Multi³: Optimizing Multimodal Single-Objective Continuous Problems in the Multi-objective Space by Means of Multiobjectivization

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Abstract. In this work we examine the inner mechanisms of the recently developed sophisticated local search procedure SOMOGSA. This method solves multimodal *single-objective* continuous optimization problems by first expanding the problem with an additional objective (e.g., a sphere function) to the *bi-objective* space, and subsequently exploiting local structures and ridges of the resulting landscapes. Our study particularly focusses on the sensitivity of this multiobjectivization approach w.r.t. (i) the parametrization of the artificial second objective, as well as (ii) the position of the initial starting points in the search space.

As SOMOGSA is a modular framework for encapsulating local search, we integrate Gradient and Nelder-Mead local search (as optimizers in the respective module) and compare the performance of the resulting hybrid local search to their original single-objective counterparts. We show that the SOMOGSA framework can significantly boost local search by multiobjectivization. Combined with more sophisticated local search and metaheuristics this may help in solving highly multimodal optimization problems in future.

Keywords: Multiobjectivization · Multimodal optimization · Local search

1 Introduction

The basic idea of multiobjectivization for single-objective (SO) optimization problems is simple [13,19]: instead of optimizing the desired objective alone, introduce a second objective and solve the resulting multi-objective (MO) – more precisely bi-objective – optimization problem using MO solvers (e.g., EMOAs). There are multiple reasons for doing this: First and foremost, local optima are obstacles in search space, which may lead to premature convergence of SO local search methods. And even for global methods, multimodality can be a curse [17].

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A first promising report on the benefits of transforming SO problems into the MO domain was provided by Knowles et al. [13]. The authors empirically showed that multiobjectivization can reduce the amount of local optima in search space. Follow-up studies showed that helper-objectives can be beneficial [8], while others theoretically demonstrate that an additional objective can improve the search behavior of evolutionary algorithms [16].

A second reason for multiobjectivization is to exploit the power of EMOAs, which are capable of solving many difficult problems [21]. However, the result of multiobjectivization may be ambivalent, and thus have positive and negative effects on an algorithm's performance [1,5]. Still, a central property of multiobjectivization remains: if we introduce an additional objective, there is often more information available that may help in guiding the search. Some authors even report on plateau networks that may level out local optima and make it easier to avoid them [2]. Using new visual representations of MO landscapes [4,10], we were recently able to show that MO landscapes in fact comprise structures that can be exploited to escape local optima [20]. In that work, we not only described the observations in the MO landscapes, but also integrated this behavior in a local search method and demonstrated the general working principle.

Given a SO problem $f_1(x)$ that is to be optimized, with $x \in \mathbb{R}^n$, we additionally introduce a sphere function $f_2(x) = (x_1 - y_1^*)^2 + \cdots + (x_n - y_n^*)^2$ as second objective, with $y^* \in \mathbb{R}^n$ denoting the position of the sphere's center and thus only optimum of f_2. Then, the resulting bi-objective problem $F(x) = (f_1(x), f_2(x))^T$ is solved by a multi-objective local search approach called *multi-objective gradient sliding algorithm* (MOGSA) [3], which essentially moves from a starting point in decision space towards the nearest local efficient set (in the MO sense), explores that local efficient set, and moves on to the next (and dominating) locally efficient set of $F(x)$. Therefore, it exploits the special structure of MO landscapes (for details, see Sect. 2). Tracing the search path from multiple starting points, we were able to show in [20], that we pass better local optima for f_1 in that process than standard local search mechanisms (like Nelder-Mead [15]) could possibly reach for many starting points. Depending on the structure of f_1, those trajectories oftentimes even crossed the global optimum.

In this work, we extend the aforementioned approach (presented in detail in [20]) towards an effective SO local search mechanism. By combining multiobjectivization and MOGSA, our modularized heuristic enables boosting of simple SO local search mechanisms like Gradient Search (GS) and Nelder-Mead (NM).

To assess the performance gain caused by our approach, we evaluate the method for two highly multimodal BBOB problems [6], as well as for the classical Rastrigin function [7]. All three functions posses multiple local optima, which certainly are traps for GS and NM. Using specifically developed measures to systematically examine the behaviour of our approach, we show that the SO variant of MOGSA (SOMOGSA) significantly outperforms both local search mechanisms. Our systematic study of starting points in search space, as well as the examinations of the approach's sensitivity to different positions of the helper objective f_2, suggests that further, possibly more advanced, SO local search mechanisms can easily be incorporated in SOMOGSA. Alternatively, our algorithm could be used within global procedures to support global convergence.

The remainder of this work is structured as follows: Sect. 2 details the idea of SOMOGSA and briefly explains the characteristics of MO landscapes that are exploited by our algorithm. Section 3 describes the conducted experiments and the corresponding results (including performance measures), before Sect. 4 summarizes our findings and highlights perspectives for future work.

2 Single-Objective Optimization via Multiobjectivization

Within this section, we first summarize the fundamental concepts of multiobjectivization. Afterwards, the core components of our hybrid and modularized local search algorithm SOMOGSA will be outlined.

Concept of Multiobjectivization: In the remainder of this work, we aim for the optimization of box-constrained continuous single-objective optimization problems of the form $\min_{x \in [l,u]} f(x)$ with $f : \mathbb{R}^n \rightarrow \mathbb{R}$, and $l, u \in \mathbb{R}^n$ being the problem's (lower and upper) box constraints.

Instead of optimizing the single-objective problem directly – w.l.o.g. we denote this objective f_1 – we herein transform the problem into a bi-objective problem $F = (f_1, f_2)$ by introducing a second objective f_2, which w.l.o.g. shall be minimized as well. This concept is known as *multiobjectivization* [8,13,16,20] and its motivation is that the resulting bi-objective problem landscape possesses structural properties which could potentially be exploited.

One of these characteristics are so-called *locally efficient sets*, i.e., the multiobjective pendants of local optima. Per definition, each of these sets is a connected set of locally efficient points. A *locally efficient point* in turn is an observation, which is not dominated[1] by any other point within the ε-neighborhood $B_\varepsilon(x) \subseteq \mathbb{R}^n$ of that point [11,12]. Interestingly, the existence of locally efficient sets within a MO problem can be very beneficial for optimization algorithms as – in contrast to their SO counterparts – these optima oftentimes do not pose traps (to the algorithms that are optimizing the problem), but instead guide the way to more promising regions of the search space [4].

By making use of the Fritz John [9] necessary conditions, locally efficient points can be identified easily: let $x \in \mathbb{R}^n$ be a locally efficient point and all objective functions of F, i.e., f_1 and f_2, continuously differentiable in $\mathbb{R}^n$. Then, there is a weight vector $v \in [0,1]^m$ with $\sum_{i=1}^{m} v_i = 1$, such that

$$\sum_{i=1}^{m} v_i \nabla f_i(x) = 0. \qquad (1)$$

That is, in case of locally efficient points, the (single-objective) gradients cancel each other out given a suitable weighting vector v. This property provides

[1] For two points $a, b \in \mathbb{R}^m$ we state that a dominates b, if $a_i \leq b_i$ for all $i \in \{1, \ldots, m\}$ and $a_j < b_j$ for at least one $j \in \{1, \ldots, m\}$. As a reminder, within this work, we only consider bi-objective problems, i.e., $m = 2$.

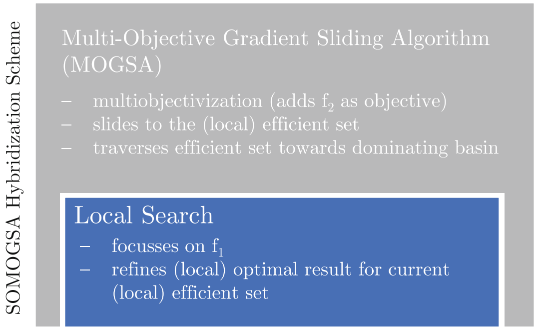

Fig. 1. Hybridization concept of SOMOGSA: While the *multi-objective* local search algorithm MOGSA realizes a descent towards dominating MO basins by approaching and traversing local efficient sets, the encapsulated *single-objective* local search focuses on the refinement of the f_1 values in the visited MO basins.

useful fundamentals for understanding and optimizing multi-objective optimization problems and (as will be shown) for single-objective problems as well. For instance, it can be used for visualizing MO landscapes [10], and is essential for the recently proposed *multi-objective gradient sliding algorithm (MOGSA)* [3,4].

As recently shown in [20], multiobjectivization enables the aforementioned multi-objective algorithm to even optimize single-objective problems. In the following subsection, we will describe this single-objective variant of MOGSA – dubbed SOMOGSA – in more detail.

The Modularized Search Heuristic SOMOGSA: Contrary to previous research (for an extensive review, we refer to Segura et al. [18,19]), we will use a deterministic MO local search algorithm. It efficiently exploits properties of MO landscapes, which we previously identified using a recently developed visualization method based on *gradient field heatmaps* [4]. In our setting the multi-objective problem (MOP) degenerates to a bi-objective problem $F(x) = (f_1(x), f_2(x))^T \in \mathbb{R}^2$. To ensure a simple usage and maximal comprehensibility, we used a simple sphere function $f_2(x) = \sum_{i=1}^{n}(x_i - y_i^*)^2$ with $x, y^* \in \mathbb{R}^n$ as second objective. It comes with the benefits that it is sufficient to guide a MO algorithm, simple enough to avoid unwanted distractions, and allows for simple, analytical determination of the corresponding gradient (which is utilized by SOMOGSA).

The general idea of our proposed hybrid and modularized search heuristic SOMOGSA is given schematically in Fig. 1. While SOMOGSA enables the exploitation of the multiobjective landscape structures, it can encapsulate an arbitrary local search for refinement of f_1 results. In Sect. 3, we will show this for two local searches. The SOMOGSA framework is described in more detail in Algorithm 1. Apart from adding a sphere as second objective (line 1), SOMOGSA essentially (repeatedly) performs the following steps:

1. Perform a MO gradient descent (i.e., 'slide down') into the vicinity of the attracting locally efficient set (lines 5 and 6).

Algorithm 1. SOMOGSA

Require: **a)** start point $x_s \in \mathbb{R}^n$, **b)** function f_1 to be optimized **c)** termination angle $t_\angle \in [0, 180]$ for switching to local search w.r.t. f_1, **d)** step size $\sigma_{MO} \in \mathbb{R}$ for MO gradient descent, **e)** step size $\sigma_{SO} \in \mathbb{R}$ for SO gradient descent w.r.t. f_2, **f)** $y^* \in \mathbb{R}^n$ optimum of f_2

1: $f_2(x) = (x_1 - y_1^*)^2 + \cdots + (x_n - y_n^*)^2$ ▷ *use sphere function for multiobjectivization*
2: $x = x_s$
3: **while** optimum of f_2 not yet reached **do**
4:     $x' = x$
5:     **while** $|\nabla f_1(x)| > 0$ and $\angle(\nabla f_1(x), \nabla f_2(x)) \leq t_\angle$ **do**
6:         $x = x - \sigma_{MO} \cdot \left(\frac{\nabla f_1(x)}{|\nabla f_1(x)|} + \frac{\nabla f_2(x)}{|\nabla f_2(x)|} \right)$ ▷ *MO gradient descent*
7:     $x^{t-1} = x = LocalSearch(x, f_1)$ ▷ *local search w.r.t.* f_1
8:     **if** $f_1(x) < f_1(x')$ **then** ▷ *check for decreasing* f_1 *value*
9:         **if** $|\nabla f_2(x)| > 0$ **then**
10:             **while** $\angle(\nabla f_1(x), \nabla f_2(x)) \geq 90°$ and $\angle(\nabla f_2(x^{t-1}), \nabla f_2(x)) \leq 90°$ **do**
11:                 $x^{t-1} = x$
12:                 $x = x - \sigma_{SO} \cdot \frac{\nabla f_2(x)}{|\nabla f_2(x)|}$ ▷ *gradient descent towards* f_2
13:         **else**
14:             $x' = x$
15:     **else**
16:         leave outer while-loop ▷ f_1 *value deteriorated: break*
17: **return** x', $f_1(x')$

2. Once an (almost) locally efficient point has been reached, SOMOGSA will perform a single-objective local search towards the corresponding (single-objective) local optimum of f_1 (line 7). Here, the user can choose his/her favorite local search strategy.
3. As the local optimum defines one end of the locally efficient set, SOMOGSA now can traverse that set towards the neighboring (better) attraction basin (lines 10–12) by performing a single-objective gradient descent in the direction of the second objective (f_2).

All these steps are repeated until either (a) SOMOGSA has reached the sphere's optimum (line 3), or (b) the objective value of f_1 got worse between two subsequently found local optima of f_1 (line 8). In the latter case, we interrupt the optimization, as SOMOGSA wouldn't improve any longer w.r.t. f_1 but instead waste the remaining budget to eventually reach the optimum of f_2.

As described above, SOMOGSA basically provides a modularized framework, which allows to make use of the strengths of MOGSA. However, the performance of SOMOGSA obviously depends on its configuration (e.g., which problem is used as objective f_2, where the optimum of f_2 is located, which local search strategy is used, etc.). Therefore, in the following, we will investigate the sensitivity of our method w.r.t. different parameters and module choices. In addition, we experimentally demonstrate that SOMOGSA can significantly boost the potential of simple single-objective local search algorithms.

3 Experiments and Results

Setup: Following the general setup in previous work [20], we conduct our experiments on the highly multimodal BBOB functions 21 and 22 [6] (also called Gallagher's 21 and 101 Peak functions) as well as on the classical, regular, but also highly multimodal Rastrigin function [7] in 2D decision space. This Rastrigin version was also used in [20] and provides a simple enough structure for visual interpretation of the algorithms' behavior. For SOMOGSA these functions are fixed as objective f_1 in the multiobjectivized problem. As second objective, we consider $f_2(x) = \sum_{i=1}^{n}(x_i - y_i^*)^2$ with $x, y^* \in \mathbb{R}^n$ (here: $n = 2$). Besides investigating the principal benefits of applying SOMOGSA together with some classical SO local search, we specifically focus on the sensitivity of the approach w.r.t the starting position of the search, as well as the location of the f_2 optimum. We thus discretize the decision space using a regular grid X of $N = d \times d$ starting points with $d = 50$, as larger values of d did not provide additional insights and lower values did not reveal all desired structures. The methods to be assessed are executed for all grid centers of X. Ten positions y^* of the f_2 optimum were generated[2] by using Latin Hypercube Sampling [14] and subsequently mapping those points to their nearest neighbors in X: $(3.5, -1.5)$, $(-1.5, 0.5)$, $(-0.5, 2.5)$, $(2.5, -2.5)$, $(-4.5, -0.5)$, $(-2.5, -3.5)$, $(1.5, 3.5)$, $(4.5, -4.5)$, $(-3.5, 4.5)$, $(0.5, 1.5)$.

As local search mechanisms inside the SOMOGSA framework Gradient Search (GS) and Nelder-Mead (NM) [15] were used, resulting in two variants of SOMOGSA: SOMOGSA+GS and SOMOGSA+NM. As baseline, we also evaluate GS and NM as stand-alone methods on each SO problem. All variants (including stand-alone GS and NM) are allowed a maximum of 4 000 function evaluations, as we observed that especially gradient search may expose slow convergence. As all considered algorithms remain deterministic local searches, a second termination criterion is activated if the method stagnates (often near a local or global SO optimum). In order to exclude this criterion as decisive influence, we evaluated all experiments for precision values $p = 0.01$ and $p = 0.001$. Fortunately, the results qualitatively exhibited the same level of performance due to the simultaneous adjustment of the tolerance of the evaluation metric r_N (see Sect. 3), such that we only report the results for $p = 0.01$.

Methodology: We investigate the sensitivity of SOMOGSA regarding (a) the parametrization of the second objective, (b) the position of the starting point, and (c) the local search strategy. We define well-suited aggregate metrics capturing the performances of each variant in all considered settings (see Fig. 2).

We define the *gain* ($g_{LS} \rightarrow \max$) and the *global gap* ($G_{LS} \rightarrow \min$) as

$$g_{LS}(x_s) = \frac{|f_1(x_b) - f_1(x_s)|}{|f_1(x^*) - f_1(x_s)|}, \qquad G_{LS}(x_s) = \frac{|f_1(x^*) - f_1(x_b)|}{|f_1(x^*) - \max_{x \in X} f_1(x)|},$$

where x_s is a starting point, x_b the best local search result and x^* the known global optimum w.r.t. f_1. In a nutshell, regarding x_b, g_{LS} provides the proportion

[2] LHS implementation of the pyDOE package: https://pythonhosted.org/pyDOE/.

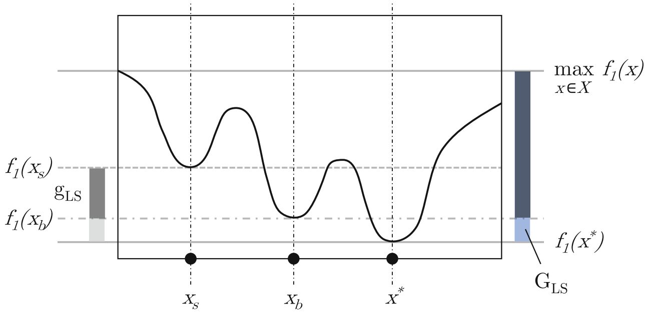

Fig. 2. Illustration of g_{LS} and G_{LS} in a one-dimensional setting.

of the gap between the function value $f(x^*)$ of the optimal solution and the function value $f(x_s)$ of the starting point. G_{LS} expresses the distance of x_b to x^* w.r.t the global maximum distance of any starting point in X to the optimum.

Both measures are evaluated for all combinations of N starting points and problem. The overall aggregated performance of each method can be statistically analyzed and visualized in the decision space, see, e.g., Fig. 3.

Furthermore, we assess the algorithm's capability to reach the optimal solution (of f_1) from any of the starting points of the (discretized) search space X by determining the relative frequency of success, denoted as (success) *ratio*, where $H_N(LS)$ is the absolute frequency of the N algorithm runs that successfully converged to the optimum of f_1 w.r.t. the precision $p = 0.01$:

$$r_N(LS) = \frac{H_N(LS)}{N}$$

Results: Figure 3 shows heatmaps of the g_{LS} measure for the considered search space of Gallagher's 101 Peak function (BBOB function 22). For each SOMOGSA variant and stand-alone LS, we color all starting points x_s – and thus pixels of the corresponding heatmap – according to its $g_{LS}(x_s)$ value, and thereby indicate the gain level – ranging from no gain (blue) to maximum gain (red).

While the first two rows of Fig. 3 show the results related to the application of GS and the corresponding hybridized method SOMOGSA+GS, the two bottom rows depict the corresponding heatmap landscapes regarding NM and the hybridized method SOMOGSA+NM. Note that, for both cases, the respective top left heatmap merely shows the single-objective problem landscape itself, while the second heatmap depicts the g_{LS} values for any starting point, when applying the stand-alone versions of GS or NM, respectively. The remaining heatmaps show the results for each of the considered ten position of f_2.

The heatmaps of the original local search techniques show that local optima are clear traps for these approaches. This is different for SOMOGSA+GS and SOMOGSA+NM. Trapping areas (denoted as blue or green-yellowish structures for GS and NM) vanish from the heatmaps and become red. This indicates that

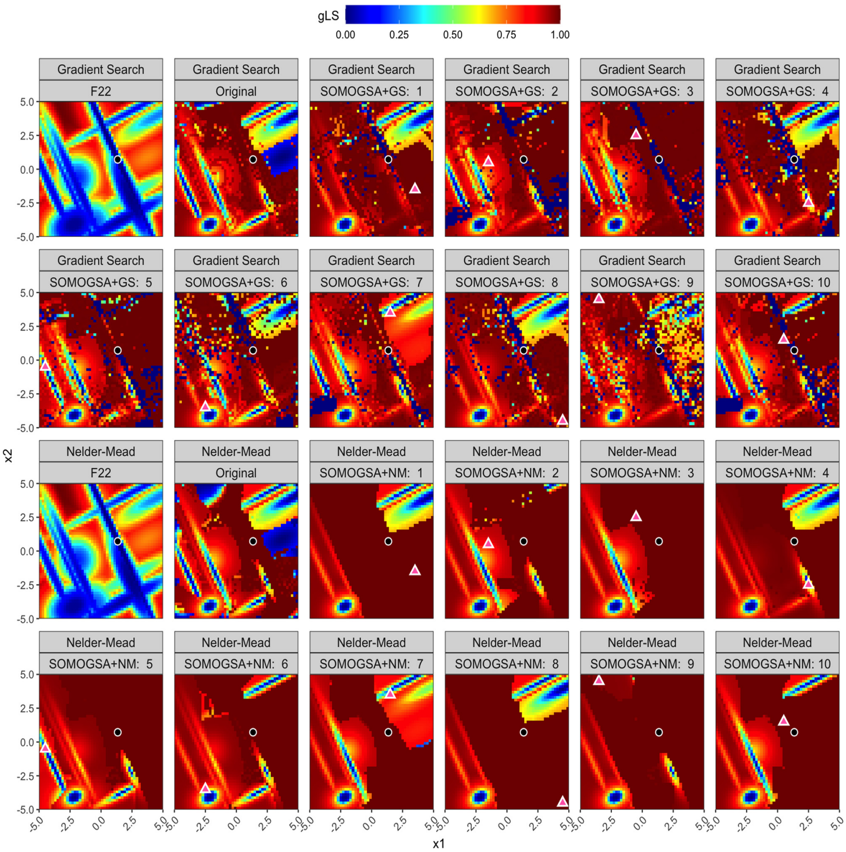

Fig. 3. Heatmaps of the g_{LS} measure for BBOB function 22. First two rows: The top left image shows the landscape of the function itself (the black dot indicates the function's optimum), followed by a heatmap with the g_{LS} performance of the original version of GS on f_1 (F22). The subsequent ten panels display the g_{LS} values of SOMOGSA+GS applied to all ten bi-objective problems. The pink triangles indicate the position of the respective optimum of f_2. Last two rows: Same heatmaps as above, but for NM and its SOMOGSA variants. (Color figure online)

for those starting points a gain is realized by using the SOMOGSA framework. As we observe the complete decision space, we can state that multiobjectivization and using SOMOGSA has the effect of removing traps for the single-objective optimizer. Although we see different resulting structures for varying locations of f_2, the general behaviour is the same for all multiobjectivized problems. Nevertheless, we can also observe an influence of the embedded local search: SOMOGSA+NM seems to produce clearer structures (and thus more robust results) than the simple gradient search mechanism. For the latter we observe many (not red colored) artefacts, which reflect premature convergence.

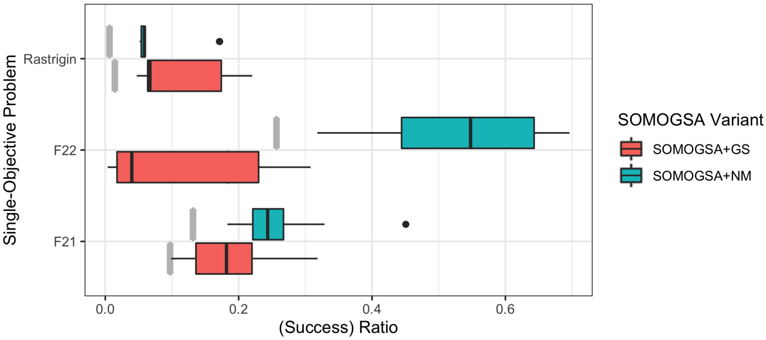

Fig. 4. Boxplots of the ratio values for all considered algorithms w.r.t. BBOB functions 21 and 22, and the Rastrigin function. The gray lines indicate the (success) ratios of the corresponding local search method (GS/NM).

This is also underlined by Fig. 4, which depicts boxplots of the (success) ratio values for all considered cases. More precisely, the red boxplots show the ratios for the three considered functions, solved by SOMOGSA+GS for each of the ten multiobjectivized (bi-objective) problem instances. Accordingly, the blue boxplots show the ratio values w.r.t. SOMOGSA+NM. For each boxplot, the ratio of the respective (original) stand-alone method, GS and NM (applied only to f_1), is shown as gray line. Figure 4 also shows that, for all considered positions of f_2, the multiobjectivization approach reaches the global optimum more often than the pure local search. An exception is SOMOGSA+GS for BBOB problem 22. Here the boxplot reflects what we already observed in Fig. 3: GS seems to get stuck with minimal gain. Furthermore, according to Fig. 4, SOMOGSA+NM proves to be better than or comparable to SOMOGSA+GS regarding all three functions. Therefore, in the following, we focus on this optimizer and take a closer look at its performance in Fig. 5, which displays both g_{LS} and G_{LS} values as boxplots. For each function, the original local search (indicated by red boxes) is compared to the hybridized method (indicated by the blue boxes). For all three functions and all considered sphere positions, this figure also reveals a significant improvement of the performance by adopting multiobjectivization. We tested this by means of a (pairwise) paired Wilcoxon rank sum test (significance level $\alpha = 5\%$) and indicated the significantly better performing variant by a blue *.

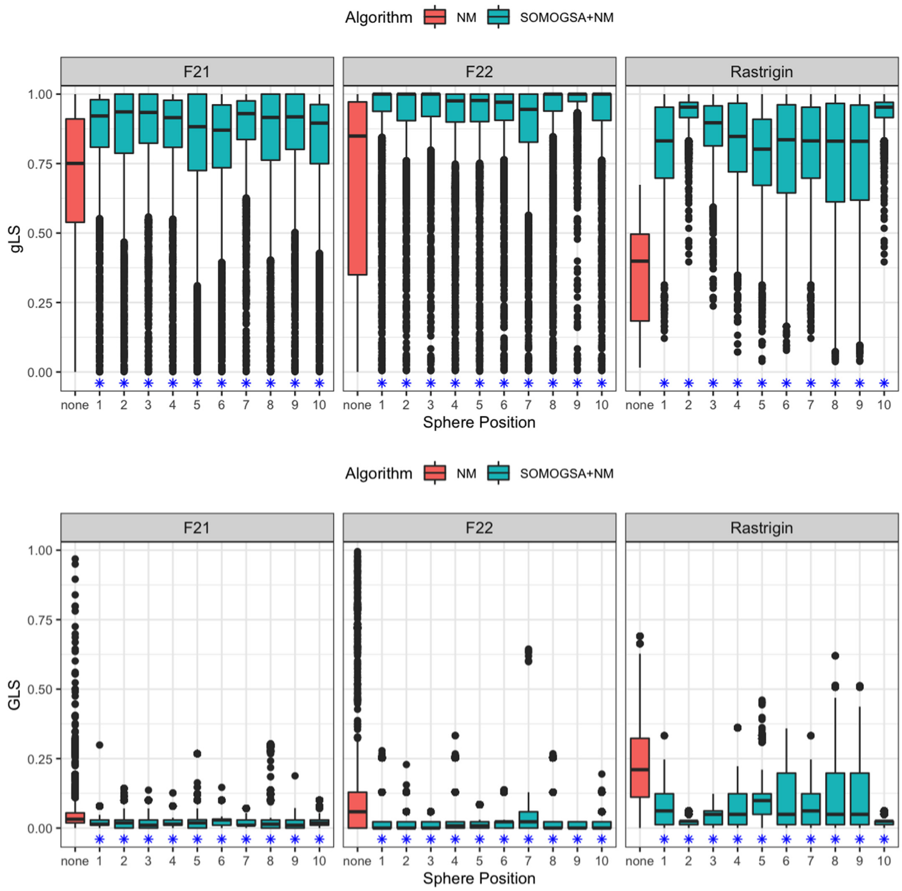

Fig. 5. Boxplots of the g_{LS} (top) and G_{LS} (bottom) measure for BBOB functions 21 and 22, as well as for the Rastrigin function. For each function, the boxplots display the values of NM (red boxplot) and SOMOGSA+NM (blue), respectively. The ten different positions of the helper function are indicated by the numbers 1 to 10. The blue * indicates, which method performs significantly better. (Color figure online)

4 Conclusion

This paper supports previous findings on the benefits of transforming multimodal single-objective problems into multi-objective problems. On selected multimodal BBOB problems we empirically show that SOMOGSA, a hybridization of the previously introduced MOGSA solver, which exploits local structures inside the multi-objective landscape, with simple single-objective local search algorithms like Gradient Search and Nelder Mead, substantially outperforms the single-objective local search optimizers themselves, while the Nelder Mead variant SOMOGSA+NM turned out to be superior to Gradient Search and the respective SOMOGSA variant. For this purpose, we specifically developed suitable performance indicators to assess solver performances on an aggregated level.

Moreover, the experiments revealed that although the performance of SOMOGSA+NM varies w.r.t. the location of the optimum of the artificial second objective – i.e., the sphere function – the extent of variation is not tremendous. This is good news as thus the multi-objective optimization problem is not largely sensitive w.r.t. the location of the sphere optimum. However, an individual configuration of this parameter based on landscape characteristics (ELA features) of the original single-objective problem is a very promising perspective to reach optimal SOMOGSA performance.

Of course, SOMOGSA itself is still a local search mechanism even after hybridization. The proximity to the optimum of individual runs depends on the starting position within the search space. Next steps will include the integration of SOMOGSA into a meta-heuristic which will be able to determine suitable starting points in a sophisticated manner including systematic restarts. Also, the underlying set of multimodal single-objective functions will be largely extended.

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