Statistical Methods for Convergence Detection of Multi-Objective Evolutionary Algorithms

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Abstract

In this paper, two approaches for estimating the generation in which a multi-objective evolutionary algorithm (MOEA) shows statistically significant signs of convergence are introduced. A set-based perspective is taken where convergence is measured by performance indicators. The proposed techniques fulfill the requirements of proper statistical assessment on the one hand and efficient optimisation for real-world problems on the other hand. The first approach accounts for the stochastic nature of the MOEA by repeating the optimisation runs for increasing generation numbers and analysing the performance indicators using statistical tools. This technique results in a very robust offline procedure. Moreover, an online convergence detection method is introduced as well. This method automatically stops the MOEA when either the variance of the performance indicators falls below a specified threshold or a stagnation of their overall trend is detected. Both methods are analysed and compared for two MOEA and on different classes of benchmark functions. It is shown that the methods successfully operate on all stated problems needing less function evaluations while preserving good approximation quality at the same time.

Keywords

Convergence detection, termination criterion, evolutionary algorithms, multi-objective optimisation, performance indicators, performance assessment.

1 Introduction

In the last decade, the application of evolutionary multi-objective algorithms has become widely accepted by academia as well as industry. However, an autonomous quality-orientated termination criterion, which could further increase the power of these methods, is still missing. The current standard approach is to fix the maximum number of allowed function evaluations with respect to some time constraint.
In order to perform the optimisation in an efficient manner, the MOEA should be stopped when

1. No improvement can be gained by further iterations, or
2. The approximation quality has reached a desired level.

In this paper, two convergence detection methods are presented and compared. A systematic offline convergence analysis called offline convergence detection (OFCD) is introduced. OFCD can be applied to optimisation problems that require high accuracy on the one hand and allow time for such a systematic and computationally intensive approach on the other hand. Furthermore, it is a sophisticated tool for experimental analysis and comparisons of different MOEAs. Moreover, an online convergence detection (OCD) method is presented. OCD makes a decision about convergence based on information from the running optimisation process. The comparison aims to show the justification and compatibility of both methods. Furthermore, it is investigated whether both methods can be brought in accordance by parameter adaptations.

The paper is organised as follows. In the next section, techniques for multi-objective convergence detection are presented. First, the present state of the art is summarised. Then OFCD and OCD are detailed and their algorithmic steps are presented. Both methods are compared and analysed by experiments on established test functions (Section 3). Finally, conclusions are drawn and the results are summarised in Section 4.

2 Methodology

In this section, both procedures for convergence detection are presented. The state of the art is summarised in advance to allow a classification of the novel methods and describe shortcomings of the existing techniques.

2.1 State of the Art

Since MOEAs are still a recent phenomenon, only a limited amount of mathematical convergence theories exist. Rudolph and Agapie (2000) and Rudolph (2001) proved that MOEAs with elitism and positive variation kernel can have the property of converging to the true Pareto front in a finite number of function evaluations in finite search spaces. Further rigorous results are available for $t \to \infty$ (Hanne, 1999; Laumanns, 2003; Laumanns et al., 2002). In order to guarantee (local) optimality of solutions, hybrid MOEA using quadratic programming methods have been developed (Wanner et al., 2006; Deb et al., 2007). These approaches are formally converged as soon as the corresponding mathematical convergence criteria hold. However, due to aggregation, they cannot guarantee the quality of the set of solutions.

Deb and Jain (2002) propose to investigate so-called running performance metrics for convergence and diversity of solutions in the course of the optimisation run. The algorithm is stopped when convergence is observed. An automated procedure for detecting convergence has not been proposed. For this purpose, Rudenko and Schoenauer (2004) survey possible online termination criteria for elitist MOEA, such as the disappearance of all dominated individuals or the deterioration of the number of newly produced non-dominated individuals. Based on this survey, they suggest a technique for determining stagnation based on stability of the maximum crowding distance. Its application is tested only with NSGA-II, which uses the crowding distance as the
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selection criterion as well (Deb et al., 2002a). It is an open issue whether a stability of the maximum crowding distance can be observed in MOEA, which does not directly use this measure in the selection process. Another approach is the application of Kalman filter techniques to performance indicators of the optimisation process. In Marti et al. (2007, 2009) the MGBM criterion is introduced, which is based on a combination of the mutual dominance rate (MDR) with a simplified Kalman filter. The concept is extended by Guerrero et al. (2009) by transforming the hypervolume and the $\varepsilon$ indicators into progress indicators. By means of a Kalman filter, a final global stopping decision is made, based on the behavior of MDR and the transformed indicators.

Different approaches have been introduced in single-objective theory (Deb, 2001). The basic idea of using dominance-related metrics to compare sets (Zitzler et al., 2003) has recently been used to reduce the multi-objective to a single-objective problem on sets (Zitzler et al., 2008). This allows for the use of convergence criteria from single-objective optimisation. However, the use of stopping criteria in this domain is far from unambiguous. The theoretically motivated approaches are not well suited for real-valued search spaces as they require recognizing coalescent paths (Hernandez et al., 2005) or potential complete exploration (Safe et al., 2004). As already proposed by Schwefel (1995), movement criteria are employed in most practical applications (see, e.g., Sastry, 2007; Zielinski and Laur, 2007). That is, differences between single individuals, aggregated fitness values, or location properties are observed and stagnation is detected if they fall below a certain threshold or stay below a threshold for a predefined number of generations. Some approaches, such as Schwefel’s ES or the CMA-ES (Hansen and Ostermeier, 2001; Hansen, 2008), also take adapted strategy parameters into account. If the step sizes become too small, no further movement is possible and the algorithm is stopped. Hoos and Stützle (2004) introduced the concept of (qualified) runtime distributions which characterises the distribution of the time an optimisation algorithm requires to reach a candidate solution within a specific bound on the quality of the solution. By this means, algorithm stagnation can be analysed. Apart from that, trivial resource-based conditions as the maximum runtime or number of generations or evaluations are still prevalent in single-objective metaheuristics.

Recently, a new method for multi-objective offline convergence detection has been introduced (Trautmann et al., 2008). This method, called testing-based runlength detection (TRD) and herein referred to as OFCD, is based on statistical testing of the similarity in the distribution of performance measures for consecutive generations relying on multiple parallel runs of the MOEA. Simulations on standard test cases show the intuitiveness and the high reliability of the proposed method. It is designed for a well-founded and reliable comparison between different MOEA on given test problems with regard to the required generations until convergence is reached. However, it is computationally intensive and thus designated for problems that require high accuracy and can afford the time for a detailed and systematic evaluation of the algorithm performance. Furthermore, a novel method for OCD has been successfully tested on benchmark functions, where about half of the recommended function evaluations for common test cases can be saved without a considerable loss of quality (Wagner et al., 2009). This method is based on two statistical tests and was also applied to two industrial test cases from aerodynamics. Here, the former results have been confirmed and the requirement of both statistical tests within OCD was accentuated (Naujoks and Trautmann, 2009).
2.2 OFCD: An Algorithm for Offline Convergence Detection

The design task of the offline method for convergence detection as suggested in Trautmann et al. (2008) is not to stop a concrete run in a timely manner but rather to attain knowledge about the maximum meaningful runtime (in generations) of a specific algorithm configuration based on a large number of repeated runs. This knowledge is valuable when setting up comparisons, as it would be unfair to compare algorithm A with a runtime proposed by OFCD of \(a\) with algorithm B with a proposed runtime of \(b\) when \(a \ll b\) or vice versa. When running for only \(a\) generations, \(B\) is generally not finished, and running algorithm \(A\) for \(b\) generations uses up computational resources without any expected further progress. The method is designed for an accurate detection of the generation in which convergence of a given algorithm can be expected, and thus deliberately needs much higher computational effort than the online method OCD presented below.

**Algorithm 1** OFCD: Algorithm for Offline Convergence Detection

Require:  
\[GL = 1\] /*initial generation number, usually 1*/

\[S\] /*step-width \(S\) for subsequent generations*/

\[GU\] /*preliminary upper generation limit*/

\(m\) /*number of MOEA repetitions*/

\((PI_1, \ldots, PI_n)\) /*vector of performance indicators*/

1: for all \(G \in \{GL, GL+S, GL+2S, \ldots, GU\}\) do /*produce data*/
2:   for all \(i \in \{1, \ldots, m\}\) do
3:     run MOEA for \(G\) generations /*always starting MOEA anew*/
4:     compute performance indicator values \((PI^G_1, \ldots, PI^G_n)\)
5:   end for
6:   \[PI^G_j = \bigcup_{i=1,\ldots,m} PI^G_{ji}\]
7: end for

8: for all \(G^* \in \{GL+5S, GL+6S, \ldots, GU\}\) do /*investigate data, not possible for prior generations*/
9:   for all \(j \in \{1, \ldots, n\}\) do /*separate test for each indicator*/
10:  perform K-S test for \(H_0: F(PI^G_j) = F(PI^{G-1.5S}_j)\) /*both samples from same distribution \(F?\)*/
11: end for
12: if \(p\) value is greater than \(\alpha = .05\) for three subsequent \(G^*\) for all \(n\) tests then
13:   break
14: end if
15: end for
16: return \(G^*\) /*Optimal generation number*/

OFCD is given in pseudocode in Algorithm 1. It employs two parameters, namely \(m\), the number of runs out of which the test sample is derived, and \(S\), the generation steps that are tested. As \(S\) determines the minimal detectable difference in run lengths, it ideally equals 1 in order to prevent the inevitable delay of at least \(S\) generations before a decision can be made. However, for long runs, this increases the computational effort unnecessarily. Even for a higher \(S\), a reasonable discriminatory power can be assumed while reducing the total workload. We assume that data are available over a reasonable run length interval from generation \(GL\) to generation \(GU\), and that we have suitable performance indicators \(PI_1\) to \(PI_n\) available.

OFCD is based on the two-sided Kolmogorov-Smirnov test (Sheskin, 2000; KS test in the following), which is a very robust nonparametric test method able to detect distribution differences between two samples. For \(p\) values below the significance level
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The null hypothesis of both samples coming from the same distribution can be rejected. The samples thus most likely originate from different distributions. The KS test requires independent samples, so that the results have to be generated separately for each tested run length.

The overall procedure is as follows. For each tested run length \((G_L + l \cdot S)\), \(m\) runs are performed and the performance indicator values (PIs) are recorded (lines 1–7 of Algorithm 1). Then, starting from generation \(G_L + 5S\), for each indicator, the distribution of the last \((1:5)S\) recorded generations over all runs \((5 \cdot m\) values) is tested against the indicator values for the current generation by means of a KS test. If the attained \(p\) value is lower than the predefined \(\alpha\) level (\(\alpha = .05\) has been used in all tests of Trautmann et al., 2008), we indirectly conclude there is a significant development in time and continue with the generation counter increased by \(S\). Precisely, equality of the respective performance indicator distributions can be rejected. Confirmed by experimental results, we wait until the rejection fails three times in a row in order to robustly diagnose stagnation. The generation where this has occurred for all indicators then is the optimal stopping point \(G^*\).

The \(\alpha\) (significance) level of \(.05\) may also be treated as a parameter whereby a lower \(\alpha\) results in earlier stops, entailing a higher risk of halting algorithms prematurely. The data from different time steps are accumulated into one sample for the test (line 10 of Algorithm 1). However, for small resolutions, that is, for high \(S\) values, the distributions of the accumulated indicator values tend to be not that close to each other as is the case for small \(S\). Thus, a small bias toward a higher stop generation has to be accepted in this case.

2.3 OCD: An Algorithm for Online Convergence Detection

In contrast to OFCD, OCD aims at directly detecting the point of convergence during the run. Wagner et al. (2009) have shown that two different criteria are necessary to robustly detect convergence. The first one focuses on a small variance within the preceding performance indicator values. The second one tests whether no significant trend of the performance indicators can be detected over the last generations. This is necessary to avoid situations of cyclic effects or even deterioration, which can be observed for MOEA based on the dominance relation of many-objective problems (Wagner et al., 2007). Furthermore, this test is the only one that regards the longitudinal nature of the indicator values over the generations. The algorithm stops if at least one of the tests indicates the convergence of the MOEA for the generations \(i\) and \((i - 1)\) or if a predefined maximum number of generations has elapsed. OCD returns the stopping generation \(i\) and the method that initiated the MOEA termination. In the case of termination based on the maximum number of generations, the user is informed about the fact that the MOEA has not yet converged and further generations may further improve the Pareto front approximation.

Before OCD can be applied, some input parameters have to be specified. The variance limit \(VarLimit\) corresponds to the desired approximation accuracy in single-objective optimisation. Termination occurs when the standard deviation of the indicator values over the given time window of \(nPreGen\) generations is significantly below \(\sqrt{VarLimit}\). Based on comprehensive experiments, Wagner et al. (2009) suggest using \(\sqrt{VarLimit} = 10^{-3}\). An adaptation of \(VarLimit\) due to the expected range of objective values is not necessary since OCD applies an internal normalisation of the \(d\)-dimensional Pareto front approximations to the interval \([1, 2]^d\) (line 8 and 10 of Algorithm 2). The
The resulting detailed formulas for both methods are presented in pseudocode. In order to allow the straightforward implementation of the tests, the statistical tests are applied to the resulting difference between the indicator values of the tested and the reference set is calculated. If a specific PI does not require a reference set (e.g., the hypervolume indicator), the set (line 13). This adaptive procedure makes OCD applicable on a stand-alone basis.

The PI are calculated for each generation falling into the time window of size \( n_{\text{PreGen}} \) as ideal, and \( 2.1 \) as nadir point. The maximum generation number \( \text{MaxGen} \) expresses the maximum runtime resources. The number and types of desired performance indicators (PI) can be selected to evaluate the solution quality concerning the requirements of the user. OCD initialises these with the standard set of PI as defined by Knowles et al. (2005), which is compared of the hypervolume, the additive \( \varepsilon \), and the R2 indicator.

The PI are calculated for each generation falling into the time window of size \( n_{\text{PreGen}} \) using the Pareto front approximation of the current generation as reference set (line 13). This adaptive procedure makes OCD applicable on a stand-alone basis. If a specific PI does not require a reference set (e.g., the hypervolume indicator), the difference between the indicator values of the tested and the reference set is calculated. The statistical tests are applied to the resulting \( n_{\text{PreGen}} \) vectors of PI at each generation (lines 14 and 16). In order to allow the straightforward implementation of the tests, detailed formulas for both methods are presented in pseudocode.

**Variance Criterion.** The resulting \( n_{\text{PreGen}} \) vectors of \( n \) indicator values are (separately for each indicator) checked against the alternative hypothesis that the variance \( \text{var} \) of these values is lower than the predefined threshold \( \text{VarLimit} \) using the \( \chi^2 \) variance test (Sheskin, 2000), which is detailed in Algorithm 3. The global significance

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**Algorithm 2 OCD: Algorithm for Online Convergence Detection**

Require: \( \text{VarLimit} \) /*maximum variance limit*/

\( n_{\text{PreGen}} \) /*number of preceding generations for comparisons*/

\( \alpha \) /*significance level of the tests*/

\( \text{MaxGen} \) /*maximum generation number*/

\( \{\text{PI}_1, \ldots, \text{PI}_n\} \) /*vector of performance indicators, e.g., (HV, \( \varepsilon \), R2)*/

1: \( i = 0 \) /*initialise generation number*/
2: repeat
3: \( i = i + 1 \)
4: Compute \( d \) objective Pareto front \( \text{PF}_i \) of \( i \) th MOEA generation
5: \( \text{lb} = \min\{\text{lb} \cup \text{PF}_i\} \) /*update lower bound vector*/
6: \( \text{ub} = \max\{\text{ub} \cup \text{PF}_i\} \) /*update upper bound vector*/
7: if \( (i > n_{\text{PreGen}}) \) then
8: \( \text{PF}_i = 1 + (\text{PF}_i - \text{lb})/(\text{ub} - \text{lb}) \) /*normalise \( \text{PF}_i \) to \([1, 2]^d\)*/
9: for all \( k \in [i - n_{\text{PreGen}}, \ldots, i - 1] \) do
10: \( \text{PF}_k = 1 + (\text{PF}_k - \text{lb})/(\text{ub} - \text{lb}) \) /*normalise \( \text{PF}_k \) to \([1, 2]^d\)*/
11: end for
12: for all \( j \in [1, \ldots, n] \) do
13: \( \text{PI}_{j,i} = (\text{PI}_j(\text{PF}_{i-n_{\text{PreGen}}}, \text{PF}_i, 1, 2.1), \ldots, (\text{PI}_j(\text{PF}_{i-n_{\text{PreGen}}}, \text{PI}_i, 1, 2.1))) \) /*compute \( \text{PI}_j \) for \( \text{PF}_{i-n_{\text{PreGen}}}, \ldots, \text{PF}_{i-1} \) using \( \text{PF}_i \) as reference set, 1 as ideal, and 2.1 as nadir point*/
14: \( p\text{Chi2}(j, i) = \text{call } \text{Chi2(PI}_{j,i}, \text{VarLimit}) \) /*p value of the \( \chi^2 \) test*/
15: end for
16: \( p\text{Reg}(i) = \text{call } \text{Reg(PI}_{1,i}, \ldots, \text{PI}_{n,i}) \) /*p value of the t test on the generation’s effect on the \( \text{PI}_{j,i} \)*/
17: end if
18: until \( \forall j \in [1, \ldots, n]: (p\text{Chi2}(j, i) \leq \alpha/n) \land (p\text{Reg}(i) \leq \alpha) \)
19: Terminate MOEA
20: return \{\text{MaxGen}, \text{Chi2}, \text{Reg}\} /*criterion which terminates the MOEA*/
21: \( i \) /*generation in which the criterion holds*/

...
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Algorithm 3 Chi2: One-sided $\chi^2$ variance test for

$H_0 : \text{var}(\text{PI}) \geq \text{VarLimit}$ vs. $H_1 : \text{var}(\text{PI}) < \text{VarLimit}$

Require: PI
  /*vector of performance indicator values*/
  VarLimit
  /*variance limit*/
1: $N = \text{length}(\text{PI}) - 1$
  /*determine degrees of freedom*/
2: $p = \chi^2(\text{Chi}, N)$
  /*look up $\chi^2$ distribution function with N degrees of freedom*/
3: $\text{return } p$

Algorithm 4 Reg: Two-sided $t$ test on the significance of the linear trend

$H_0 : \beta = 0$ vs. $H_1 : \beta \neq 0$

Require: PI$_j$, $j = (1, \ldots, n)$
  /*vectors of performance indicator values*/
1: $N = \text{length}(\bigcup_{j=1}^n \text{PI}_j) - 1$
  /*determine degrees of freedom*/
2: for all $j \in \{1, \ldots, n\}$ do
3:   $\text{PI}'_j = (\text{PI}_j - \text{mean}(\text{PI}_j))/\text{std}(\text{PI}_j)$
   /*standardise*/
4: end for
5: $\bar{Y} := \text{concatenate}(\text{PI}'_1, \ldots, \text{PI}'_n)$
   /*row vector of all PI'$_j$*/
6: $\bar{X} = (1, \ldots, \text{length}(\text{PI}_1), \ldots, 1, \ldots, \text{length}(\text{PI}_n))$
   /*row vector of generations corresponding to each PI'$_j$*/
7: $\hat{\beta} = (\bar{X}^T\bar{X})^{-1} \ast \bar{X} \ast \bar{Y}^T$
   /*linear regression without intercept*/
8: $\epsilon = \bar{Y} - \bar{X} \ast \hat{\beta}$
   /*compute residuals*/
9: $s^2 = (\epsilon \ast \epsilon^T)/N$
   /*mean squared error of regression*/
10: $t = \frac{\hat{\beta}}{s/\sqrt{\text{length}(\bar{X})}}$
    /*compute test statistic*/
11: $p = 2 \cdot \min(t_N(v), 1 - t_N(v))$
    /*look up p value from t distribution with N degrees of freedom*/
12: return $p$

level $\alpha$ has to be adjusted due to the multiplicity of the test problem using a Bonferroni correction (Dudoit and van der Laan, 2008). Thus, there is an individual significance level of $\alpha/n$ for each PI variance test result (line 18 of Algorithm 2). However, a correction with respect to the sequential testing over all generations is impossible concerning a reasonable applicability of OCD. Since the MOEA is terminated when the $p$ value drops below this threshold, a lower value of $\alpha$ leads to a later termination.

Regression Criterion. The significance of the improving trend in the indicators is checked by a linear regression analysis without intercept and a respective $t$ test on the estimated regression coefficient $\hat{\beta}$, which is detailed in lines 7–11 of Algorithm 4. In a preprocessing step, the indicator values PI$_j$ are standardised, that is, they are linearly transformed to mean zero and standard deviation one, so that the regression can be performed for all indicators at once (lines 2–6). Due to a termination in cases where the $p$ value is higher than $\alpha$ (line 18 of Algorithm 2), a more conservative $\alpha$ leads to an earlier termination. However, a combination of the $\alpha$ levels of both tests with respect to multiple test theory (Dudoit and van der Laan, 2008) cannot be performed. The goal is not to directly control the $\alpha$ error, but to find reasonable critical values of the test statistics in order to make OCD applicable and successful within industrial applications.
Runtime. The update, normalisation, and standardisation of the objective sets within each iteration can be performed in $O(N)$, where $N$ denotes the population size. The calculation of the Pareto front requires $O(N \log^d N)$ (Kung et al., 1975; Jensen, 2003), but is already part of most known MOEA. The hypervolume indicator can become the crucial part of OCD, due to the runtime in $O(n^{d/2} \log n)$ time for $d > 3$, and can be computed in $O(n \log n)$ time for $d > 3$ (Beume et al., 2009). For time-critical optimisation tasks, this indicator may be omitted. Thus, the dependence of the convergence detection approaches proposed in this paper with respect to the indicators is also analysed in the following experiments.

3 Experiment: Comparison of Offline and Online Convergence Detection

Pre-Experimental Planning. Offline and online convergence detection methods have been comprehensively evaluated separately (Trautmann et al., 2008; Wagner et al., 2009; Naujoks and Trautmann, 2009). Since both methods are reported to operate successfully, a systematic comparison seems appropriate.

Task. The experiments at hand aim to work out similarities and differences of the two different approaches. It has to be tested whether both approaches terminate the optimisation at a reasonable generation number and if major differences between the methods can be observed. The behaviour of both methods using different parameterisations should be investigated. Another important topic in the experiments is the analysis of the dependence of the approaches with respect to the performance indicators. In addition, strengths and weaknesses of both approaches have to be summarised.

Setup. Two EMO algorithms, namely NSGA-II ( Deb et al., 2002a) and SMS-EMOA (Beume et al., 2007) are analysed on a set of five test functions, that is, Fonseca (Fonseca and Fleming, 1995), ZDT1, ZDT2, ZDT4 (Zitzler et al., 2000), and DTLZ2 (Deb et al., 2002b). Different population sizes and selection strategies $([\mu + \mu]$ for the NSGA-II and $(\mu + 1)$ in the SMS-EMOA) are incorporated according to their appearance in the literature, that is, $\mu \in \{60 \text{ (Fonseca)}, 100 \text{ (ZDT1, ZDT2, DTLZ2), 200 (ZDT4)}\}$ ( Deb et al., 2003). For the sake of comparability, we define a generation of the SMS-EMOA to equal a sequence of $\mu$ function evaluations. Each combination of MOEA and test function has been run 50 times independently (OCD). For OFCD, 50 runs of each MOEA/test function combination were carried out for each generation number (see Algorithm 1), always restarting from generation one.

An NSGA-II implementation in R (Ihaka and Gentleman, 1996)\(^1\) was employed, which uses SBX and polynomial mutation ( Deb, 2001) with $p_c = 0.7$ and $p_m = 0.2$ as well as crossover and mutation distribution indices $\eta_m = \eta_c = 20$. A yet unpublished MATLAB implementation of the SMS-EMOA was used ($p_m = 1/|x|$, $p_c = 0.9$, $\eta_m = 20$, $\eta_c = 15$, and $p_{swap} = 0.5$).

In the first step, all parameters were set to the default levels of Trautmann et al. (2008) and Wagner et al. (2009) (OC: $VarLimit = 0.001^2$, $\alpha = .05$, $nPreGen = 10$; OFCD: $\alpha = .05$, $S = 1$). In addition, the parameters were altered to $VarLimit = 0.0001^2$ (OCD)

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\(^1\)NSGA-II is taken from the package mco (http://cran.r-project.org/web/packages/mco/index.html).
Table 1: Stop Generations of OFCD and OCD (VarLimit = 0.001²) for Both MOEA

<table>
<thead>
<tr>
<th>Problem</th>
<th>NSGA-II</th>
<th>SMS-EMOA</th>
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<tbody>
<tr>
<td></td>
<td>OFCD</td>
<td>OCD</td>
</tr>
<tr>
<td></td>
<td>α = .05 (.01)</td>
<td>med(OCD)</td>
</tr>
<tr>
<td>ZDT1</td>
<td>152 (108)</td>
<td>78 (85/85)</td>
</tr>
<tr>
<td>ZDT2</td>
<td>136 (136)</td>
<td>92 (96/96)</td>
</tr>
<tr>
<td>ZDT4</td>
<td>62 (49)</td>
<td>86 (110/118)</td>
</tr>
<tr>
<td>DTLZ2</td>
<td>23 (21)</td>
<td>14 (14/14)</td>
</tr>
<tr>
<td>Fonseca</td>
<td>28 (26)</td>
<td>19 (19/19)</td>
</tr>
</tbody>
</table>

and α = .01 (OFCD) in order to investigate the dependence on the parametrisation. For measuring the performance of the algorithms, the following PI have been used: hypervolume (HV; Zitzler and Thiele, 1998), additive ε (Eps; Zitzler et al., 2003), and R2 (Hansen and Jaszkiewicz, 1998). OCD terminates if and only if at least one of the tests (χ² variance or t test on ˆβ) indicates convergence with respect to all three metrics simultaneously.

In order to enable the computation of the quality loss of the stop generation compared to MaxGen in the online approach, the PIs were additionally calculated at MaxGen and the OCD stop generation for all runs using a discrete approximation of the true Pareto front as the reference front. These reference fronts also used within OFCD have been calculated via equidistant sampling of the known Pareto fronts.

Results/visualisation. Table 1 compares the stop generations obtained for different parameterisations of OFCD and OCD. For OCD, the percentage of runs terminated by variance criterion is given in addition; for OFCD, different values of α are tested, brackets reveal results for (VarLimit = 0.0001²/Only Regression Criterion) within the columns of OCD. Table 2 displays the saved function evaluations that have been possible applying the corresponding convergence detection methods and the resulting loss in quality, which has to be accepted. The table consists of three subtables, where the two upper ones provide the results from OCD featuring different VarLimit values (0.001² upper table, 0.0001² middle one), the lower one presents the results for OFCD featuring α = .05. The loss of quality is calculated by the difference of the normalised performance indicators (Wagner et al., 2009) at the computed stop generation and the ones obtained performing all function evaluations (MaxGen) suggested in the literature (Deb et al., 2003). In addition, the number of saved function evaluations and their percentage of the recommend ones are reported; for VarLimit = 0.0001² only the problems where the variance criterion terminates in some of the runs are given.

Figures 1 and 2 provide a visual analysis of the different stopping criteria. The results for the ZDT test functions (ZDT1 in the upper group, ZDT2 in the middle group, and ZDT4 in the lower group) are provided in Figure 1. Figure 2 depicts the corresponding plots for the Fonseca test function (upper group) and DTLZ2 (lower group).

Observations. OCD with default settings manages to save at least 20% of the function evaluations recommended in literature (Deb et al., 2003)—in most cases a lot more (Table 2). Simultaneously, a high accuracy of the optimisation result is ensured by keeping the PI loss with respect to the maximum generation number (MaxGen) in the range of the specified variance limit (VarLimit) of the χ² variance test. With decreasing VarLimit, the OCD stop generation increases if OCD terminates due to the variance.
Table 2: (a) OCD, \( \text{VarLimit} = 0.001^2 \); (b) OCD, \( \text{VarLimit} = 0.0001^2 \); (c) OFCD, \( \alpha = .05 \); Summary of PI and Generation Differences at the Stop Generation and MaxGen, where \( \text{PIDiff} = \text{PI}_{j,\text{Stop}} - \text{PI}_{j,\text{MaxGen}} \) and \( \text{GenDiff} = \text{MaxGen} - \text{Stop} \), \( j = \{HV, Eps, R2\} \).

<table>
<thead>
<tr>
<th>Problem</th>
<th>MaxGen</th>
<th>NSGA-II</th>
<th>SMS-EMOA</th>
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<th>SMS-EMOA</th>
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<th>Problem</th>
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Figure 1: Median, lower, and upper quartile of the indicator values of all 50 runs on (a) ZDT1, (b) ZDT2, and (c) ZDT4 at each generation (NSGA-II: top, SMS-EMOA: bottom). Overall (solid vertical line) and PI-specific offline (OFCD, $\alpha = .05$) stop generation (dashed vertical line) are marked. Vertical boxplots (light gray: $VarLimit = 0.0001^2$, dark gray: $VarLimit = 0.001^2$) show the distribution of online (OCD) stop generations.
Figure 2: Median, lower, and upper quartile of indicator values of all 50 runs on (a) Fonseca and (b) DTLZ2 at each generation (NSGA-II: top, SMS-EMOA: bottom). Overall (solid vertical line) and PI-specific offline (OFCD, $\alpha = .05$) stop generation (dashed vertical line) are marked. Vertical boxplots (light gray: $\text{VarLimit} = 0.00012$, dark gray: $\text{VarLimit} = 0.0012$) show the distribution of online (OCD) stop generations.

criterion (Table 1, Figures 1 and 2). This leads to a smaller PI loss, approximately in the interval of $[10^{-04}, 10^{-03}]$. For ZDT2, the recommended MaxGen are closest to OCDStop, whereas the opposite is true for DTLZ2 where more than 90% of the generations are spent without improvement.

The chosen set of test functions reveals the necessity of both OCD termination criteria. While for the ZDT problems with OCD default settings in most cases the variance criterion initiates MOEA termination (Table 1), the regression criterion is dominant for DTLZ2 and Fonseca. For these two problems, the NSGA-II is never stopped due to the variance criterion. Table 1 also lists the median OCD stopping generation in case the variance criterion has been deactivated. These numbers equal upper limits of the possibility of shifting OCDStop in the direction of the offline stop generation (OFCDStop).

It becomes obvious that a perfect match of OCDStop and OFCDStop will be impossible by only altering VarLimit, even in case each test problem is focused individually.
The OCD boxplots in Figures 1 and 2 often show increasing variability in the distribution of OCD stop generations with decreasing \textit{VarLimit}. Also, a shift of the distribution toward higher generation numbers can be observed, except for the test problems that are nearly exclusively terminated by the regression criterion.

The stop generations of OFCD with \( \alpha = .05 \) (default) match with an intuitive MOEA termination received from visually analysing Figures 1 and 2. Except for ZDT4, OFCD-Stop is higher than the median OCD stop generation. Surprisingly, the SMS-EMOA is stopped on ZDT4 although it progresses in all three PI. Note that at the same time, the variance between runs increases. However, a case of divergence (NSGA-II on DTLZ2) is detected—the suggested stop generation generally fits well with human intuition.

The median PI differences are approximately of size \( 10^{-3} \) (Table 1). There is a wide range of saved FE with regard to the test problems (24\% up to even more than 90\%), and generally these values are slightly smaller than the ones for OCD. In case the \( \alpha \) level of the KS tests is decreased to a level of \( \alpha = .01 \), the OFCD criterion becomes less sensitive and results in lower stop generations (Table 1).

The KS test is performed separately for each PI leading to a PI-specific offline stop generation, which is marked in Figures 1 and 2 by a dashed vertical line. The termination of SMS-EMOA is nearly always indicated by the hypervolume (HV) indicator, but for the NSGA-II, the last satisfied criterion can be the HV or \( \varepsilon \) indicator (ZDT4, DTLZ2). \( R^2 \) indicator curves show the most fluctuating shape over time, especially for the Fonseca problem.

**Discussion.** OCD and OFCD show obvious differences. It can be generally concluded that OFCD detects convergence later than OCD. This is no surprise as OFCD always takes a set of runs into account and should detect the point when continuing any of the runs is unreasonable. Furthermore, the observation is related to the fact that the dependencies of PIs of successive generations are not taken into consideration in order to ensure the applicability of the KS test. In contrast, OCD always acts on the level of one concrete run. A spread of OCD stop generations is thereby intended and reflects the differences between runs. The experiment shows that most investigated cases comply with this expectation, the only exception being ZDT4. While for OCD, the desired level of approximation quality can be expressed by \textit{VarLimit} and stagnation is assessed in the regression analysis, OFCD detects stationarity in the distribution of indicator values over all performed runs. Thereby, both situations, which are separately analyzed by OCD, can be detected by the KS test of OFCD. On the one hand, the indicator values indeed stagnate, but on the other hand, the variation of indicator values over different runs gives a limit for improvements that can be detected. Figures 1 and 2 document this fact. Whenever OFCD detects convergence in cases of further improvements, the variation of indicator values over the runs, which is depicted by the interquartile ranges, exceeds the current median value. This can be observed for the SMS-EMOA on ZDT4 or the \( R^2 \) indicator on Fonseca. This fact is particularly interesting with respect to the application of OFCD for algorithm comparison. Whenever statistical tests are used to evaluate the significance of the results, the variation of indicator values within each algorithm gives a limit for detectable differences. A higher accuracy in the detection of the optimum would not provide a benefit, but spends unnecessary computational resources.

Another difference between both approaches is due to the combination of the indicator values before the test is performed, in particular when only the regression criterion of OCD is considered. In OFCD, each indicator is analysed separately and
the run is terminated if all tests detect convergence. In OCD, the indicators are combined before the test is conducted. Thus, it realises a kind of majority decision. This is advantageous in the given tests because the method stops when the $\varepsilon$ and hypervolume indicator stagnate, despite the R2 indicator continuing to improve. As Table 2 shows, no unbounded improvement of the R2 indicator has been given away. This behavior is related to the selection scheme applied in the corresponding MOEA. While the SMS-EMOA is hypervolume-based, the NSGA-II utilises the nondominated sorting procedure. Thus, it especially focuses on the hypervolume and $\varepsilon$ indicator. No specific aggregation-based algorithm has been considered. Surprisingly, the indicators actually applied in the MOEA are those for which convergence is detected last when OFCD is used. This may be due to a lower variation in these indicators as described above.

The parameter variation documents that both methods can be intuitively adjusted by their control parameters. The fact that OFCD becomes less sensitive with decreasing $\alpha$ level is due to the termination in cases when the null hypothesis of equal distributions can no longer be rejected. The VarLimit of OCD shows a close relation to the results that can be expected. In cases where the regression criterion has not stopped the run before, the maximum quality difference to the result after the recommended number of generations can be limited to the magnitude of VarLimit (Table 2[a,b]). The larger confidence regions in the boxplots can be explained by two reasons. A lower VarLimit entails a higher influence of the stochastic effects. Furthermore, more and more runs are terminated due to the regression criterion if VarLimit decreases.

4 Conclusions

In this paper, two recently proposed methods for convergence detection are analysed and systematically compared. The application of these methods to different MOEA and a wide range of test problems documents their successful application as well as their robustness with respect to changing characteristics of performance-indicator trajectories. The systematic differences between the methods are revealed and described. According to their different application levels (OFCD: many runs, offline, OCD: one run, online), the two methods show different characteristics. The method for offline convergence detection efficiently detects the generation in which all indicators stagnate or the improvement falls below the level of variation between the runs. In contrast, the online method has to respond to the course of one concrete run. The experimental analysis shows that stagnation can be detected or the desired accuracy can be obtained by the interplay of a criterion based on variance and one that indicates if the majority of indicator values has converged (regression criterion). In summary, OFCD and OCD each are well suited to their corresponding application area and reliably stop MOEA runs according to a maximum loss, which is predefined (OCD) or detected from the data (OFCD).

References


