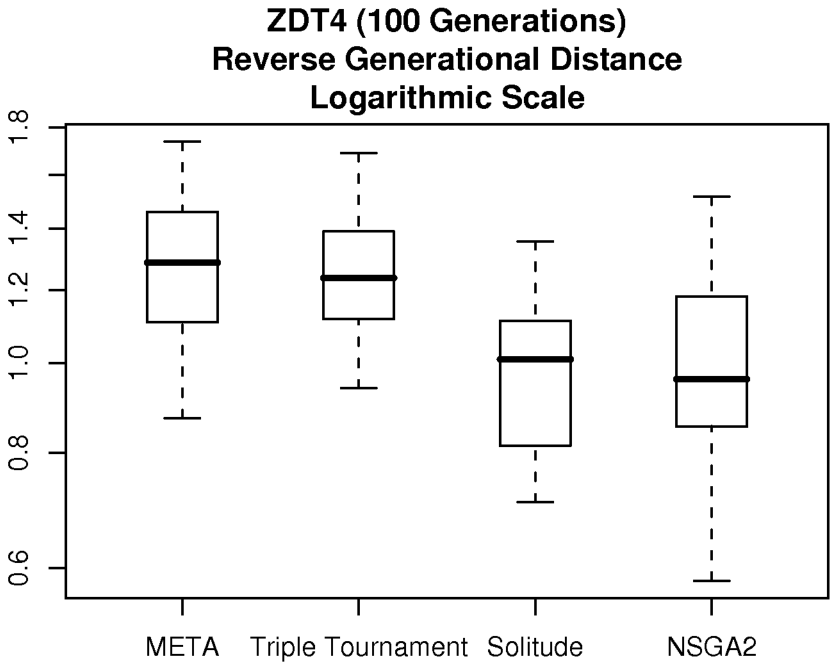
0.10
0.05
META
Triple Tournament
Solitude
NSGA2


ZDT4 (100 Generations)
Reverse Generational Distance
Logarithmic Scale
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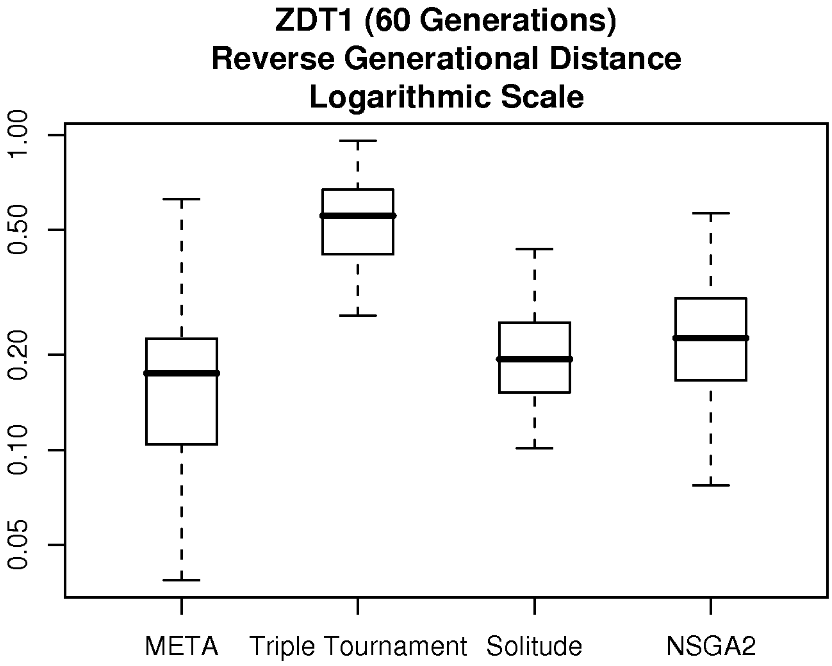
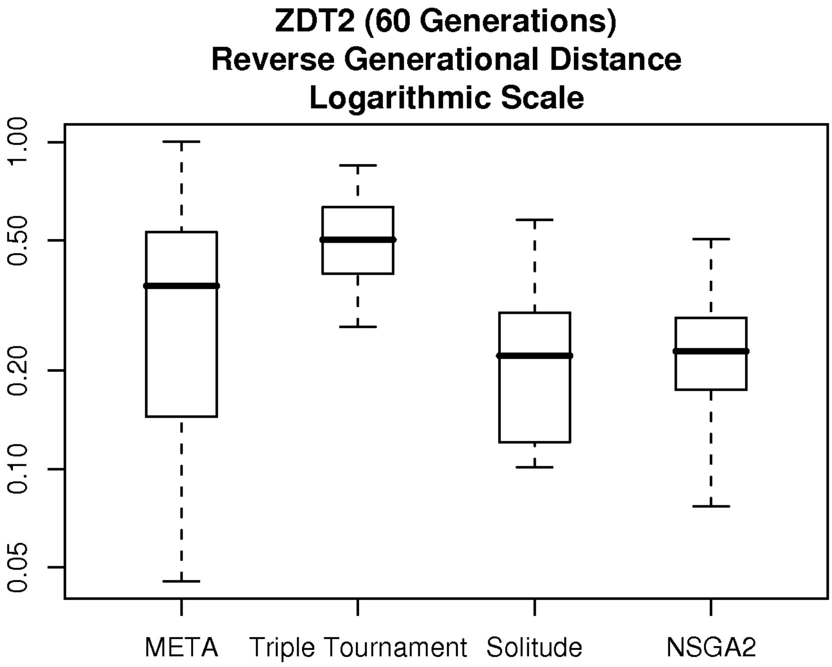
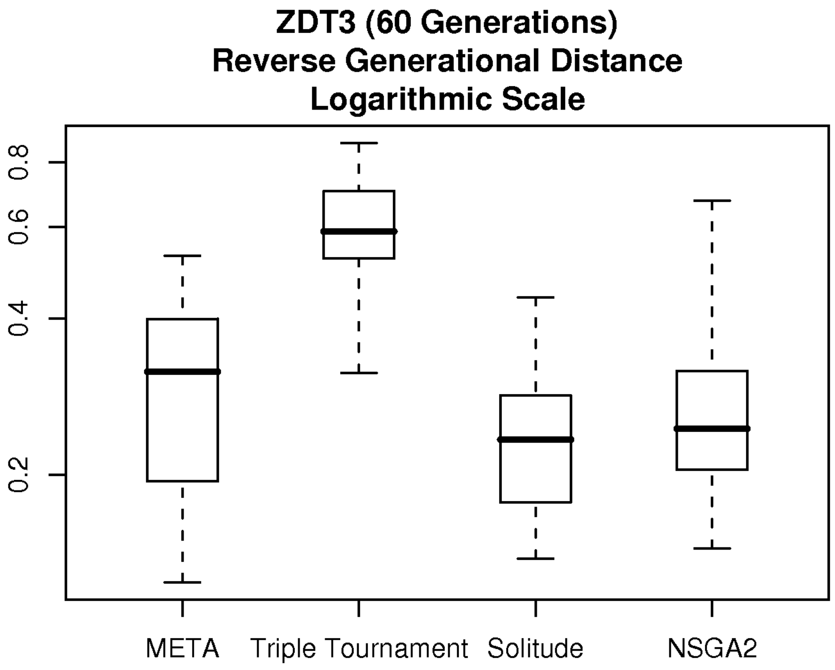
1.4
1.2
1.0
0.8
0.6
META
Triple Tournament
Solitude
NSGA2

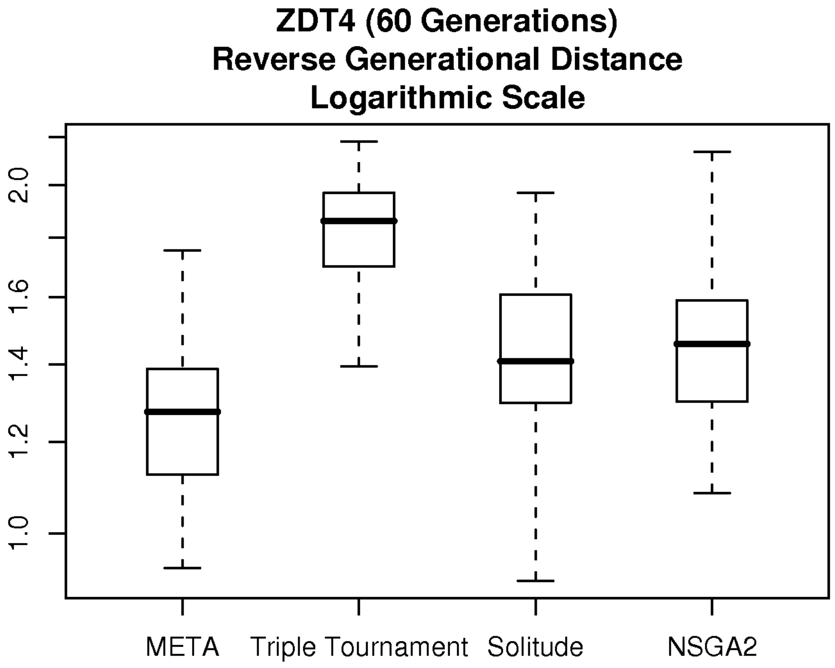


ZDT1 (60 Generations)
Reverse Generational Distance
Logarithmic Scale



ZDT2 (60 Generations)
Reverse Generational Distance
Logarithmic Scale


ZDT3 (60 Generations)
Reverse Generational Distance
Logarithmic Scale
0.2
0.4
0.6
0.8
META
Triple Tournament
Solitude
NSGA2


ZDT4 (60 Generations)
Reverse Generational Distance
Logarithmic Scale
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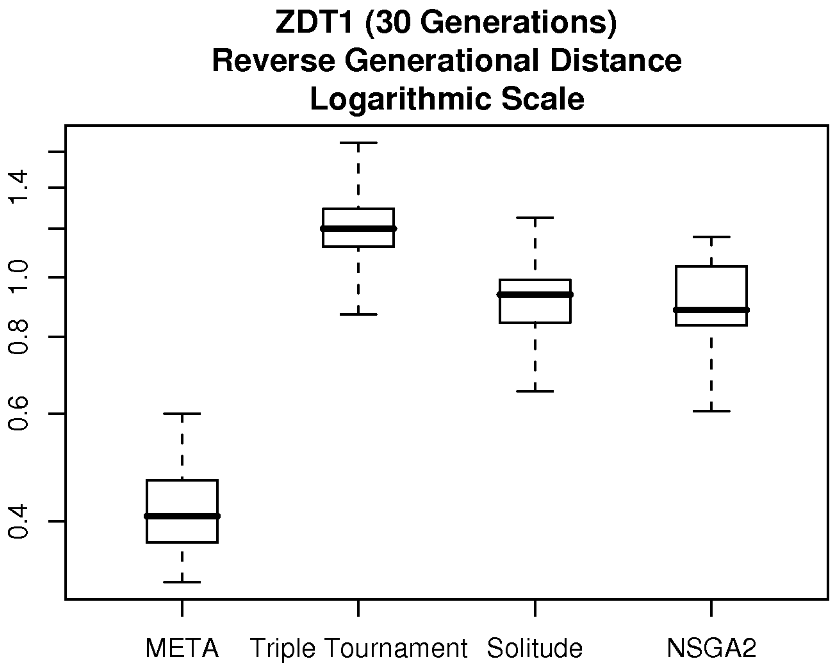
1.6
2.0
META
Triple Tournament
Solitude
NSGA2


ZDT1 (30 Generations)
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Logarithmic Scale
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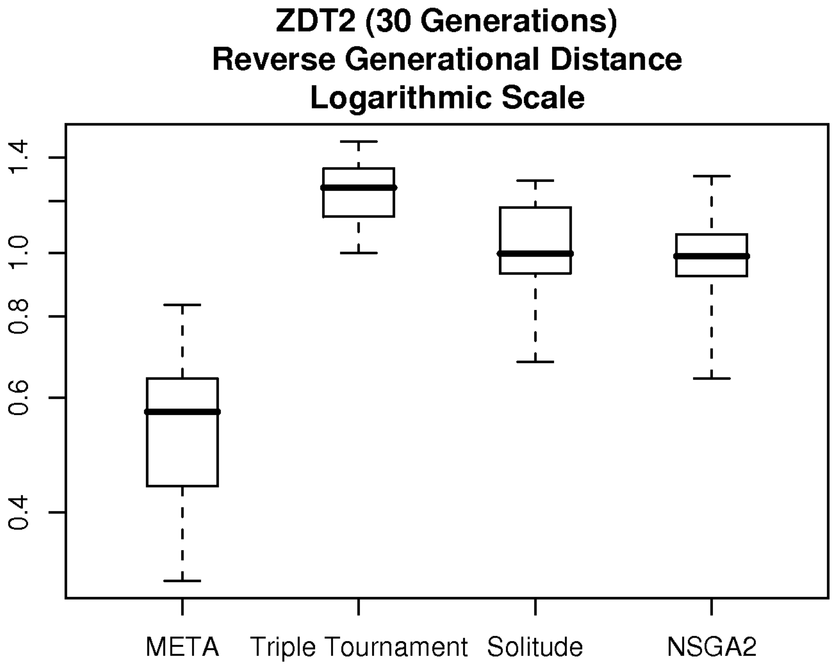
0.6
0.8
1.0
1.4
META
Triple Tournament
Solitude
NSGA2


ZDT2 (30 Generations)
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Logarithmic Scale
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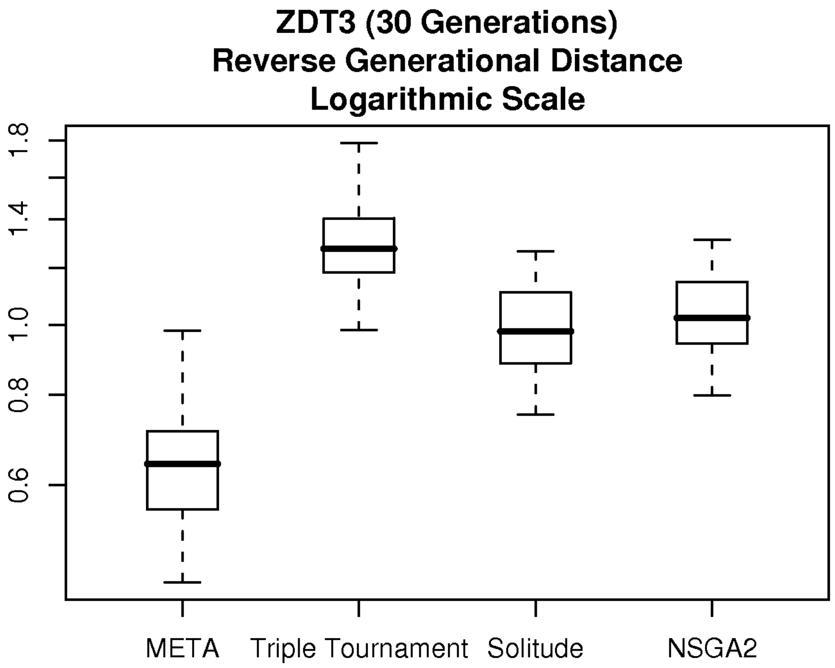
1.4
META
Triple Tournament
Solitude
NSGA2


ZDT3 (30 Generations)
Reverse Generational Distance
Logarithmic Scale
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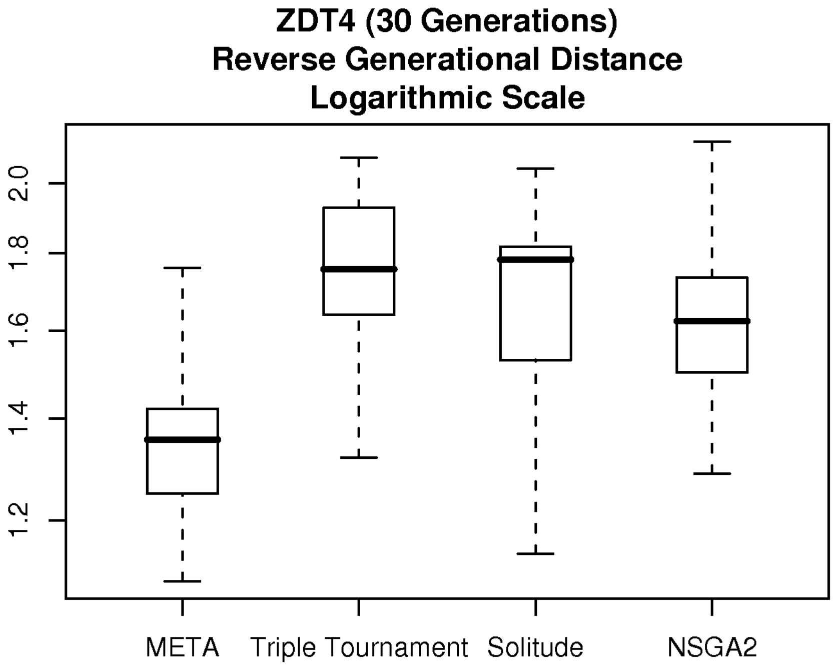
0.8
1.0
1.4
1.8
META
Triple Tournament
Solitude
NSGA2


ZDT4 (30 Generations)
Reverse Generational Distance
Logarithmic Scale
1.2
1.4
1.6
1.8
2.0
META
Triple Tournament
Solitude
NSGA2

Appendix B