

# A Multi-Tier Adaptive Grid Algorithm for the Evolutionary Multi-Objective Optimisation of Complex Problems

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**Abstract** The multi-tier Covariance Matrix Adaptation Pareto Archived Evolution Strategy (m-CMA-PAES) is an evolutionary multi-objective optimisation (EMO) algorithm for real-valued optimisation problems. It combines a non-elitist adaptive grid based selection scheme with the efficient strategy parameter adaptation of the elitist Covariance Matrix Adaptation Evolution Strategy (CMA-ES). In the original CMA-PAES, a solution is selected as a parent for the next population using an elitist adaptive grid archiving (AGA) scheme derived from the Pareto Archived Evolution Strategy (PAES). In contrast, a multi-tiered AGA scheme to populate the archive using an adaptive grid for each level of non-dominated solutions in the considered candidate population is proposed. The new selection scheme improves the performance of the CMA-PAES as shown using benchmark functions from the ZDT, CEC09, and DTLZ test suite in a comparison against the  $(\mu + \lambda)$  Multi-Objective Covariance Matrix Adaptation Evolution Strategy (MO-CMA-ES). In comparison to MO-CMA-ES, the experimental results show that the proposed algorithm offers up to a 69% performance increase according to the Inverse Generational Distance (IGD) metric.

**Keywords** Multi-objective optimisation · evolutionary algorithms · evolution strategies · covariance matrix adaptation · adaptive grid archiving

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## 1 Introduction

The quality of the set of candidate solutions to a multi-objective optimisation problem can be assessed using three criteria: proximity to the true Pareto front (i.e. how close the set of candidate solutions is to the true global solution set), diversity (i.e. how well distributed the set of candidate solutions is over the true Pareto-optimal front), and pertinency (i.e. how relevant the set of candidate solutions is to a decision maker). An ideal approximation set should be uniformly spread across the true Pareto-optimal front (Deb, 2001), or - in real-world problems at least - that part of it that represents a useful subset of solutions to the problem<sup>1</sup> (Purshouse and Fleming, 2007).

The vast majority of the current state-of-the-art Evolutionary Multiobjective Optimisation (EMO) algorithms employ elitism to enhance convergence to the true Pareto-optimal front. Elitism ensures some or all of the fittest individuals in a population at generation  $g$  are inserted into generation  $g + 1$ . Using this method, it is possible to prevent the loss of the fittest individuals which are considered to have some of the most valuable chromosomes in the population. However, in many multi-objective optimisation problems, solutions exist which may not be considered elite due to their objective value in regards to the population, but may contain useful genetic information. This genetic information can be utilised later in the search to move into unexplored areas of the objective-space, but due to elitism and non-

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<sup>1</sup> For example, in the design of automotive engines there is typically a trade-off between torque generated and emissions produced. Designs at the extreme ends of this trade-off surface (i.e. with good emissions but poor torque - or vice versa) are usually not very useful for production automobiles.

dominated sorting schemes it may be abandoned in the early stages of the search.

The aim of this study is to counter the potential negative effects resulting from elitist approaches to selection (for example, the bounded Pareto archive used in the Covariance Matrix Adaption - Pareto Archived Evolution Strategy (CMA-PAES)) by not only preserving elite solutions but also focusing part of the function evaluation budget on non-elitist solutions that have the potential to contribute useful genetic information in the future. To achieve this, a novel multi-tier adaptive grid selection scheme is developed and combined with the existing CMA-PAES algorithm, in a new augmented algorithm named the Multi-tier Covariance Matrix Adaption Pareto Archived Evolution Strategy. This novel algorithm sacrifices a portion of the function evaluation budget in favour of producing diverse approximation sets consisting of solutions from areas of the objective space which are difficult or impossible to obtain with an elitism approach. With this feature, the final approximation set offers a better representation of the trade-off surface, therefore allowing the decision maker to make a more informed selection. The performance of this new algorithm is then evaluated on several benchmarking test suites from the literature.

The paper is organised as follows: Section 2 introduces the field of evolutionary multi-objective optimisation and its performance characteristics, Section 3 introduces the CMA-PAES algorithm and novel multi-tier adaptive grid algorithm, Section 4 contains the experimental set-up and methods of performance assessment, Section 5 presents and discusses the results, and Section 6 draws some conclusions as well as suggesting future research direction.

## 2 Background

### 2.1 Evolutionary algorithms

Evolutionary Algorithms (EAs) are an optimisation technique inspired by some of the concepts behind natural selection and population genetics and are capable of iteratively evolving a population of candidate solutions to a problem (Goldberg, 1989). They both explore the solution space of a problem (by using variation operators such as mutation and recombination) and exploit valuable information present in the previous generation of candidate solutions (by using a selection operator which gives preference to the best solutions in the population when creating the next generation of solutions to be evaluated).

One of the main reasons evolutionary algorithms are applicable across many different problem domains

(including those where conventional optimisation techniques struggle) is their direct use of evaluation function information, rather than derivative information or other auxiliary knowledge. Derivative information (for example) can be extremely difficult to calculate in many real-world problems because the evaluation of candidate solutions can be expensive. Evolutionary algorithms are also robust to noisy solution spaces because of their population based nature. This means that each generation contains more information about the shape of the fitness landscape than would be available to conventional, non-population based optimisation methods (Michalewicz and Fogel, 2000).

Evolutionary algorithms have also been used in combination with other approaches to optimisation to form hybrid algorithms which have been applied successfully to real-world problems (Sfrent and Pop, 2015). Hyperheuristics are a methodology in search and optimisation which are concerned with choosing an appropriate heuristic or algorithm in any given optimisation context (Burke et al, 2003), and can operate on meta-heuristics. Hybrid algorithms indicate the benefits of using an approach which aim to combine existing algorithms and heuristics such that a more general approach can be taken to optimisation.

### 2.2 Evolutionary multi-objective optimisation

Many real-world optimisation problems involve the satisfaction of several objectives which, in a general form, can be described by a vector of objective functions  $f$  and a corresponding set of decision variables  $v$ , as illustrated in equation 1.

$$\min_f(v) = (f_1(v), f_2(v), \dots, f_M(v)) \quad (1)$$

In many problems conflicts occur between objectives such that it is not possible to find a single ideal solution to the problem. In this case, the solution consists of a set of Pareto optimal points - where any improvement in one objective will lead to a deterioration in one or more of the other objectives.

The quality of the set of non-dominated solutions (known as the *approximation set*) can be characterised by considering three main measures (Purshouse, 2003):

- The **proximity** of the approximation set to the true Pareto front.
- The **diversity** of the distribution of solutions in the approximation set.
- The **pertinence** of the solutions in the approximation set to the decision maker.

These concepts are illustrated graphically in Fig. 1, where a single objective value is defined as  $x_m$  and an objective vector of  $M$  objectives can be defined as  $\mathbf{X} = \langle x_1, x_2, \dots, x_M \rangle$ . A preference vector can be defined as  $\mathbf{P} = \langle \rho_1, \rho_2, \dots, \rho_M \rangle$ , where every entry  $\rho_m$  refers to the goal which the corresponding objective values  $x_m$  must satisfy.

An ideal approximation set should contain solutions that are as close as possible to the true Pareto front (i.e. having good *proximity*) and provide a uniform spread of solutions across the region of interest of the decision maker (i.e. having a *diverse* set of candidate solutions that are *pertinent* to the decision maker).

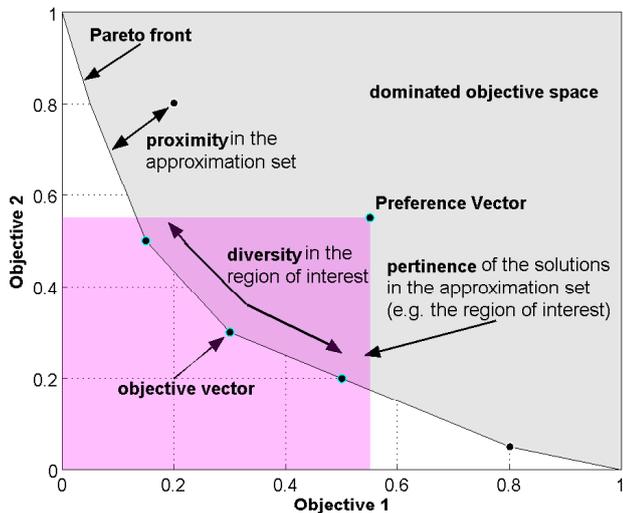


Fig. 1: Characterising the approximation set for a bi-objective problem

Conventional multi-objective optimisation methods often fail to satisfy all these requirements, with methods such as the weighted sum method (Hwang and Masud, 1979) and the goal attainment method (Gembicki, 1974) only capable of finding a single point from the approximation set rather than a diverse distribution of potential solutions. This means that such algorithms do not fully capture the shape of the trade-off space without running the optimisation routine many times. In contrast, Evolutionary Algorithms (EAs) iteratively evolve a population of candidate solutions to a problem in parallel and are thus capable of finding multiple non-dominated solutions. This results in a diverse set of potential solutions to choose from, rather than a single solution that may not meet the required performance criteria.

### 2.3 Obtaining good proximity

The primary goal in evolutionary multi-objective optimisation is finding an approximation set that has good proximity to the Pareto front. This ensures that the candidate solutions in this approximation set represent optimal trade-offs between objectives. The early approaches to evolutionary multi-objective optimisation were primarily concerned with guiding the search towards the Pareto front, reflecting the importance of this goal.

Convergence to the Pareto front is mainly driven by selection for variation, where the best candidate solutions are assigned the highest fitness (and thus have the best chance of contributing to the next generation). Several techniques have been proposed to solve the problem of assigning scalar fitness values to individuals in the presence of multiple objectives - with Pareto-based methods generally being considered the best. Several variants of Pareto based fitness assignment methods exist (see Zitzler et al (2004) for more information), but the general procedure is to rank individuals in the approximation set according to some dominance criterion, and then map fitness values to these ranks (often via a linear transformation). Mating selection then proceeds using these fitness values.

The proximity of the approximation set to the true Pareto front can be enhanced by the use of *elitism*. Elitism aims to address the problem of losing good solutions during the optimisation process (Zitzler et al, 2004), either by maintaining an external population of non-dominated solutions (commonly referred to as an *archive*), or by using a  $(\mu + \lambda)$  type environmental selection mechanism. Studies have shown that elitist MOEAs perform favourably when compared to their non-elitist counterparts (Zitzler and Thiele, 1999; Zitzler et al, 2000a). Elitism has also been shown to be a theoretical requirement to guarantee convergence of an MOEA in the limit condition (Rudolph and Agapie, 2000).

In archive based elitism, the archive can be used either just to store good solutions generated by the MOEA, or can be integrated into the algorithm with individuals from the archive participating in the selection process. Some mechanism is often needed to control the number of non-dominated solutions in the archive, since the archive is usually a finite size and the number of non-dominated individuals can potentially be infinite. Density based measures to preserve diversity are commonly used in this archive reduction - for example, the Pareto Archived Evolution Strategy (Knowles and Corne, 2000a) uses an adaptive crowding procedure to preserve diversity (see later).

An alternative elitist strategy is the  $(\mu + \lambda)$  population reduction scheme, where the parent population and the child population compete against each other for selection. This scheme originated in Evolution Strategies and forms the basis of the environmental selection scheme used in algorithms such as NSGA-II (Deb et al, 2002a) and, more recently, the Multi-Objective Covariance Matrix Adaptation Evolutionary Strategy (MO-CMA-ES) (Igel et al, 2007). In both these algorithms a two level sorting process is used, with Pareto dominance as the primary sorting criteria and population density as a secondary sorting criteria (used as a tie-breaker amongst individuals having the same level of non-dominance).

MO-CMA-ES is a state-of-the-art elitist multiobjective evolutionary optimisation technique that builds upon the powerful covariance matrix adaptation evolution strategy (CMA-ES) real-valued single objective optimiser (Hansen and Ostermeier, 2001; Hansen et al, 2003). The key features of CMA-ES are that it is invariant against linear transformations of the search space, performs extremely well across a broad spectrum of problems in the continuous domain (Auger and Hansen, 2005), and is robust to the initial choice of parameters (due to its advanced self-adaptation strategy). These make the CMA-ES algorithm an excellent choice to base a multi-objective evolutionary optimisation on.

Two variants of MO-CMA-ES exist in the literature: the *s*-MO-CMA-ES which achieves diversity using the contributing hypervolume measure (or *s*-metric) introduced by (Zitzler and Thiele, 1998), and the *c*-MO-CMA-ES which achieves diversity using the crowding-distance measure introduced in NSGA-II. Whilst initial results have shown that MO-CMA-ES is extremely promising, it is as yet mostly untested on real-world engineering problems. Some results show that MO-CMA-ES struggles to converge to good solutions on problems with many deceptive locally Pareto-optimal fronts - a feature that can be common in real-world problems (Voß et al, 2010).

In the original MO-CMA-ES, a mutated offspring solution is considered to be successful if it dominates its parent. In contrast, (Voß et al, 2010) introduces a new MO-CMA-ES variant which considers a solution successful if it is selected to be in the next parent population, introduces a new update rule for the self-adaptive strategy, and conducts a comparison of MO-CMA-ES variants on synthetic test functions consisting of up to three objectives. MO-CMA-ES with the improved update rule is shown to perform substantially better than the original algorithm and is thus used for comparison in Section 5 of this paper.

## 2.4 Obtaining good diversity

Most EMO algorithms use density information in the selection process to maintain diversity in the approximation set. However, diversity preservation has often been seen as a secondary consideration (after obtaining good proximity to the Pareto front). This is because, as Bosman and Thierens (2003) state:

“...since the goal is to preserve diversity *along* an approximation set that is as close as possible to the Pareto optimal front, rather than to preserve diversity in general, the exploitation of diversity should not precede the exploitation of proximity.”

Goldberg (1989) initially suggested the use of a *nicheing* strategy in EMO to maintain diversity, with most of the first generation of Pareto based EMO algorithms using the concept of fitness sharing from single objective EA theory (Fonseca and Fleming, 1993; Horn et al, 1994; Srinivas and Deb, 1994). However, the success of fitness sharing is strongly dependent on the choice of an appropriate niche size parameter,  $\sigma_{share}$ . Whilst several authors proposed guidelines for choosing  $\sigma_{share}$  (Deb and Goldberg, 1989; Fonseca and Fleming, 1993), Fonseca and Fleming (1995) were the first to note the similarity between fitness sharing and kernel density estimation in statistics which then provided the EMO community with a set of established techniques for automatically selecting the niche size parameter, such as the *Epanechnikov estimator* (Silverman, 1986).

A large number of the second generation of Pareto-based MOEAs include advanced methods of estimating the population density, inspired by statistical density estimation techniques. These can be mainly classified into *histogram techniques* (such as that used in PAES (Knowles and Corne, 2000a)) or *nearest neighbour density estimators* (such as that used in SPEA2 (Zitzler et al, 2001) and NSGA-II (Deb et al, 2002a)). Other approaches to diversity preservation include the use of hybrid algorithms, such as the Hybrid Immune-Genetic-Algorithm (HIGA) Istin et al (2011), which uses an immune component to continuously evolve new solutions and then inject them back into the population of an EA. These estimates of population density can be used in both mating selection and environmental selection. In mating selection these density estimates are commonly used to discriminate between individuals of the same rank. Individuals from a less dense part of the population are assigned higher fitness and thus have a higher chance of contributing to the next generation.

Density estimation in environmental selection is commonly used when there exists more locally non dominated solutions than can be retained in the population.

For example, in archive based elitism, density based clustering methods are often used to reduce the archive to the required size. Non-dominated solutions from sparser regions of the search space are again preferred over those from regions with higher population densities, with the aim being to ensure that the external population contains a diverse set of candidate solutions in close proximity to the Pareto front.

The Pareto Archived Evolution Strategy (Knowles and Corne, 2000a) uses an adaptive crowding procedure to preserve diversity that recursively divides up the objective space into grid segments. This bounded Pareto archiving technique then uses this adaptive grid to keep track of the density of solutions within sections of the objective space (Knowles and Corne, 1999). Since it is adaptive, this crowding procedure does not require the critical setting of a niche size parameter which was a common problem with traditional kernel based methods of diversity preservation. This Adaptive Grid Archiving (AGA) scheme uses a grid with a pre-configured number of divisions to divide the objective space and, when a solution is generated, its grid location is identified and associated with it. Each grid location is considered to contain its own sub-population, and information on how many solutions in the archive are located within a certain grid location is available during the optimisation process. Fig. 2 illustrates this grid archiving scheme in two dimensions, in this example it can be observed that the sub-population at grid location 91 holds a single solution whereas the sub-population at grid location 62 contains many more. With this additional information, it is possible to discard a solution from one of the more densely populated sub-populations in favour of a candidate solution which will be located in a sparsely populated sub-population e.g. the one located at grid location 91.

When an archive has reached capacity and a new candidate solution is to be archived, the information tracked by the AGA is used to replace a solution in the grid location containing the highest number of solutions. When a candidate solution is non-dominated in regards to the current solution and the archive, the grid information is used to select the solution from the least populated grid location as the current (and parent) solution.

The AGA concept used in PAES later inspired several researchers and was altered and deployed in multiple EMO algorithms such as the Pareto Envelope-based Selection Algorithm (PESA) (a population based version of PAES) (Corne et al, 2000), the Micro Genetic Algorithm (Coello Coello and Pulido, 2001), and the Domination Based Multi-Objective Evolutionary Algorithm ( $\epsilon$ -MOEA) (Deb et al, 2005).

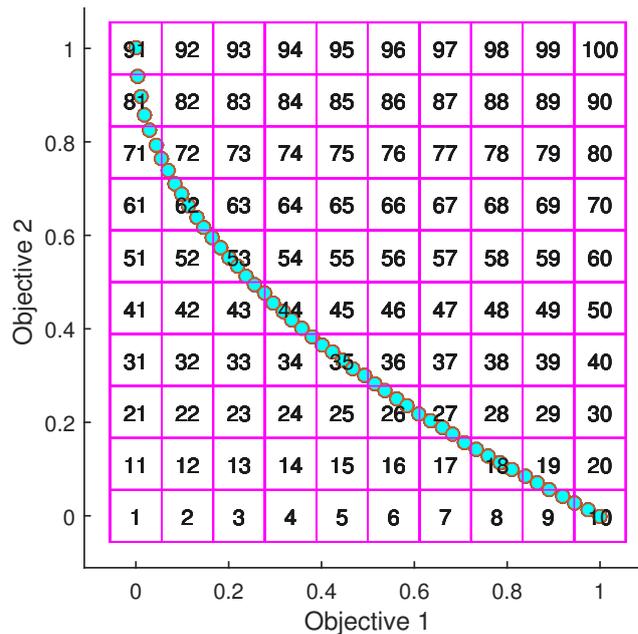


Fig. 2: An example plot of a population and visualisation of grid divisions managed by an AGA.

## 2.5 Issues with elitism

Whilst elitism has been almost universally adopted in the current state-of-the-art for evolutionary multi objective optimisers, in many multi-objective optimisation problems solutions may exist which are not considered elite due to their objective value in regards to the population but may still contain useful genetic information. This genetic information can be utilised later in the search to move into unexplored areas of the objective-space but, due to elitism and non-dominated sorting schemes, it may be abandoned in the early stages of the search.

The consequences of elitism and non-dominated sorting can be seen in Figure 3, where an elitist EMO algorithm has produced an approximation set for the CEC09 UF1 (Zhang et al, 2008b) test function with a budget of 300,000 function evaluations (in compliance with the CEC09 competition rules).

By observing this two-objective plot of the approximation set, it can be seen that the elitist EMO algorithm has converged to an approximation set which is missing three distinct areas containing solutions in comparison to the true Pareto-optimal front plotted in Figure 4. The genetic information which would have potentially found these missing areas was discarded by the algorithm during the search process due to the use of elitism and non-dominated sorting. This is a difficulty that occurs in the CEC09 UF1 test problem because of its complicated Pareto-optimal set, which has

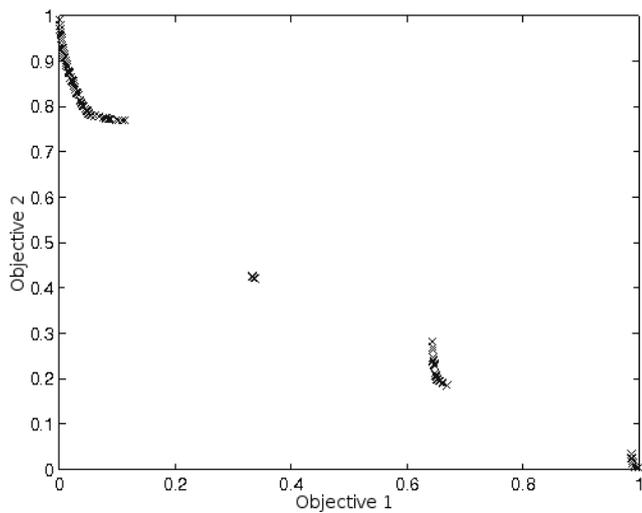


Fig. 3: An approximation set found using an elitist EMO algorithm after 300,000 function evaluations on CEC09 UF1.

some regions that are easier to reach. In these cases, elitist EMO algorithms will focus selection on these more dominant solutions and converge further into that area of the Pareto-optimal-set, discarding individuals which may have been only a few generations away from producing non-dominated solutions in unexplored areas of the objective-space.

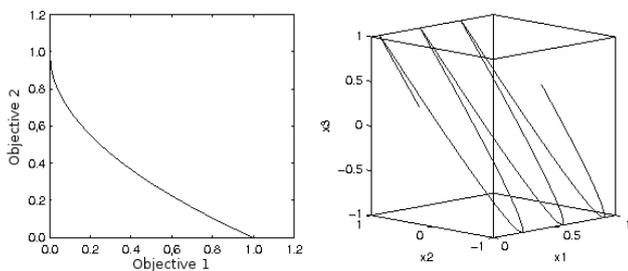


Fig. 4: The true Pareto-optimal front (left) and Pareto-optimal set (right) for CEC09 UF1.

Figure 5 illustrates an example of elitist and non-dominated selection discarding an individual that may contain valuable genetic information, which could have been exploited to produce a better quality approximation set. In this example a Pareto AGA selection scheme has been used to select parent individuals for the next generation. Because of the scheme's elitist nature, the individual between 0.6 and 0.7 on the x-axis has not been selected for reproduction, and therefore the scheme has discarded genetic information which may have ultimately produced solutions towards the missing area of the approximation set. This behaviour

over many generations can lead to convergence to incomplete approximation sets.

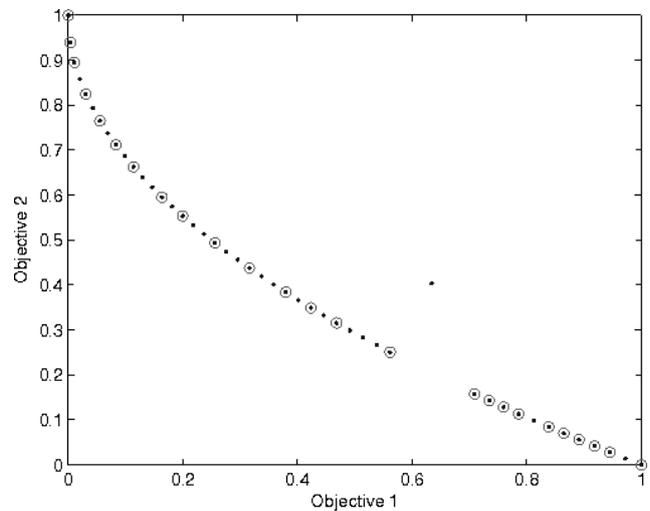


Fig. 5: An example of elitist and non-dominated selection, circled points indicate a selected individual.

### 3 CMA-PAES

The Covariance Matrix Adaptation Pareto Archived Evolution Strategy is an extensible EMO algorithm framework (Rostami and Shenfield, 2012) inspired by the simplicity of PAES (Knowles and Corne, 2000b). As a result the execution life-cycle of the optimisation process does not have a high computational cost in regards of algorithm overhead. The modular structure of the algorithm has allowed for the Covariance Matrix Adaptation (CMA) operator to be easily incorporated in order to achieve fast convergence through the powerful variation of population solutions. To manage these populations at each generational iteration, an Adaptive Grid Algorithm (AGA) approach is used in conjunction with bounded Pareto archiving with the aim of diversity preservation.

The algorithm execution life-cycle for CMA-PAES has been illustrated in Figure 6. CMA-PAES begins by initializing the algorithm variables and parameters, these include the number of grid divisions used in the AGA, the archive for storing Pareto-optimal solutions, the parent vector  $Y$  and the covariance matrix. An initial current solution is then generated at random, which is evaluated and then the first to be archived (without being subjected to the PAES archiving procedure). The generational loop then begins, the square root of the covariance matrix is resolved using Cholsky decomposition (as recommended by Beyer and Sendhoff (2008))

which offers a less computationally demanding alternative to spectral decomposition. The  $\lambda$  candidate solutions are then generated using copies of the current solution and the CMA-ES procedure for mutation before being evaluated. The archive is then merged with the newly generated offspring and subjected to Pareto ranking, this assigns a rank of zero to all non-dominated solutions, and a rank reflecting the number of solutions that dominate the inferior solutions. The population is then purged of the inferior solutions so that only non-dominated solutions remain before being fed into the PAES archiving procedure. After the candidate solutions have been subjected to the archiving procedure and the grid has been adapted to the new solution coverage of objective space, the archive is scanned to identify the grid location with the smallest population, this is considered the lowest density grid population (*ldgp*). The solutions from the lowest density grid population are then spliced onto the end of the first  $\mu - ldgp$  of the Pareto rank ordered population to be included in the adaptation of the covariance matrix, with the aim to improve the diversity of the next generation by encouraging movement into the least dense area of the grid. After the covariance matrix is updated, the generational loop continues onto its next iteration until the termination criteria is satisfied (maximum number of generations).

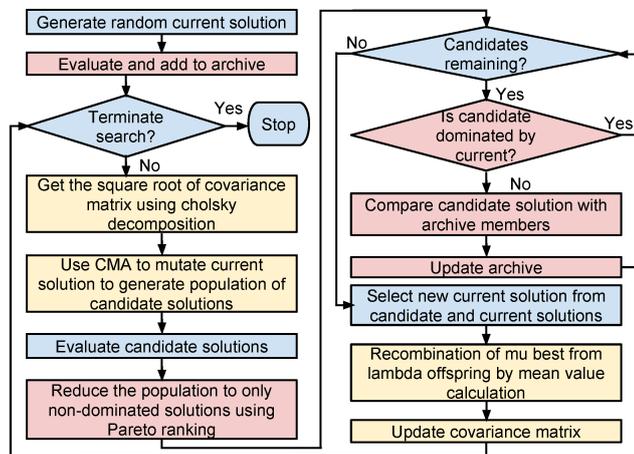


Fig. 6: Execution life-cycle for the CMA-PAES algorithm.

CMA-PAES has been benchmarked against NSGA-II and PAES in Rostami and Shenfield (2012) on the ZDT synthetic test suite. Two performance metrics were used to compare the performance in terms of proximity (using the generational distance metric) and diversity (using the spread metric). CMA-PAES displayed superior performance (the significance of which was sup-

ported with randomisation testing) in returning an approximation set close to or on the true Pareto-optimal front as well as maintaining diversity amongst solutions in the set.

CMA-PAES has also been benchmarked against the MO-CMA-ES algorithm in Rostami (2014), using the hypervolume indicator as a measure of performance. In this study, both the algorithms considered demonstrated comparable performance across multiple test problems, the significance of which was supported by the use of non-parametric testing.

### 3.1 A Novel Multi-Tier Adaptive Grid Algorithm

The new multi-tier AGA aims to prevent a population from prematurely converging as a result of following only the dominant (i.e. elite) solutions which may be discovered early in the optimisation process. This common optimisation scenario often results in genetic drift and consequently a final approximation set with solutions clustered around these elite solutions. This prevention is achieved by dividing an optimisation function evaluation budget and investing a percentage of this budget in to non-elite solutions. This solutions which appear non-elite early on in the optimisation process may potentially contain genetic information that would contribute to finding undiscovered areas of the objective space later in the search.

The algorithm pseudo-code for this new multi-tier approach is listed in Algorithm 1, which is executed from line 14 of the Multi-tier Covariance Matrix Adaptation Pareto Archived Evolution Strategy (m-CMA-PAES) execution life-cycle presented in Algorithm 2. This new optimisation algorithm which builds upon the algorithmic components (AGA and CMA) outlined in Fig. 6 is referred to as the m-CMA-PAES. First, the candidate population is divided into sub-populations based on their non-dominated rank using NSGA-II's fast non-dominated sort. If the size of any sub-population exceeds  $\mu$ , then the standard AGA scheme is applied to it with a maximum archive capacity of  $\mu$ , resulting in a number of rank-ordered archives each with a maximum capacity of  $\mu$ . Then, a single population of size  $\mu$  plus the budget for non-elite individuals  $\beta$  is produced, for example if  $\beta$  is set as 10% for a  $\mu$  population of 100, then a population of size  $100 \times 1.10$  is to be produced. Next the multi-tier archives containing the first  $\mu \times \beta$  solutions are merged with no size restriction (meaning the merged archive size can be greater than  $\mu \times \beta$ ). This merged archive is then subjected to a non-elite AGA (ensuring non-elite solutions are not instantly discarded) with an archive capacity of  $\mu$ , producing a pop-

ulation of individuals to be selected as parents for the next generation.

The configuration of  $\beta$  is important to the convergence of the algorithm - if it is too high (for example if it is greater than half of  $\mu$ ), then the majority of the function evaluation budget is spent on solutions which are dominated and the search does not progress in a positive direction, and may instead move away from the Pareto-optimal front. However if  $\beta$  is too small, the benefits of investing in non-elite solutions are not exploited to an extent which will significantly impact the performance of the optimisation process. The result of this new grid selection scheme has been illustrated in Figure 7, where the solution which may potentially contain valuable genetic information is selected, in contrast to it being discarded in Figure 5.

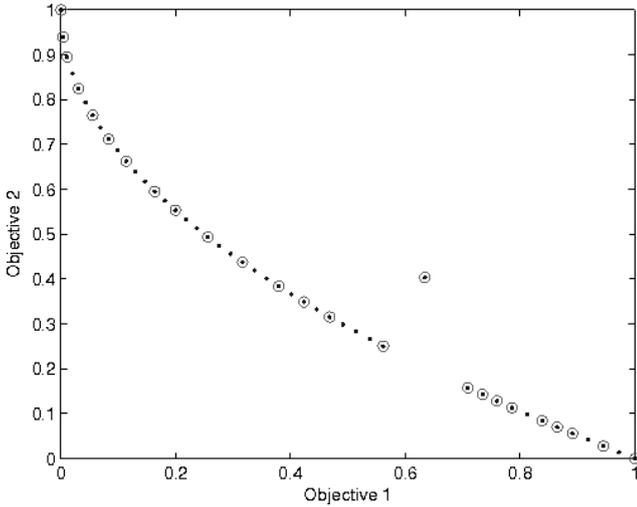


Fig. 7: An example of the multi-tiered grid selection, circled points indicate a selected individual.

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**Algorithm 1** Pseudo-code of Multi-Tier Adaptive Grid Algorithm: multiTierSelect()

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1: nonDominatedFronts = nonDominatedSort(population)
2: spaceRemaining =  $\mu \times \beta$ 
3: for all nonDominatedFront in nonDominatedFronts do
4:   if spaceRemaining > 0 then
5:     tierArchive = adaptiveGridSelection(nonDominatedFront,  $\mu$ )
6:     archive = archive + tierArchive
7:     spaceRemaining = spaceRemaining - size(archive)
8:   end if
   parentPopulation = adaptiveGridSelection(archive,  $\mu$ )
9: end for

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In m-CMA-PAES, a population of candidate solution individuals  $a_i^{(g)}$  are initialized as the structure  $[x_i^{(g)}, \bar{p}_{succ,i}^{(g)}, \sigma_i^{(g)}, p_{i,c}^{(g)}, \mathbf{C}_i^{(g)}]$ , where each individual is assigned a randomly generated problem variable  $x_i^{(g)} \in \mathbb{R}^n$  between the lower ( $x^{(L)}$ ) and upper ( $x^{(U)}$ ) variable boundaries,  $\bar{p}_{succ,i}^{(g)} \in [0, 1]$  is the smoothed success probability,  $\sigma_i^{(g)} \in \mathbb{R}_0^+$  is the global step size,  $p_{i,c}^{(g)} \in \mathbb{R}^n$  is the cumulative evolution path, and  $\mathbf{C}_i^{(g)} \in \mathbb{R}^{n \times n}$  is the covariance matrix of the search distribution.

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**Algorithm 2** m-CMA-PAES life-cycle

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1:  $g \leftarrow 0$ 
2: initialise parent population  $Q^g$ 
3: while termination criteria not met do
4:   for  $k = 1, \dots, \lambda$  do
5:      $i_k \leftarrow k$ ;
6:      $a_k^{(g+1)} \leftarrow a_{i_k}^{(g)}$ 
7:      $x_k^{(g+1)} \sim x_{i_k}^{(g)} + \sigma_{i_k}^{(g)} \mathcal{N}(0, \mathbf{C}_{i_k}^{(g)})$ ;
8:     if  $x^{(L)} \not\leq x_k^{(g+1)} \leq x^{(U)}$  then
9:        $x_k^{(g+1)} = \begin{cases} x^{(U)} & \text{if } x_k^{(g+1)} > x^{(U)} \\ x^{(L)} & \text{otherwise} \end{cases}$ 
10:    end if
11:     $Q_{\mu+k}^{(g)} \leftarrow \{a_k^{(g+1)}\}$ ;
12:  end for
13: end while
14:  $Q^{g+1} = \text{multiTierSelect}(Q^g)$  (Executes Algorithm 1)
15: updateParameters() (Executes CMA Algorithm)
16:  $g \leftarrow g + 1$ 

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## 4 Experimental design and performance assessment

### 4.1 Experimental set-up

In order to evaluate the performance of m-CMA-PAES on multi-objective test problems, a pairwise comparison between m-CMA-PAES and MO-CMA-ES on selected benchmark problems from the literature (consisting of upto 3 objectives) has been conducted. MO-CMA-ES (as outlined in Section 2.3) is a state-of-the-art algorithm which uses the CMA operator for variance much like m-CMA-PAES.

Both m-CMA-PAES and MO-CMA-ES have been configured with a budget of 300,000 function evaluations per algorithm execution, and were executed 30 times per test function as per the CEC2009 competition guidelines. The algorithm configurations are presented in Table 1, and the finer configurations for the CMA operator and MO-CMA-ES have been taken from Voß et al (2010), where the version of MO-CMA-ES used incorporates the improved step-size adaptation.

Table 1: Algorithm configurations used when benchmarking MO-CMA-ES and m-MA-PAES.

Parameter	MO-CMA-ES	m-CMA-PAES
$\mu$	2D(100),3D(300)	2D(100),3D(300)
$\lambda$	2D(100),3D(300)	2D(100),3D(300)
Archive Capacity	—	2D(100),3D(300)
Multi-tier Budget	—	10%
Divisions	—	10

The ZDT, DTLZ, and CEC2009 test suites have been selected for the benchmarking and comparison of m-CMA-PAES and MO-CMA-ES (see Section 4.2). These test suites will pose both MOEAs with difficulties which are likely to be encountered in many real-world multi-objective optimisation problems, in both two-dimensional and three-dimensional objective spaces (allowing for feasible comparison with MO-CMA-ES which relies on the hypervolume indicator for secondary sorting and is thus computationally expensive in high-dimensional search spaces).

The metric used for performance assessment is the popular Inverted Generational Distance (IGD) indicator described in Section 4.3. The IGD indicator will be used at each generation in order to assess performance, and compare both algorithms on not just the IGD quality of the final approximation set, but also the IGD quality over time. In order to comply with the CEC2009 competition rules (as described in Zhang et al (2008b)), both m-CMA-PAES and MO-CMA-ES have been executed 30 times on each test function to reduce stochastic noise. This sample size is seen as sufficient because of the limited benefit of producing more than 25 samples (discussed in Section 4.1.1).

#### 4.1.1 Sample Size Sufficiency

Selecting a sufficient number of samples when comparing optimisers is critical. The sample size of 25, in order to reduce stochastic noise, is re-occurring in the evolutionary computation literature (e.g. Yang et al (2008); Zamuda et al (2007); De Falco et al (2012); García et al (2009); Wang et al (2011)). To prove the sufficiency of this sample size, a large number of hypervolume indicator value samples have been produced by executing m-CMA-PAES 200 times on the DTLZ1 synthetic test problem.

These 200 samples were then used to identify the relationship between the Standard Error of the Mean (SEM) and the sample size using:

$$SEM = \frac{SD}{\sqrt{N}} \quad (2)$$

This relationship has been illustrated in Figure 8, which shows the limited benefit of more than 25 independent executions of the algorithm on the synthetic test problem.

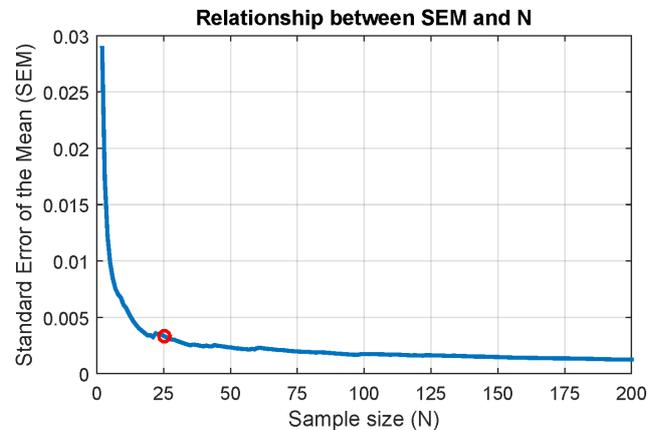


Fig. 8: Relationship between Standard Error of the Mean (SEM) and the sample size of hypervolume indicator values from 200 executions of m-CMA-PAES on the DTLZ1 synthetic test problem.

sizes, evolution paths and covariance matrices of the successful solutions are updated.

## 4.2 Multi-objective Test Suites

The performance of the novel m-CMA-PAES algorithm is compared to MO-CMA-ES across three different real-valued, synthetic, test suites: the widely used ZDT bi-objective test suite proposed in Zitzler et al (2000b), the scalable DTLZ multi-objective test suite proposed in Deb et al (2002b); and the unconstrained functions from the CEC2009 multi-objective competition test suite proposed in Zhang et al (2008b). The configurations used for these test problems and some of their salient features are shown in Table 2

Each of these test suites incorporates a different balance of features that MOEAs may find difficult to overcome during the optimisation process (for example, multi-modal search landscapes, deceptive local Pareto-fronts, non-convex Pareto-fronts, etc.). The ZDT and DTLZ test suites provide well defined Pareto-optimal fronts that have been widely used in the literature - thus allowing easy comparison with previous work. The CEC2009 multi-objective optimisation competition test suite is more recent and is predominantly made up of problems with solution sets that consist of complex curves through decision variable space. These test prob-

Table 2: Parameter configurations used for the ZDT, DTLZ and CEC09 test suites.

Problem	# Var	# Obj	Salient features
ZDT1	30	2	convex front
ZDT2	30	2	concave front
ZDT3	30	2	disconnected front
ZDT4	10	2	convex front, many local optima
ZDT6	10	2	concave front, non uniform distribution
DTLZ1	7	3	linear front
DTLZ2	12	3	spherical front
DTLZ3	12	3	spherical front, many local optima
DTLZ4	12	3	spherical front, non uniform distribution
DTLZ5	12	3	spherical front, difficult to find true front
DTLZ6	12	3	disconnected front
DTLZ7	22	3	disconnected front
UF1	30	2	nonlinear decision space
UF2	30	2	nonlinear decision space
UF3	30	2	many local fronts
UF4	30	2	non-convex front
UF5	30	2	discrete points on a linear hyperplane
UF6	30	2	disconnected front
UF7	30	2	linear hyperplane front
UF8	30	3	spherical front
UF9	30	3	disconnected front
UF10	30	3	spherical front

lems contain variable linkages and present many difficulties for multi-objective optimisation routines.

### 4.3 Performance Assessment

As the EMO process is stochastic by nature, each algorithm was executed 30 times against each test function, in an effort to minimise stochastic noise and increase the integrity of the comparison between the algorithms (see Section 4.1.1). The performance of each algorithm execution was then measured using the Inverted Generational Distance (IGD) performance metric to assess the quality of the approximation set, in terms of proximity to the true Pareto-optimal front and the diversity of solutions in the population.

The IGD metric measures how well the obtained approximation set represents the true Pareto-optimal front which is provided as a large reference set. This is calculated by finding the minimum Euclidean distance of each point of the approximation set to points in the reference set. Lower IGD values indicate a better quality approximation set with IGD values of 0 indicating all the solutions in the approximation set are in the reference set and cover all the Pareto front.

The IGD was introduced in Coello Coello and Cortés (2005) as an enhancement to the generational distance metric, measuring the proximity of the approximation set to the true Pareto-optimal front in objective space. The IGD can be defined as:

$$IGD = \frac{\sqrt{\sum_{i=1}^{n'} d_i^2}}{n'} \quad (3)$$

where  $n'$  is the number of solutions in the reference set, and  $d$  is the Euclidean distance (in objective space) between each solution in the reference set and the nearest solution in the approximation set. A GD value equal to zero indicates that all members of the approximation set are on the true Pareto-optimal front, and any other value indicates the magnitude of the deviation of the approximation set from the true Pareto-optimal front. This implementation of the GD solves an issue in its predecessor so that it will not rate an approximation set with a single solution on the reference set as better than an approximation set which has more non-dominated solutions that are close in proximity to the reference set.

Much like the GD measure, knowledge regarding the true Pareto-optimal front is required in order to form a reference set. The selection of solutions for the reference set will have an impact on the results obtained from the IGD, and therefore the reference set must be diverse. The calculation of the IGD can be computationally expensive when working with large reference sets or a high number of objectives.

The IGD measure has been employed in the performance assessment of algorithms in much of the multi-objective optimisation and evolutionary computation literature (e.g. Zhang et al (2008a, 2010); Tiwari et al (2009); Chen et al (2009); Nasir et al (2011)).

### 4.4 Statistical comparison of stochastic optimisers

Statistical comparison of the performance of the algorithms was conducted by computing the  $t$ -values<sup>2</sup> of the IGD metric produced by both the algorithms. However, when analysing stochastic systems (such as EAs) the initial conditions that ensure the reliability of parametric tests cannot be satisfied (Li et al, 2012) - therefore a non-parametric test (encouraged by Derrac et al (2011); Epitropakis et al (2012)) for pairwise statistical comparison must be used to evaluate the significance of results. The Wilcoxon signed-ranks (Wilcoxon,

<sup>2</sup> The  $t$ -value is the difference between the means of the datasets divided by the standard error.

1945) non-parametric test (counter-part of the paired t-test) can be used with the statistical significance value ( $\alpha = 0.05$ ) to rank the difference in performance between two algorithms over each approximation set.

Non-parametric testing is becoming more commonly used in the literature to statistically contrast the performance of evolutionary algorithms in many experiments (García et al, 2010; Derrac et al, 2012; Li et al, 2012; Epitropakis et al, 2012; Hatamlou, 2013; Civicioglu, 2013).

## 5 Results

The results from the experiments described in Section 4 have been produced and presented in a number of formats in order to allow for a better assessment of each algorithms performance.

The worst, mean, and best IGD indicator results for the final approximation set of each algorithm are presented in Table 3 for the two-objective test functions, and in Table 4 for the three-objective test functions. Tables 3 and 4 also present information regarding the  $p$ -value resolved by the Wilcoxon signed-ranks non-parametric test for the final approximation sets of the considered synthetic test problems, and a symbol indicating the observation of the null hypothesis. A '+' symbol indicates that the null hypothesis was rejected, and m-CMA-PAES displayed statistically superior performance at the 95% significance level ( $\alpha = 0.05$ ) on the considered synthetic test function. A '-' symbol indicates that the null hypothesis was rejected, and m-CMA-PAES displayed statistically inferior performance. An '=' symbol indicates that there was no statistically significant difference between both of the considered algorithms on the synthetic test problem. The table column "%IGD" indicates the difference in performance between m-CMA-PAES and MO-CMA-ES using m-CMA-PAES as the benchmark. This percentage can be calculated by finding the normalised mean performance of each algorithm:

$$\%IGD = 100 \times \left( \frac{mean_a - worst}{best - worst} - \frac{mean_b - worst}{best - worst} \right) \quad (4)$$

where  $mean_a$  is the mean performance for m-CMA-PAES,  $mean_b$  is the mean performance for MO-CMA-ES,  $worst$  is the highest IGD achieved by either algorithm, and  $best$  is the lowest IGD achieved by either algorithm. A positive %IGD indicates the percentage of which m-CMA-PAES outperformed MO-CMA-ES, whereas a negative %IGD indicates the percentage of

which m-CMA-PAES was outperformed by MO-CMA-ES.

Overall, m-CMA-PAES outperformed MO-CMA-ES on all but 3 (ZDT3, UF6 and UF9) of the 22 test functions, producing better performing worst, mean, and best approximation sets.

The mean of the IGD metric at each generation has been plotted and presented in Figure 9 for the two-objective test functions, and Figure 11 for the three-objective test functions. These plots illustrate the rate of IGD convergence from the initial population to the final population.

m-CMA-PAES significantly outperforms the MO-CMA-ES on most of the test-functions used in this comparison. However, as a consequence of investing a percentage of the maximum number of function evaluations in non-elite solutions, it can be observed in Figures 9 and 11 that the convergence of the algorithm is slower in most cases (more so in the two-objective test functions). This suggests that in experiments where the number of function evaluations are not constrained to a low number, the m-CMA-PAES will outperform MO-CMA-ES.

It can be observed in Figures 9 and 11 that the mean IGD for MO-CMA-ES oscillates or rises on some test functions over time. This issue is most visible on UF4 (where the mean IGD for MO-CMA-ES can be seen to oscillate over time) and on DTLZ3 (where the mean IGD for MO-CMA-ES can be seen to improve in performance until 200 generations and then worsen gradually until termination). This issue is due to MO-CMA-ES being dependent on the hypervolume indicator entirely for diversity preservation which, when paired with its elitism scheme, ends up gradually reducing the IGD quality of an approximation set once a difficult area of the search space is encountered.

The results presented in Table 3 and Table 4, as well as the box plots presented in Figure 13 and Figure 14, show that on 18 of the 22 considered test functions m-CMA-PAES significantly outperformed MO-CMA-ES in regards to the achieved mean and median IGD. The box plots show that the interquartile ranges for the m-CMA-PAES results are significantly better than the interquartile ranges for the MO-CMA-ES results. Across all test functions m-CMA-PAES produces fewer outliers - indicating a more reliable and robust algorithm than MO-CMA-ES on the considered test functions.

On the UF3 test function, it can be observed (in Figure 13) that, although the MO-CMA-ES median IGD outperforms m-CMA-PAES, m-CMA-PAES achieved a better interquartile range and a far better total range - achieving the best approximation set for that test function. A similar result can be seen in the performance

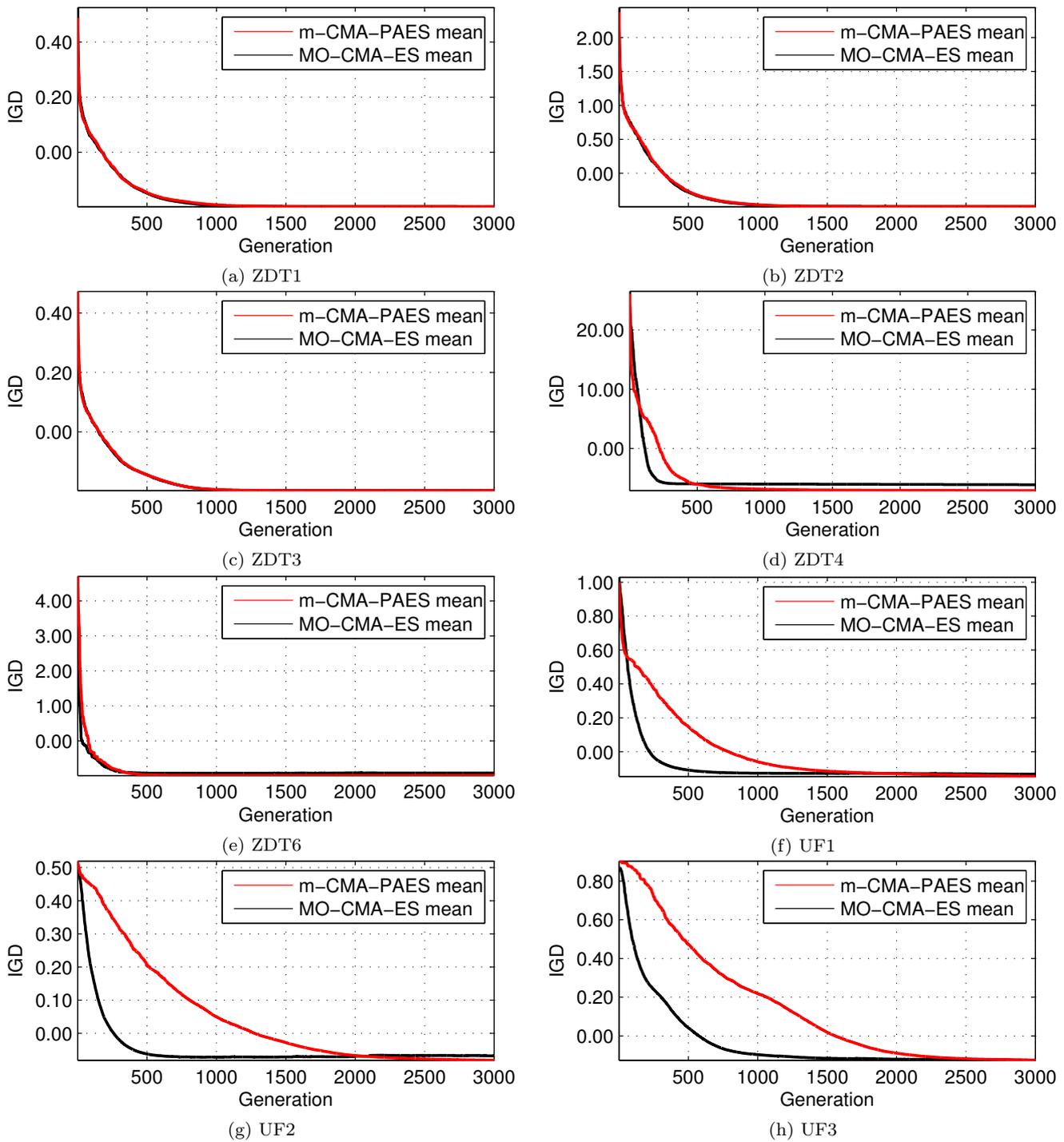


Fig. 9: IGD results at each generation visualising performance of m-CMA-PAES and MO-CMA-ES over 300,000 function evaluations on two-objective test problems, 30 runs.

Table 3: IGD results from 30 executions of m-CMA-PAES and MO-CMA-ES on the ZDT and CEC09 test suites with two problem objectives.

2D	m-CMA-PAES			MO-CMA-ES			$p$ -value	%IGD	
	Best	Mean	Worst	Best	Mean	Worst			
ZDT1	<b>0.00628</b>	<b>0.00657</b>	<b>0.00686</b>	0.00813	0.00936	0.01031	1.4e-09	69.23%	+
ZDT2	<b>0.00592</b>	<b>0.00614</b>	<b>0.00639</b>	0.00989	0.01172	0.01511	1.4e-09	60.72%	+
ZDT3	0.00574	0.00609	0.00676	<b>0.00552</b>	<b>0.00594</b>	<b>0.00643</b>	0.0625	-12.10%	=
ZDT4	<b>1.80044</b>	<b>6.17983</b>	<b>11.44563</b>	2.85512	8.35397	14.56593	0.0232	17.03%	+
ZDT6	<b>0.01132</b>	<b>0.01279</b>	<b>0.01406</b>	0.04788	0.08938	0.20901	1.4e-09	38.74%	+
UF1	<b>0.03762</b>	<b>0.05824</b>	<b>0.06579</b>	0.05044	0.07228	0.12375	1.1e-06	17.00%	+
UF2	<b>0.01359</b>	<b>0.02006</b>	<b>0.02687</b>	0.02117	0.03496	0.05235	5.5e-08	38.44%	+
UF3	<b>0.04869</b>	<b>0.07992</b>	0.12647	0.06044	0.08129	<b>0.10133</b>	0.7269	1.76%	=
UF4	<b>0.05925</b>	<b>0.06431</b>	<b>0.06942</b>	0.07661	0.08261	0.09722	1.4e-09	48.20%	+
UF5	<b>0.49880</b>	<b>0.72982</b>	<b>1.04816</b>	0.87997	1.04873	1.26644	8.3e-09	41.54%	+
UF6	<b>0.08817</b>	0.12736	0.22802	0.09314	<b>0.11268</b>	<b>0.22469</b>	0.010432	-10.50%	-
UF7	<b>0.01791</b>	<b>0.02431</b>	<b>0.03226</b>	0.03306	0.06434	0.12773	1.4e-09	36.45%	+

Table 4: IGD results from 30 executions of m-CMA-PAES and MO-CMA-ES on the DTLZ and CEC09 test suites with three problem objectives.

3D	m-CMA-PAES			MO-CMA-ES			$p$ -value	%IGD	
	Best	Mean	Worst	Best	Mean	Worst			
UF8	<b>0.13308</b>	<b>0.18188</b>	<b>0.23023</b>	0.16091	0.23432	0.24924	3.6e-08	45.14%	+
UF9	0.07381	0.07877	0.08795	<b>0.06755</b>	<b>0.07440</b>	<b>0.07911</b>	5.4e-05	-21.45%	-
UF10	<b>0.64046</b>	<b>0.97907</b>	<b>1.34102</b>	1.33073	1.90805	2.89107	1.6e-09	41.28%	+
DTLZ1	<b>0.60928</b>	<b>3.11971</b>	<b>5.72913</b>	2.11988	10.1829	20.9531	1.2e-06	34.72%	+
DTLZ2	<b>0.03919</b>	<b>0.04005</b>	<b>0.04077</b>	0.04207	0.04491	0.04939	1.4e-09	7.06%	+
DTLZ3	<b>22.4023</b>	<b>50.7571</b>	<b>102.51</b>	171.175	188.531	229.147	1.4e-09	66.64%	+
DTLZ4	<b>0.02459</b>	<b>0.03090</b>	<b>0.04093</b>	0.03181	0.04411	0.07016	5.5e-08	28.99%	+
DTLZ5	<b>0.00152</b>	<b>0.00174</b>	<b>0.00201</b>	0.00190	0.00213	0.00259	8.3e-09	11.21%	+
DTLZ6	<b>0.11059</b>	<b>0.32162</b>	<b>0.65582</b>	0.19705	0.42455	0.71631	0.01701	16.99%	+
DTLZ7	<b>0.05268</b>	<b>0.05783</b>	<b>0.06449</b>	0.05824	0.06653	0.07449	2.9e-08	39.89%	+

on UF6 where m-CMA-PAES also achieves the best approximation set but is outperformed by MO-CMA-ES on the median values of the IGD results.

The MO-CMA-ES significantly outperforms the m-CMA-PAES on UF9. This function (as well as ZDT3 and UF6) consists of disjoint true Pareto-optimal fronts as shown in Figure 15. The comparison in performance on these problems shows that the m-CMA-PAES has performance issues on some problems consisting of multiple parts in their Pareto-optimal fronts.

## 6 Conclusion

In this paper, a multi-tier AGA scheme has been introduced and incorporated into the CMA-PAES algorithm to create m-CMA-PAES. m-CMA-PAES improves the quality of the produced final approximation set by investing a percentage of the allowed function evaluation budget in non-elite but potentially successful solutions. With this approach, m-CMA-PAES is able to

find portions of the Pareto-optimal front which remain unexplored by elitist approaches. Experiments and statistical analysis presented in this study show that with CEC09 competition compliant benchmarking configurations, m-CMA-PAES significantly outperforms MO-CMA-ES on all but 4 of the 22 considered synthetic test problems, and out of these 4, MO-CMA-ES only performs statistically significantly better on 2 test functions.

When observing the IGD values at each generation, it can be seen that in some cases the IGD of the final population is higher than some of the generations before it, this is due to the non-elite solutions invested in at each generation being a factor right to the end of the algorithm. This suggests that in further work the algorithm may benefit from either an offline archive which the algorithm selects from at the end of the optimisation process or a final approximation set selection scheme which uses the last two generations of the op-

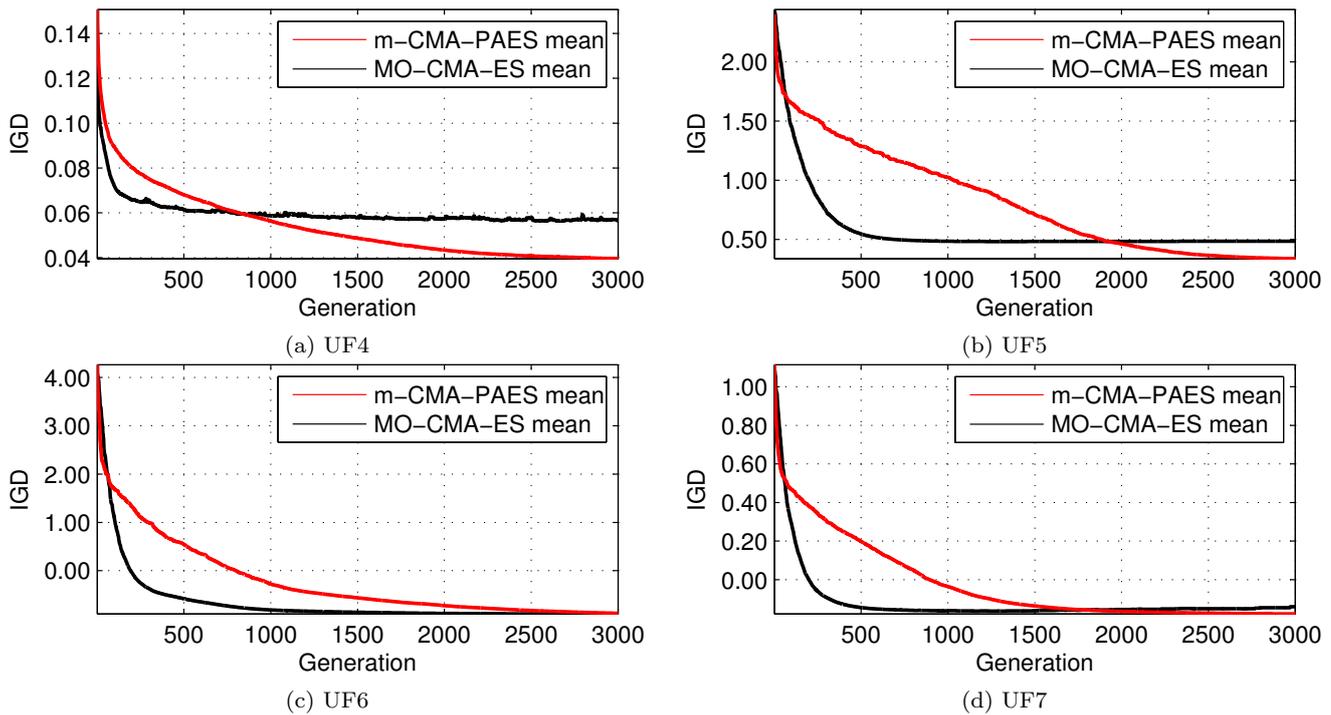


Fig. 10: IGD results at each generation visualising performance of m-CMA-PAES and MO-CMA-ES over 300,000 function evaluations on two-objective test problems, 30 runs.

timisation process, including non-dominated solutions only.

The results indicate a clear trade-off between m-CMA-PAES and MO-CMA-ES. In the majority of the benchmarks MO-CMA-ES appears to offer a faster rate of convergence. However, this comes at the cost of premature convergence very early in the optimisation process. In contrast, m-CMA-PAES offers a slower rate of convergence throughout the entire optimisation process, with steady improvement until the end of the function evaluation budget. Unlike MO-CMA-ES, m-CMA-PAES does not subject the entire non-dominated population to the contributing hypervolume indicator. By not doing so m-CMA-PAES remains computationally lightweight, unlike MO-CMA-ES which becomes computationally infeasible as the number of problem objectives increase. By investing a portion of the function evaluation budget in non-elite solutions, areas of the Pareto-optimal front which are difficult to obtain can be discovered later on in the optimisation process. This results in improved diversity and coverage in the produced approximation sets.

Future works will further investigate the possibility for self-adaptation of the m-CMA-PAES algorithm parameter which defines the budget for non-elite individuals ( $\beta$ ). A current limitation of m-CMA-PAES requires the manual configuration of the  $\beta$  parameter,

which may result in inefficient usage of the function evaluation budget when parameters such as the population size and the number of problem objectives change.

### Compliance with Ethical Standards:

Conflict of Interest: Dr. Shahin Rostami declares that he has no conflict of interest. Dr. Alex Shenfield declares that he/she has no conflict of interest.

Ethical approval: This article does not contain any studies with human participants or animals performed by any of the authors.

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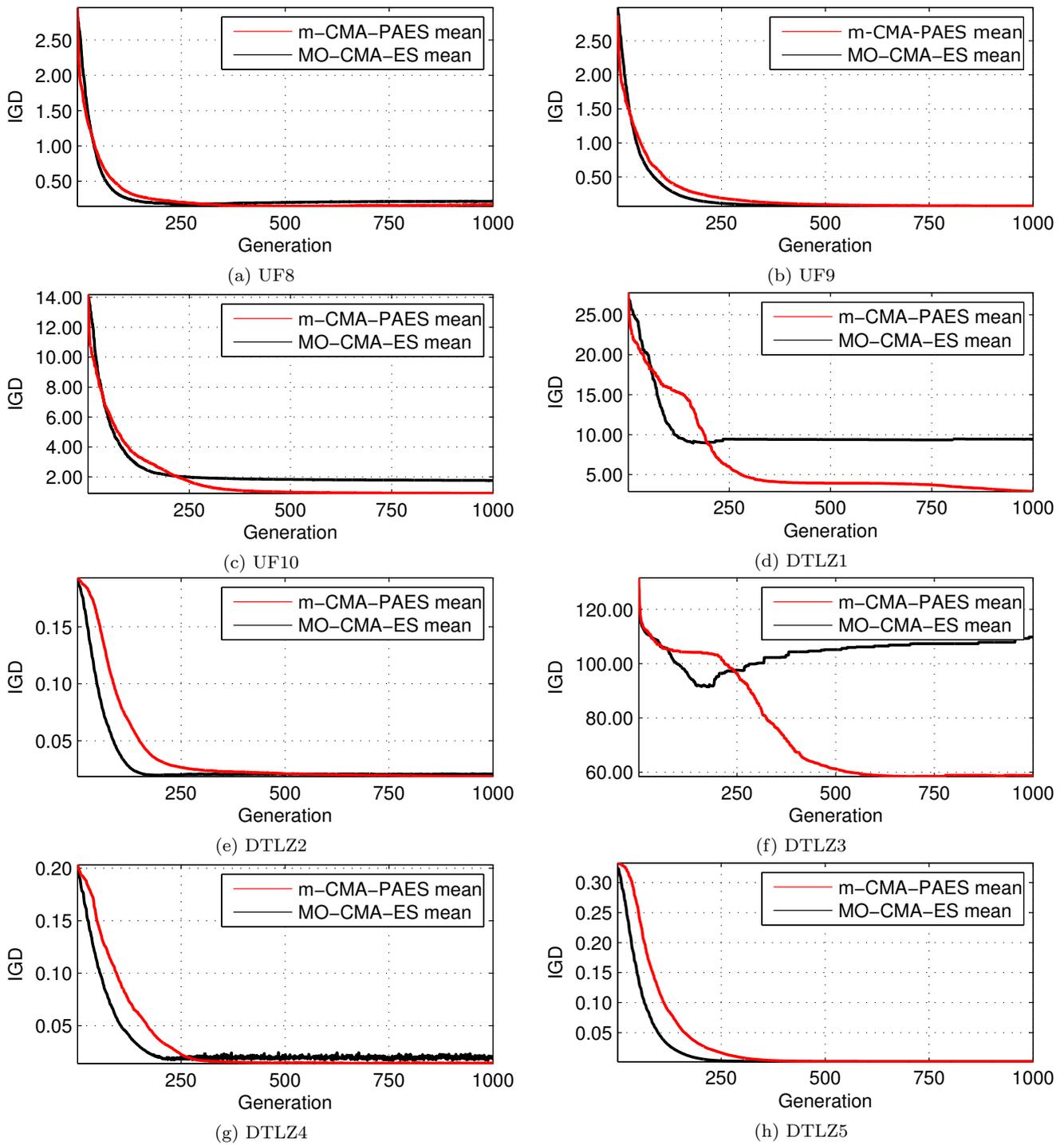


Fig. 11: IGD results at each generation visualising performance of m-CMA-PAES and MO-CMA-ES over 300,000 function evaluations on three objective test problems, 30 runs.

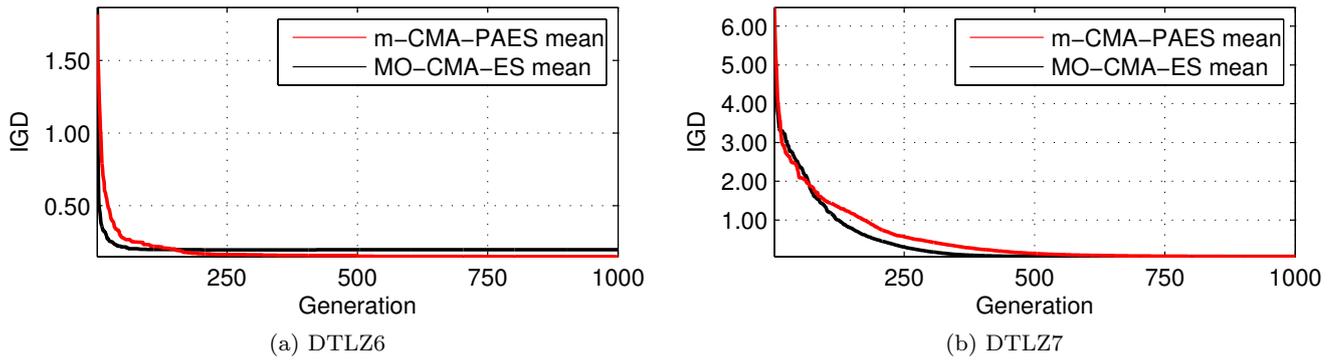


Fig. 12: IGD results at each generation visualising performance of m-CMA-PAES and MO-CMA-ES over 300,000 function evaluations on three objective test problems, 30 runs.

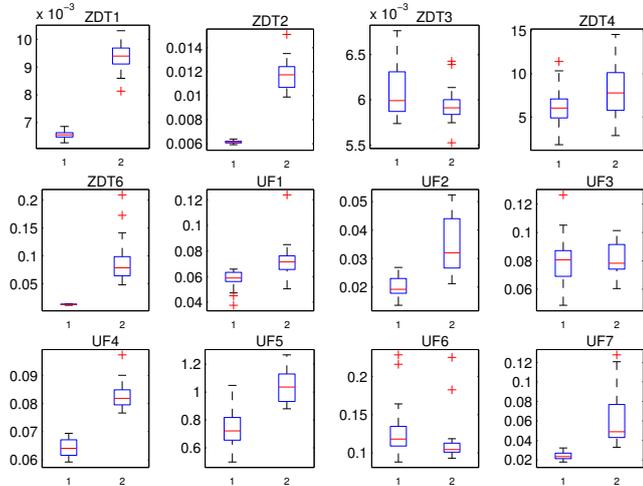


Fig. 13: Box plots of IGD indicator results for two-objective test problems (1: m-CMA-PAES; 2: MO-CMA-ES) 300,000 function evaluations, 30 runs.

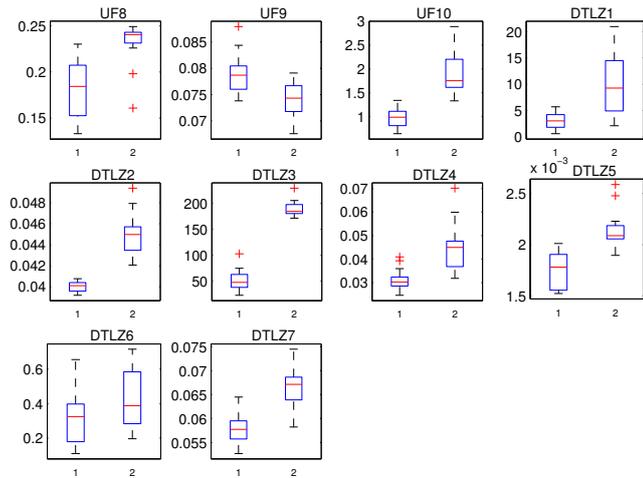


Fig. 14: Box plots of IGD indicator results for three-objective test problems (1: m-CMA-PAES; 2: MO-CMA-ES) 300,000 function evaluations, 30 runs.

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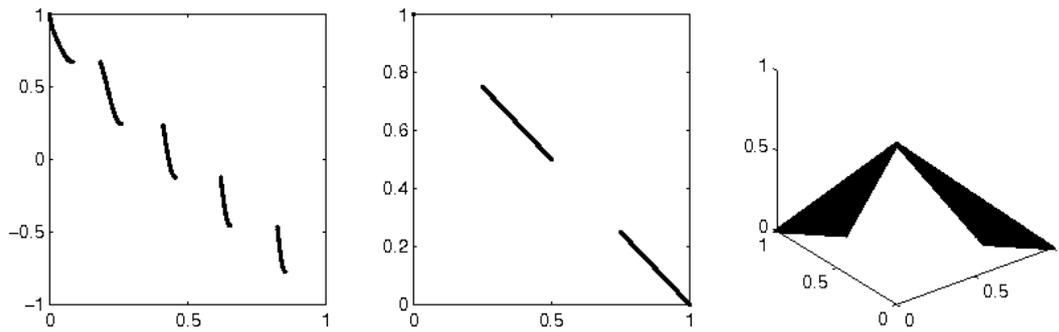


Fig. 15: True Pareto-optimal fronts plotted for problems ZDT3 (left), UF6 (middle) and UF9 (right).

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