DIRECTGO: A new DIRECT-type MATLAB toolbox for derivative-free global optimization

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In this work, we introduce DIRECTGO, a new MATLAB toolbox for derivative-free global optimization. DIRECTGO collects various deterministic derivative-free DIRECT-type algorithms for box-constrained, generally-constrained, and problems with hidden constraints. Each sequential algorithm is implemented in two ways: using static and dynamic data structures for more efficient information storage and organization. Furthermore, parallel schemes are applied to some promising algorithms within DIRECTGO. The toolbox is equipped with a graphical user interface (GUI), ensuring the user-friendly use of all functionalities available in DIRECTGO. Available features are demonstrated in detailed computational studies using a comprehensive DIRECTGOLib v1.0 library of global optimization test problems. Additionally, eleven classical engineering design problems illustrate the potential of DIRECTGO to solve challenging real-world problems. Finally, the appendix gives examples of accompanying MATLAB programs and provides a synopsis of its use on the test problems with box and general constraints.

1 INTRODUCTION

The DIRECT (DIviding RECTangles) algorithm [39] is a well-known and widely used solution technique for derivative-free global optimization problems. The DIRECT algorithm extends classical Lipschitz optimization [62–64, 68, 71, 72, 78, 81], where the Lipschitz constant is not assumed to be known. This property makes DIRECT-type methods especially attractive for solving various real-world optimization problems (see, e.g., [2, 3, 9, 14, 16, 25, 50, 61, 66, 89] and the references given therein). Moreover, a recent review and comparison in [75] revealed that, on average, DIRECT-type algorithms performance is one of the best among all tested state-of-the-art derivative-free global optimization approaches. The DIRECT-type algorithms often outperform algorithms belonging to other well-known classes, such as Genetic [34], Simulated annealing [42], and Particle swarm optimization [41].

While the original DIRECT addresses only box-constrained optimization problems, various DIRECT-type modifications and extensions have been proposed. Based on the type of constraints, DIRECT-type algorithms can be classified into four main categories:

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- Box-constrained (see, e.g., [19, 22, 25, 37, 39, 48–51, 66, 76] and the references given therein);
- Linearly-constrained/symmetric (see, e.g., [27, 60, 65–67] and the references given therein);
- Generally-constrained (see, e.g., [13, 21, 37, 44, 89] and the references given therein);
- Containing hidden constraints (see, e.g., [24, 58, 84] and the references given therein).

MATLAB [53] is one of the most broadly used mathematical computing environments in scientific and technical computing (see, e.g., [7, 33, 96]). Many widely used implementations of the original DIRECT algorithm (see, e.g., [6, 20, 24]) as well as various later introduced DIRECT-type extensions (see, e.g., [44, 47, 48, 66]), were developed using MATLAB. Motivated by this, we developed a DIRECT-type global optimization toolbox (DIRECTGO) within the MATLAB environment. The DIRECTGO toolbox is equipped with a graphical user interface (GUI), which links to a DIRECTGOLib v1.0 [86, 91] library and ensures the user-friendly use of all functionalities available in DIRECTGO. The DIRECTGOLib v1.0 library is a continuation of our previous DIRECTLib [90], which was widely used in our different previous studies (see, e.g., [88, 89, 93]). However, DIRECTLib was designed as a static library and did not offer the global optimization community comfortable opportunities to contribute to it. Therefore, a new DIRECTGOLib v1.0 is designed as an open-source GitHub repository to which other researchers can easily contribute.

The first publicly available DIRECT implementations and many others introduced later typically use static data structures for storage and organization. Our recent work [93] showed that the MATLAB implementation of the same DIRECT-type algorithm based on dynamic data structure often has a significant advantage over implementation based on the static data structure. Therefore, each algorithm in DIRECTGO is implemented using both static and dynamic data structures. As various applications can benefit from parallel computing, the SPMD (Single Program Multiple Data) parallel scheme (see [93] for more information) is used to implement some approaches.

1.1 Contributions and structure

We summarize our main contributions below:

- We develop a new MATLAB toolbox (DIRECTGO) for derivative-free global optimization, consisting of 36 different DIRECT-type algorithms (see Table 1 for the details).
- We implement each DIRECT-type algorithm using two types of data structures, static and dynamic [30, 93].
- We adapt the SPMD parallel scheme [93] for selected DIRECT-type algorithms.
- We create a new library (DIRECTGOLib v1.0 [91]) of test and engineering global optimization problems for usage with DIRECTGO and convenient contribution to it through GitHub [86].
- We perform a comprehensive experimental study on the effectiveness of various DIRECT-type approaches.
- We design a user-friendly application with a graphical user interface (GUI).
- We make DIRECTGO open-source, i.e., freely available to anyone [85].

The rest of the paper is organized as follows. Section 2 provides the classification of existing DIRECT-type algorithms and describes the algorithms implemented within our toolbox in more detail. The parallel scheme used in implementing some algorithms is also discussed here. DIRECTGO toolbox is introduced and described in Section 3. The detailed computational study of the DIRECTGO toolbox using classical global optimization test and engineering design problems DIRECTGOLib v1.0 [91] are presented in Sections 4 and 5, respectively. Finally, in Section 6, we conclude the work and discuss the possible future directions.

Table 1. Classification of DIRECT-type implementations (within the DIRECTGO toolbox) based on the type of constraints.

Problem type	Algorithm name	Implementation			Description and References
		st	dy	pa	
Box constrained	DIRECT v4.0	+	+	+	Finkel's implementation [20] of the original DIRECT [39] algorithm
	DIRECT-restart	+	+	+	Our implementation of the algorithm from [19] (based on Finkel's DIRECT [20] implementation)
	DIRECT-m	+	+	+	Our implementation of the algorithm from [22] (based on Finkel's DIRECT [20] implementation)
	DIRECT-l	+	+	+	Our implementation of the algorithm from [25] (based on Finkel's DIRECT [20] implementation)
	DIRECT-rev	+	+	+	Our implementation of the algorithm from [37] (based on Finkel's DIRECT [20] implementation)
	DIRECT-a	+	+	+	Our implementation of the algorithm from [46] (based on Finkel's DIRECT [20] implementation)
	DIRMIN	+	+	+	Our implementation of the algorithm from [50] (based on Finkel's DIRECT [20] implementation)
	PLOR	+	+	+	Our implementation of the algorithm from [56] (based on Finkel's DIRECT [20] implementation)
	glbSolve	+	+	−	Björkman's implementation [6] of the original DIRECT [39] algorithm
	glbSolve-sym, glbSolve-sym2	+	+	−	Our implementation of algorithms from [27] (based on Björkman's glbSolve [6] implementation)
	MrDIRECT, MrDIRECT$_{075}$	+	+	−	Our implementation of algorithms from [48, 49] (based on Björkman's glbSolve [6] implementation)
	BIRECT	+	+	−	Our implementation of the algorithm from [59] (based on Björkman's glbSolve [6] implementation)
	GB-DISIMPL-C, GB-DISIMPL-V	+	+	−	Our implementation of algorithms from [60] (based on Björkman's glbSolve [6] implementation)
	Gb-BIRECT, BIRMIN, Gb-glbSolve	+	+	−	Our implementation of algorithms from [61] (based on Björkman's glbSolve [6] implementation)
	DISIMPL-C, DISIMPL-V	+	+	−	Our implementation of algorithms from [65] (based on Björkman's glbSolve [6] implementation)
	ADC	+	+	−	Our implementation of the algorithm from [76] (based on Björkman's glbSolve [6] implementation)
	Aggressive DIRECT	+	+	+	Our implementation of the algorithm from [2]
	DIRECT-G, DIRECT-L, DIRECT-GL	+	+	+	Our implementation of algorithms from [88]
Linearly constrained	Lc-DISIMPL-C, Lc-DISIMPL-V	+	+	−	Our implementation of algorithms from [66, 67] (based on Björkman's glbSolve [6] implementation)
Generally constrained	DIRECT-L1	+	+	+	Finkel's implementation of the algorithm from [20]
	DIRECT-GLc, DIRECT-GLce, DIRECT-GLce-min	+	+	+	Our implementation of algorithms from [89] (based on our DIRECT-GL [88] implementation)
Hidden constraints	DIRECT-NAS	+	+	−	Finkel's implementation of the algorithm from [24]
	DIRECT-Barrier	+	+	−	Our implementation of the algorithm from [24] (based on Finkel's DIRECT [20] implementation)
	subDIRECT-Barrier	+	+	−	Our implementation of the algorithm from [58] (based on Finkel's DIRECT [20] implementation)
	DIRECT-GLh	+	+	−	Our implementation of the algorithm from [84] (based on our DIRECT-GL [88] implementation)

st - implementation using static data structures.
dy - implementation using dynamic data structures.
pa - parallel implementation using dynamic data structures.

2 THEORETICAL AND ALGORITHMIC BACKGROUNDS

This section provides the classification of existing DIRECT-type algorithms and describes the algorithms implemented within our DIRECTGO toolbox in more detail. For a thorough review, we refer to a recent survey [38].

The derivative-free DIRECT algorithm [39] is an efficient deterministic technique to solve global optimization [36, 79, 94] problems subject to simple box constraints

$$\min_{\mathbf{x} \in D} \quad f(\mathbf{x}), \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ denotes the objective function and the feasible region is an n-dimensional hyper-rectangle $D = [\mathbf{a}, \mathbf{b}] = \{\mathbf{x} \in \mathbb{R}^n : a^j \leq x^j \leq b^j, j = 1, \ldots, n\}$. The objective function $f(\mathbf{x})$ is supposed to be Lipschitz-continuous (with an unknown Lipschitz constant) but can be non-linear, non-differentiable, non-convex, and multi-modal.

The DIRECT algorithm includes three main steps: selection, sampling, and partitioning (subdivision). At the initial iteration, the DIRECT algorithm normalizes the feasible region D to be the unit hyper-cube $\bar{D}$ and refers to the original space D only when evaluating the objective function. Regardless of the dimension, the first evaluation of the objective function is done at the midpoint $\mathbf{c}_1 \in \bar{D}$ (see the left panel of Fig. 1). Then DIRECT selects $\bar{D}$ and samples at $\mathbf{c}_1 \pm \delta e^j, j = 1, \ldots, n$, where e^j is the jth unit vector and δ is equal to one-third of the maximum side length of $\bar{D}$. The subdivision procedure in DIRECT is based on n-dimensional trisection along all longest dimensions (sides). When several dimensions have the maximum side length, DIRECT starts trisection from the dimension with the lowest w^j and continues to the highest [38, 39]. Here w^j is defined as the best function values sampled along dimension j

$$w^j = \min\{f(\mathbf{c}_i + \delta_i \mathbf{e}^j), f(\mathbf{c}_i - \delta_i \mathbf{e}^j)\}, \tag{2}$$

where $\mathbf{c}_i$ is the center of the hyper-rectangle $\bar{D}_i$, and $j \in M -$ set of dimensions with the maximum side length. Figure 1 illustrates the DIRECT algorithm's selection, sampling, and subdivision (trisection) for a two-dimensional *Rosenbrock* test function.
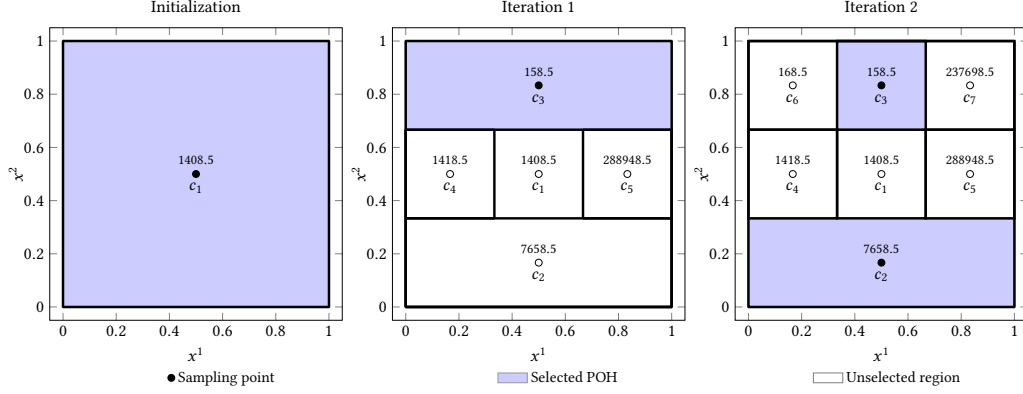

Fig. 1. Illustration of selection, sampling, and subdivision (trisection) used in the original DIRECT algorithm [39] on a two-dimensional *Rosenbrock* test function in the first two iterations.

The selection procedure at the initial step is trivial as we have only one candidate $\bar{D}$. To formalize the selection of potentially optimal hyper-rectangles (POHs) in the future iterations, we define the current partition at the iteration k

$$\mathcal{P}^k = \{\bar{D}_i^k : i \in \mathbb{I}^k\},$$

where $\bar{D}_i^k = [\mathbf{a}_i, \mathbf{b}_i] = \{\mathbf{x} \in \mathbb{R}^n : 0 \le a_i^j \le x^j \le b_i^j \le 1, j = 1, \ldots, n, \forall i \in \mathbb{I}^k\}$ and $\mathbb{I}^k$ is the index set identifying the current partition $\mathcal{P}^k$. The next partition $\mathcal{P}^{k+1}$ is obtained after the subdivision of the selected POHs from the current partition $\mathcal{P}^k$. DIRECT assesses the potentiality based on the lower bound estimates for the objective function f over each hyper-rectangle $\bar{D}_i^k$ as stated in Definition 2.1.

Definition 2.1. (Potentially optimal hyper-rectangle) Let $\mathbf{c}_i^k$ denote the center sampling point and δ_i^k be a measure of the hyper-rectangle $\bar{D}_i^k$. Let $\varepsilon > 0$ be a positive constant and $f_{\min}$ be the best currently found value of the objective function. A hyper-rectangle $\bar{D}_j^k, j \in \mathbb{I}^k$ is said to be potentially optimal if there exists some rate-of-change (Lipschitz) constant $\tilde{L} > 0$ such that

$$f(\mathbf{c}_j^k) - \tilde{L}\delta_j^k \quad \le \quad f(\mathbf{c}_i^k) - \tilde{L}\delta_i^k, \quad \forall i \in \mathbb{I}^k, \tag{3}$$

$$f(\mathbf{c}_j^k) - \tilde{L}\delta_j^k \quad \le \quad f_{\min} - \varepsilon|f_{\min}|, \tag{4}$$

where the measure of the hyper-rectangle $\bar{D}_i^k$ is

$$\delta_i^k = \frac{1}{2}\|\mathbf{b}_i^k - \mathbf{a}_i^k\|_2. \tag{5}$$

The hyper-rectangle D_j^k is potentially optimal if the lower Lipschitz bound for the objective function computed by the left-hand side of (3) is the smallest one with some positive constant $\tilde{L}$ among the hyper-rectangles of the current partition $\mathcal{P}^k$. In (4), the parameter ε is used to protect from an excessive refinement of the local minima [39, 60]. Authors obtained good results for ε values ranging from 10^{-3} to 10^{-7} in [39].
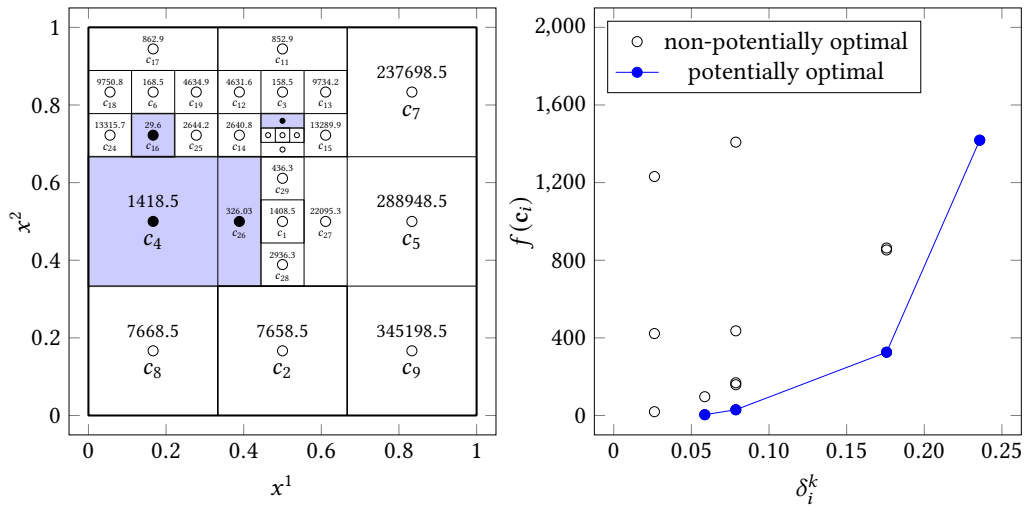
Fig. 2. Visualization of selected potentially optimal rectangles in the fifth iteration of the `DIRECT` algorithm on a two-dimensional *Rosenbrock* test problem.

A geometric interpretation of the selection procedure is given on the right panel of Fig. 2. Here, each hyper-rectangle is represented as a point. The x-axis shows the measure (δ_i^k) while the y-axis – the objective function value attained at the midpoint (c_i^k) of a certain hyper-rectangle. The hyper-rectangles meeting conditions (3) and (4) are points on the lower-right convex hull (highlighted in blue color). Condition (4) prevents wasting function evaluations on tiny hyper-rectangles where only a negligible improvement can be expected.

Then at each subsequent iteration, `DIRECT` performs a selection of POHs, which are sampled, evaluated, and trisected. Almost all `DIRECT`-type extensions and modifications follow the same algorithmic framework, summarized in Algorithm 1.

Algorithm 1: Main steps of `DIRECT`-type algorithms

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1 **Initialization**. Normalize the search space D to be the unit hyper-rectangle $\bar{D}$, but refer to the original space D when making function calls. Evaluate the objective f at the center point c_1. Set $f_{\min} = f(c_1)$, $c_{\min} = c_1$. Initialize algorithmic performance measures, and *stopping criteria.*

2 **while** *stopping criteria are not satisfied* **do**

3   **Selection**. *Identify* the sets S of POHs (subregions of $\bar{D}$).

4   **Sampling**. For each POH ($\bar{D}_j \in S$) *sample* and *evaluate* the objective function at new domain points. Update $f_{\min}, c_{\min}$, and algorithmic performance measures.

5   **Subdivision**. Each POH ($\bar{D}_j \in S$) subdivide (trisect) and update the partition ($\mathcal{P}$).

6 **end**

7 **Return** $f_{\min}, c_{\min}$, and performance measures.

2.1 DIRECT-type algorithms for box-constrained global optimization

Many different `DIRECT` extensions have been suggested. Most of them focused on improving the selection of POHs, while others introduced new partitioning and sampling strategies. The summary of all box-constrained proposals

considered in the DIRECTGO toolbox is given in Table 2. Most algorithms are based on the trisection of n-dimensional POHs, and just ADC, BIRECT, and both DISIMPL versions use different partitioning strategies. Below we briefly review the DIRECT-type approaches for box-constrained global optimization implemented in the current release of the DIRECTGO toolbox.

Adaptive diagonal curves (ADC) based algorithm with a new two-phase technique balancing local and global information was introduced in [76]. Independently on dimensionality, the ADC algorithm evaluates the objective function at two vertices $\mathbf{a}_i^k$ and $\mathbf{b}_i^k$ of the main diagonal, as shown in Fig. 3. Notice that up to 2^n hyper-rectangles can share the same vertex, leading (in a long sequence) to a smaller number of sampled points than the total number of hyper-rectangles in the current partition. Furthermore, as in the revised version of DIRECT [37], ADC trisects each selected POH along just one of the longest dimensions. Such a diagonal scheme potentially obtains more comprehensive information about the objective function than center-based sampling, which sometimes may take many iterations to find the solution. For example, a hyper-rectangle containing the optimum with a bad function value at the midpoint makes him undesirable for further selection. The ADC algorithm intuitively reduces this chance for both sampling points in the hyper-rectangle containing the optimum solution.
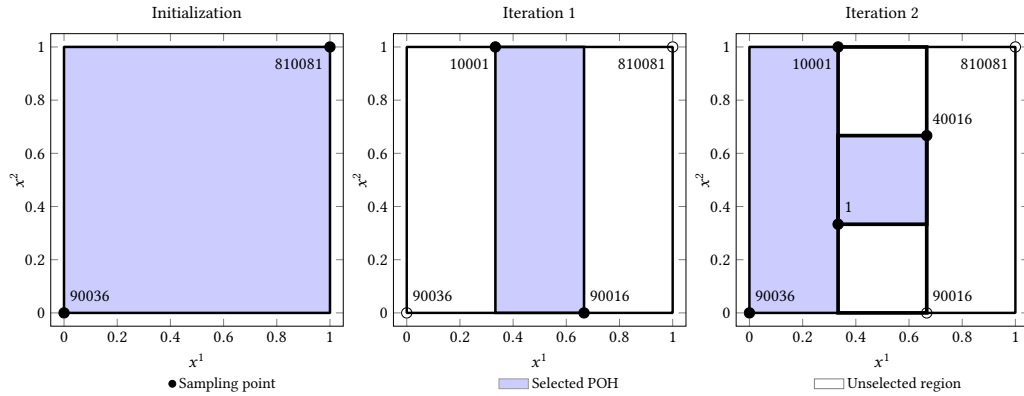

Fig. 3. Illustration of the diagonal trisection strategy introduced in the ADC algorithm on a two-dimensional *Rosenbrock* test function in the first two iterations.

BIRECT (BIsecting RECTangles) [59] is motivated by the diagonal partitioning strategy [76, 77, 79]. As the name suggests, the bisection is used instead of a trisection typical for DIRECT-type algorithms. In BIRECT, the objective function is evaluated at two points on the diagonal equidistant between themselves and a diagonal's vertices, as shown in Fig. 4. Such a sampling strategy enables the reuse of sampling points in descendant hyper-rectangles. Moreover, as in the ADC case, using two-points-based diagonal sampling, potentially more comprehensive information about the objective function is considered than in the center-based sampling.

In DISIMPL [65], simplicial partitions are considered instead of hyper-rectangles. The hyper-cube $\bar{D}$ is partitioned into $n!$ simplices by the standard face-to-face simplicial division based on the combinatorial vertex triangulation at the first iteration. After this, all simplices share the diagonal of the feasible region and have equal hyper-volume. In [65], we proposed two different sampling strategies. Both are included in the DIRECTGO toolbox: i) DISIMPL-C evaluating the objective function at the geometric center of the simplex; ii) DISIMPL-V evaluating the objective function on all unique vertices of the simplex. For box-constrained problems, the total number of initial simplices grows speedily with the
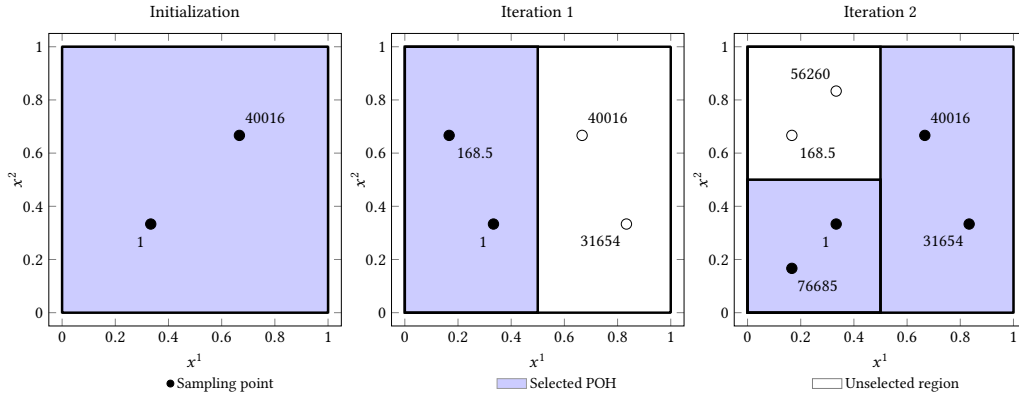
Fig. 4. Illustration of the diagonal bisection strategy used in the BIRECT algorithm on a two-dimensional *Rosenbrock* test function in the first two iterations.

dimension increase. Therefore, DISIMPL effectively can be used only for small box-constrained problems. However, the DISIMPL approach is auspicious (among all DIRECT-type methods) for symmetric optimization problems [65, 66] and problems with linear constraints [67].

In the DIRECT-restart algorithm [19], the authors introduced an adaptive scheme for the ε parameter. Condition (4) is needed to stop the DIRECT from wasting function evaluations on minor hyper-rectangles where only a negligible improvement can be expected. The DIRECT-restart algorithm starts with $\varepsilon = 0$, and the same value for ε is maintained while improvement is achieved. However, if five consecutive iterations have no improvement in the best function value, the search may be stagnated around a local optimum. Therefore, the algorithm switches to $\varepsilon = 0.01$ value to prevent an excessive local search. If the algorithm finds an improvement or fails to see the progress within 50 iterations in this phase, DIRECT-restart switches to $\varepsilon = 0$. Then, if another 50 iterations pass without improvement, this may indicate that the global minimum has been found, and one should work on refining it to higher accuracy.

The authors of MrDIRECT [49] and MrDIRECT$_{075}$ [45] algorithms introduced three different levels to perform the selection procedure:

- At level 2, DIRECT is run as usual, with $\varepsilon = 10^{-5}$.
- At level 1, the selection is limited to only 90% of $\bar{D}_i^k \in \mathcal{P}^k$; 10% of the largest hyper-rectangles are ignored. Here, $\varepsilon = 10^{-7}$ is used.
- At level 0, the selection is limited to 10% of the largest hyper-rectangles (ignored at level 1) using $\varepsilon = 0$.

Both algorithms cycle through these levels using "*W-cycle*": 21011012. The main difference between the proposed algorithms is that MrDIRECT uses fixed $\varepsilon = 10^{-4}$ value at all levels, while MrDIRECT$_{075}$ follows above-mentioned rules.

In [2], the authors relaxed the selection criteria of POHs and proposed an aggressive version of the DIRECT algorithm. Aggressive DIRECT's main idea is to select and divide at least one hyper-rectangle from each group of different diameters (δ_i^k) having the lowest function value. Therefore, using Aggressive DIRECT in the situation presented in Fig. 2, a hyper-rectangle with the slightest measure δ_i^k would also be selected and divided. The aggressive version performs more function evaluations per iteration than other DIRECT-type methods. From the optimization point of view, such an approach seems less favorable since it "wastes" function evaluations by exploring unnecessary (non-potentially optimal) hyper-rectangles. However, such a strategy is much more appealing in a parallel environment, as was shown

in [28, 29, 31, 98]. Note that the authors did not specify which hyper-rectangle should be selected from the same group (δ_i^k) if more than one with identical objective function values exist. Thus, the hyper-rectangle with the larger index value was selected in our implementations.

In [25], the algorithm named `DIRECT-l` was proposed. In most `DIRECT`-type algorithms, the measure of the hyper-rectangle is calculated by a half-length of a diagonal (see (5)). In `DIRECT-l`, this measure is evaluated by the length of its longest side. This measure corresponds to the infinity norm and allows the `DIRECT-l` algorithm to group more hyper-rectangles with the same measure. Thus, there are fewer different measures, so fewer POHs are selected Moreover, with `DIRECT-l` at most one hyper-rectangle selected from each group, even if there is more than one POH in the same group. Such a strategy allows a reduction in the number of divisions within a group. Once again, the same rule is adapted [88] to determine which hyper-rectangle to select from several possible ones.

In [22], the authors concluded that the original `DIRECT` algorithm is sensitive to the objective function's additive scaling. Additionally, the algorithm does not operate well when the objective function values are large enough. The authors proposed a scaling of function values by subtracting the median (f_{median}) of the collected function values to overcome this. `DIRECT-m` replaces the equation (4) in Definition 2.1 to:

$$f(\mathbf{c}_j) - \tilde{L}\delta_j \le f_{\min} - \varepsilon|f_{\min} - f_{\mathrm{median}}|. \tag{6}$$

Similarly, in [46], the authors extended the same idea in `DIRECT-a` to reduce the objective function's additive scaling. Instead of the median value, the authors proposed to use the average value (f_{average}) at each iteration

$$f(\mathbf{c}_j) - \tilde{L}\delta_j \le f_{\min} - \varepsilon|f_{\min} - f_{\mathrm{average}}|. \tag{7}$$

Another extension of the `DIRECT` algorithm was proposed in [27]. The authors introduced `glbSolve-sym` (`glbSolve-sym2`) as `DIRECT` extensions for symmetric Lipschitz continuous functions. When solving symmetric optimization problems, there exist equivalent subregions in the hyper-rectangle. The algorithm determines which hyper-rectangles can be safely discarded, considering the problem's symmetrical nature, and avoids exploration over equivalent subregions.

In the `PLOR` algorithm [56], the set of POHs is reduced to just two, corresponding to the first and last point on the Pareto front (see the right panel in Fig. 2). Therefore, only hyper-rectangles with the lowest function value and the most extensive measure, breaking ties in favor of a better center-point function value, are selected.

Our recent extension, `DIRECT-GL` [88], introduced a new approach to identifying the extended set of POHs. Here, using a novel two-step-based strategy, the set of the best hyper-rectangles is enlarged by adding more medium-measured hyper-rectangles with the smallest function value at their centers and, additionally, closest to the current minimum point. The first step of the selection procedure forces the `DIRECT-GL` algorithm to work more globally (compared to the selection used in `DIRECT` [39]). In contrast, the second step assures a faster and broader examination around the current minimum point. The original `DIRECT-GL` version performs a selection of POHs in each iteration twice [88], and the algorithm separately handles the found independent sets G (using Definition 2 from [88] - `DIRECT-G`) and L (using Definition 3 from [88] - `DIRECT-L`). Following the same trend from [93], the version used in this paper slightly differs compared to [88]. In the current version of `DIRECT-GL`, identifying these two sets is performed in succession, and the unique union of these two sets ($S = G \cup L$) is used in Algorithm 1, Line 3. This modification was introduced to reduce the data communication between the computational units in the parallel algorithm version [83]. At the same time, we found that this way modified `DIRECT-GL` was, on average, more effective than the original one.

Several globally biased (Gb-) versions of DIRECT-type algorithms were introduced and investigated [60, 61]. Proposed approaches are primarily oriented for solving extremely difficult global optimization problems and contain a phase that constrains itself to large subregions. The introduced step performs until a sufficient number of divisions of hyper-rectangles near the current best point is done. Once those subdivisions around the current best minima point are performed, the neighborhood contains only small measure hyper-rectangles and all larger ones located far away from it. Therefore, the two-phase strategy makes the DIRECT-type algorithms examine larger hyper-rectangles and return to the general phase only when an improved minimum is obtained. The proposed globally biased strategy is combined with glbSolve, BIRECT, DISIMPL-C, and DISIMPL-V algorithmic frameworks within our DIRECTGO toolbox.

Finally, three different hybridized DIRECT-type algorithms are proposed (DIRECT-rev [37], DIRMIN [50], BIRMIN [61]). In our implementation, all algorithms are combined with the same local search routine – *fmincon*. The DIRMIN algorithm suggests running a local search starting from the midpoint of every POH. However, such an approach likely generates more local searches than necessary, as many start points will converge to the same local optimum. The other authors of the DIRECT-rev and BIRMIN algorithms tried to minimize the usage of local searches. They suggested using *fmincon* only when some improvement in the best current solution is obtained. The authors in [37] additionally incorporated the following two enhancements. First, in the DIRECT-rev algorithm, selected hyper-rectangles are trisected only on one longest side. Second, only one POH is selected if several equally good exist (the same measure and objective values) in Definition 2.1. We have applied the same rule from [88] to determine which hyper-rectangle to select from several ones when needed.

2.2 DIRECT-type algorithms for generally constrained global optimization

The original DIRECT algorithm [39] only solves optimization problems with the variables' bounds. In this subsection, we consider a generally constrained global optimization problem of the form:

$$\min_{\mathbf{x} \in D} f(\mathbf{x})$$
$$\text{s.t. } \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \tag{8}$$
$$\mathbf{h}(\mathbf{x}) = \mathbf{0},$$

where $f : \mathbb{R}^n \to \mathbb{R}$, $\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^m$, $\mathbf{h} : \mathbb{R}^n \to \mathbb{R}^r$ are (possibly non-linear) continuous functions. The feasible region is a non-empty set, consisting of points that satisfy all constraints, i.e., $D^{\text{feas}} = D \cap \Omega \neq \emptyset$, where $\Omega = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0}\}$. As for the box-constrained problems, it is also assumed that the objective and all constraint functions are Lipschitz-continuous (with unknown Lipschitz constants) but can be non-linear, non-differentiable, non-convex, and multi-modal.

The first DIRECT-type algorithm for problems with general constraints was introduced in [37]. Finkel in [21] investigated three different constraint handling schemes within the DIRECT framework. The comparison revealed various disadvantages of the initial proposals. Recently, various new promising extensions for general global optimization problems were introduced (see, e.g., [4, 13, 44, 69, 70, 89] and the references given therein). Below we briefly review approaches implemented in the current release of the DIRECTGO toolbox (see Table 1).

An exact L1 penalty approach DIRECT-L1 [20] is transforming the original constrained problem (8) in the form:

$$\min_{\mathbf{x} \in D} f(\mathbf{x}) + \sum_{i=1}^{m} \max\{\gamma_i g_i(\mathbf{x}), 0\} + \sum_{i=1}^{r} \gamma_{i+m} |h_i(\mathbf{x})|, \tag{9}$$

Table 2. Summary of main characteristics of DIRECT-type algorithms for box-constrained global optimization

Step / **Alg.**	*Partitioning scheme*	*Sampling scheme*	*Selection of POH & comments on additional steps, if any*	*Input param.*
`Aggressive DIRECT`	Hyper-rectangular partitions-based on n-dimensional trisection	Samples midpoints of the hyper-rectangles	Relaxed criteria of POH selection. At each iteration, the algorithm selects and divides the best hyper-rectangles of each size (δ_i^k).	No input parameters
`DIRECT-G`			Uses enhanced global selection (Definition 2 in [88]).	
`DIRECT-L`			Uses enhanced local selection (Definition 3 in [88]).	
`DIRECT-GL`			Uses the unique union of two sets obtained using enhanced global and local selection (Definitions 2 and 3 [88]).	
`DIRECT`			Uses Definition 2.1	Balance parameter ϵ
`DIRECT-restart`			Uses two different ε values during the selection: 0 if there is an improvement in the solution, and 0.01 otherwise.	
`DIRECT-m`			Uses the median value f_{median} in (6).	
`DIRECT-l`			Uses the infinity norm in (5) and selects at most one POH from each group having the same measure (δ_i^k)	
`DIRECT-rev`	Hyper-rectangular partitions-based on 1-dimensional trisection		Selects at the most one POH from each group of (δ_i^k). Additional minimization procedure `fmincon` is employed.	
`DIRECT-a`	Hyper-rectangular partitions-based on n-dimensional trisection		Uses the average value f_{average} in Eq. (7).	
`DIRMIN`			`fmincon` is performed from each selected POH.	
`PLOR`			The set of POH is reduced to just two: with the maximal ($\delta_{\max}^k$) and the minimal ($\delta_{\min}^k$) measures.	
`glbSolve`			Uses the function *conhull* to return all points on the convex hull, even redundant ones. *conhull* is based on the extended version of the GRAHAMSHULL [73] algorithm.	
`glbSolve-sym`			Discards unnecessary hyper-rectangles for symmetric functions.	
`glbSolve-sym2`				
`MrDIRECT`			Performs the selection of POH on three different sets ("levels"). `MrDIRECT`$_{075}$ uses different ε values at each level.	
`MrDIRECT`$_{075}$				
`Gb-glbSolve`			Uses an adaptive scheme for balancing the local and global search. Local minimization procedure `fmincon` is embedded into the `BIRMIN` algorithm.	
`Gb-BIRECT`	Hyper-rectangular partitions-based on 1-dimensional bisection	Samples hyper-rectangle at two points lying on diagonals		
`BIRMIN`				
`BIRECT`				
`ADC`		Sample hyper-rectangle at two vertices	Uses an adaptive scheme for balancing the local and global search.	
`DISIMPL-C`	Simplicial partitions-based on n-dimensional trisection	Samples midpoints of the simplices		
`GB-DISIMPL-C`			Uses an adaptive scheme for balancing the local and global search.	
`GB-DISIMPL-V`		Samples at vertices of the simplices		
`DISIMPL-V`				

where γ_i are penalty parameters. Experiments in [21] showed promising results of this approach. Nevertheless, the biggest drawback is the users' requirement to set penalty parameters for each constraint function manually. In practice, choosing penalty parameters is an essential task and can significantly impact the algorithm's performance [21, 44, 66, 67, 89].

In [89], we have introduced a new DIRECT-type extension based on the DIRECT-GL [88] algorithm. The new DIRECT-GLce algorithm uses an auxiliary function approach that combines objective and constraint functions and does not require penalty parameters. The DIRECT-GLce algorithm works in two phases, where during the first phase, the algorithm finds feasible points and in the second phase improves a feasible solution. A separate step for handling infeasible initial points is beneficial when the feasible region is small compared to the entire search space. In the first phase, DIRECT-GLce samples the search space and minimizes the sum of constraint violations, i.e.:

$$\min_{\mathbf{x} \in D} \varphi(\mathbf{x}), \tag{10}$$

where

$$\varphi(\mathbf{x}) = \sum_{i=1}^{m} \max\{g_i(\mathbf{x}), 0\} + \sum_{i=1}^{r} |h_i(\mathbf{x})|. \tag{11}$$

The algorithm works in this phase until at least one feasible point ($\mathbf{x} \in D_{\varepsilon_\varphi}^{\text{feas}}$) is found, where

$$D_{\varepsilon_\varphi}^{\text{feas}} = \{\mathbf{x} : 0 \leq \varphi(\mathbf{x}) \leq \varepsilon_\varphi, \mathbf{x} \in D\}. \tag{12}$$

The ε_φ is a small user-specified tolerance for the sum of constraint functions Eq. (11). When feasible points are located, the effort is switched to improve the feasible solutions. In the second phase, DIRECT-GLce uses the transformed problem (8):

$$\min_{\mathbf{x} \in D} f(\mathbf{x}) + \tilde{\xi}(\mathbf{x}, f_{\min}^{\text{feas}}),$$

$$\tilde{\xi}(\mathbf{x}, f_{\min}^{\text{feas}}) = \begin{cases} 0, & \mathbf{x} \in D_{\varepsilon_\varphi}^{\text{feas}} \\ 0, & \mathbf{x} \in D_{\varepsilon_{\text{cons}}}^{\inf} \\ \varphi(\mathbf{x}) + \Delta, & \text{otherwise,} \end{cases} \tag{13}$$

where

$$D_{\varepsilon_{\text{cons}}}^{\inf} = \{\mathbf{x} : f(\mathbf{x}) \leq f_{\min}^{\text{feas}}, \varepsilon_\varphi < \varphi(\mathbf{x}) \leq \varepsilon_{\text{cons}}, \mathbf{x} \in D\}, \tag{14}$$

and $\varepsilon_{\text{cons}}$ is a small tolerance for constraint function sum, which automatically varies during the optimization process. An auxiliary function $\xi(\mathbf{x}, f_{\min}^{\text{feas}})$ depends on the sum of the constraint functions and the parameter $\Delta = |f(\mathbf{x}) - f_{\min}^{\text{feas}}|$, equal to the absolute difference between the best feasible function value found so far ($f_{\min}^{\text{feas}}$) and the objective value at an infeasible center point. The purpose of the parameter Δ is to forbid the convergence to infeasible regions by penalizing the objective value at infeasible points. In such a way, the formulation (13) does not require any penalty parameters and determines the convergence of the algorithm to a feasible solution. The value of $\xi(\mathbf{x}, f_{\min}^{\text{feas}})$ is updated when a smaller value of $f_{\min}^{\text{feas}}$ is found. This way, the new DIRECT-GLce algorithm divides more hyper-rectangles with center points lying close to the boundaries of the feasible region, i.e., the potential solution.

The proposed `DIRECT-GLce` algorithm has two extensions: The first one is `DIRECT-GLc` (see Table 1), which is a simplified version of `DIRECT-GLce` and instead of (13) minimizes the transformed problem:

$$\min_{\mathbf{x} \in D} f(\mathbf{x}) + \xi(\mathbf{x}, f_{\min}^{\text{feas}}),$$

$$\xi(\mathbf{x}, f_{\min}^{\text{feas}}) = \begin{cases} 0, & \mathbf{x} \in D_{\varepsilon_\varphi}^{\text{feas}} \\ \varphi(\mathbf{x}) + \Delta, & \text{otherwise,} \end{cases} \tag{15}$$

Experimental investigation in [89] showed that the algorithm has the most wins in this comparison and can solve about 50% of the problems with the highest efficiency. Unfortunately, the `DIRECT-GLc` algorithm's efficiency decreases, solving more challenging problems (with non-linear constraints and $n \geq 4$), where `DIRECT-GLce` is significantly better. Therefore, `DIRECT-GLc` should be used only for simpler optimization problems (with linear constraints and $n \leq 4$). The second extension of the `DIRECT-GLce` algorithm is `DIRECT-GLce-min`, where the algorithm is incorporated with `MATLAB` optimization solver `fmincon`. In [89], we observed that embedding a local minimization procedure into `DIRECT-GLce-min` (see Table 1) significantly reduces the total number of function evaluations compared to `DIRECT-GLce` and can significantly improve the quality of the final solution.

2.2.1 `DIRECT`*-type algorithms for linearly constrained global optimization.* Let us note that all previously described algorithms for a generally constrained problem can be directly applied to solve linearly constrained problems. In this section, we consider optimization problems with only linear constraints.

In [67], we have extended the original simplicial partitioning-based `DISIMPL` algorithm [65, 66] for such problems with linear constraints. Simplices may cover a search space defined by linear constraints. Therefore, a simplicial approach may tackle such linear constraints very subtly. In such a way, the new algorithms (`Lc-DISIMPL-C` and `Lc-DISIMPL-V`) [67] perform the search only in the feasible region, in contrast to other `DIRECT`-type approaches. Nevertheless, the authors in [67] showed that the feasible region's calculation requires solving $2n + m$ linear n-dimensional systems, and such operation is exponential in complexity. Therefore, the proposed algorithm can be effectively used for relatively small n and m values.

2.3 DIRECT-type algorithms for problems with hidden constraints

Optimization problems with hidden constraints often occur when the objective function is not defined everywhere [10]. Typical examples of such situations are the simulation crashes [17] and failure of computations within the objective function [9, 11, 15, 82]. As in [10, 17], we call these internal to f constraints "hidden constraints" and assume that f fails to return a value when evaluated at $\mathbf{x} \notin D^{\text{feas}}$. Some authors alternatively may use other terms like "crash," "unknown," "unspecified," and "forgotten" constraints [1, 17].

In this subsection, we consider the solution to the constrained global optimization problem:

$$\min_{\mathbf{x} \in D^{\text{feas}}} f(\mathbf{x}), \tag{16}$$

where $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ denotes an extended real-valued, most likely "black-box" objective function. A priori an unknown feasible region D^{feas} is defined as a non-empty set

$$D^{\text{feas}} = D \setminus D^{\text{hidden}} \neq \emptyset,$$

and D^{hidden} are not given by explicit formulae hidden constraints. Such a problem formulation leads to a complex and analytically undefined feasible region. Hidden constraints are typically handled by returning NaN or ∞ evaluating

the objective function at $\mathbf{x} \notin D^{\text{feas}}$. Therefore, using NaN hyper-rectangles with an infeasible center point would not be selected as potential optimal at all [84]. In the case of ∞ (or any other high value), they would be left unexplored as long as there are the same size hyper-rectangles with feasible centers [21, 84]. Unfortunately, most DIRECT-type algorithms cannot be directly (without any modifications) applied for the problem's (16) solution. In the current version of the DIRECTGO toolbox, four such algorithms are available (see Table 1).

One of the first proposed modifications for such problems was the barrier method (DIRECT-Barrier) [24]. The DIRECT-Barrier is relatively straightforward and assigns a predefined high value to infeasible hyper-rectangles. However, such an approach produces other well-known problems discussed and reviewed by a few authors [21, 66, 89]. The main issue is that the barrier approach makes exploration around the edges of feasibility very slow. Significant penalties used by the barrier method ensure that no infeasible hyper-rectangle can be potentially optimal as long as there is the same measure hyper-rectangle with the feasible center midpoint. For DIRECT-Barrier, the priority is the examination of regions where feasible points are found already. Another critical issue concluded in [21] is that hyper-rectangles, even with the sizeable feasible region, will not be explored in a reasonable number of function evaluations. To sum up, the barrier approach is not the best fit for the problem (16).

The second DIRECT-type approach for hidden constraints is based on Neighbourhood Assignment Strategy (NAS) [24]. DIRECT-NAS's main idea is to assign the value at infeasible point $\mathbf{x}^{\text{inf}} \notin D^{\text{feas}}$ relative to the objective values attained in the feasible points from the neighborhood of $\mathbf{x}^{\text{inf}}$. DIRECT-NAS iterates over all infeasible midpoints by creating surrounding hyper-rectangles around them by keeping the same center points in every iteration. These hyper-rectangles are increased by doubling the length of each dimension. If more than one feasible center point inside the enlarged region, DIRECT-NAS assigns the smallest function value to the infeasible midpoint plus a small epsilon $f(\mathbf{x}^{\text{feas}}) + \epsilon f(\mathbf{x}^{\text{feas}})$, where $\epsilon = 10^{-6}$ was proposed to use. If inside the enlarged region has no feasible points, DIRECT-NAS assigns the largest objective function value found so far $f_{\max} + \lambda$, where $\lambda = 1$ was proposed to use. This strategy does not allow the DIRECT-NAS algorithm to move beyond the feasible region by penalizing infeasible midpoints with large values. However, the algorithm's principal concern is the slow convergence caused by many additional calculations.

Another recent idea to handle hidden constraints within the DIRECT framework is to use a subdividing step for infeasible hyper-rectangles. The proposed subDIRECT-Barrier [58] incorporates the previously mentioned barrier approach techniques. Specifically, if the center point is identified as infeasible, then subDIRECT-Barrier assigns a considerable penalty value to it. An extra subdividing step is performed only in specific iterations, during which all infeasible hyper-rectangles are identified as potentially optimal and subdivided together with others POHs. The sub-dividing step can decompose the boundaries of the hidden constraints quite efficiently. Still, subDIRECT-Barrier has several apparent drawbacks. The algorithm performance depends on when (how often) the subdividing step is performed. Therefore, new subdivisions can grow drastically, especially for higher dimensionality problems.

The most recent version for hidden constraints DIRECT-GLh [84] is based on our previous DIRECT-GL [88] algorithm. For hyper-rectangles with infeasible midpoints, DIRECT-GLh assigns a value depending on how far the center is from the current best minima $\mathbf{x}_{\min}$. Such a technique does not require any additional computation. Simultaneously, distances from the $\mathbf{x}_{\min}$ point are already known, as they are used to selecting potential optimal hyper-rectangle schemes adapted from DIRECT-GL [88]. In such a way, DIRECT-GLh does not penalize infeasible hyper-rectangles with large values (as was suggested by previous proposals), which are close to the $\mathbf{x}_{\min}$ and assure a faster and more comprehensive examination of hidden regions. Moreover, this approach employs additional procedures to efficiently handle infeasible initial points (see [84] for experimental justification).

2.4   Implementation of `DIRECT`-type algorithms within `DIRECTGO`

2.4.1   Sequential implementation of the algorithms. The performance of `DIRECT`-type algorithms highly depends on computer implementation. Most publicly available `DIRECT` implementations (see, e.g., `DIRECT v4.0` [20] and `glbSolve` [6]) use static data memory management [6, 20, 24]. In the "Impelmentation" column of Table 1, we provide information on which data structures were used in our implementations and whether a particular algorithm was implemented in parallel. Below we look at the main advantages and disadvantages of each of them.

   With static data management, all information received after the domain partitioning is stored in the contiguous memory blocks. This includes objective and constraint function values, index numbers, center point coordinates, side lengths of hyper-rectangles, and so on. Such implementation can quickly access the elements for further selection, sampling, and subdivision steps. An apparent drawback of the static data structure is unpredictable memory demand due to different characteristics of the optimization problems. Thus many `DIRECT`-type algorithmic implementations use large static arrays to store the current state of the space partitioning. If any array is insufficient to store the required information, this can lead to code failure.

   Another disadvantage of static data structures used in `DIRECT` implementations is that they require unnecessary recalculations in each iteration. One of the essential tasks in the `DIRECT`-type algorithms is the selection step. This step requires sorting all existing hyper-rectangles by the same size of diameter. Such sorting becomes especially inefficient when the optimization process is longer and the amount of data gets large, e.g., for higher dimensionality problems or when a solution with high accuracy is required.

   In [30], the authors proposed using dynamic data structures. Information received after space partitioning is sorted by hyper-rectangle diameters and stored in columns. All rectangles of the same diameter are stored in the column in any order. In [30], the authors mentioned the idea of sorting columns by function values in descending order or inserting all new data in sorted sequences separately. However, any of these ideas have not been investigated further. With dynamic data structures, the selection step is much more efficient. It can be performed only in the set consisting of the best function values from each column. Such implementation saves lots of time compared with the static data structure-based implementation.

   In [93], we have compared two different implementations (static and dynamic) of the same `DIRECT-GLce` algorithm. The dynamic implementation of the code required, on average, 62% less total execution time than static-based. The difference was even more significant when the number of function evaluations was high.

   One of the apparent drawbacks of the dynamic data structure is unpredictable columns size. Fully processed POHs must be removed from the previous columns and added to a new/existing column. During the algorithm's execution, there can be many hyper-rectangle diameters. Depending on the dimension of the problem, usually, the initial array is allocated of reasonably large size. If the array provides insufficient size, new blocks of columns will be reallocated as needed. In practice, only a few of these columns need reallocation at any given time.

2.4.2   Parallel implementations of the algorithms. We use the MathWorks official extension to the `MATLAB` language – the Parallel Computing Toolbox [53] for parallel implementations. The Parallel Computing Toolbox provides several parallel programming paradigms [52], like threads, parallel `for`-loops, and SPMD (Single Program Multiple Data). In [93], we concluded that the SPMD-based parallel implementation of the `DIRECT-GLce` is the most efficient and significantly outperforms the other two based on `parfor`-loops.

   Therefore, in the `DIRECTGO` toolbox, parallel implementations are based on the SPMD functionality within the Parallel Computing Toolbox, used to allocate the work across multiple labs in the `MATLAB` software environment. Each lab stores

Fig. 5. Flowchart diagram for the parallel implementations of selected `DIRECT`-type algorithms.

information on its main memory block, and data is exchanged through the message passing over the interconnection network [53]. The master-slave paradigm is used to implement dynamic load balancing. The flowchart of the parallel algorithmic framework is illustrated in Fig. 5. One lab is the master, denoted by lab_1, and the other labs are slaves $lab_i, i = 2, \ldots, \rho$. The master also acts as a slave. Each iteration must be done in a sequence to preserve the determinism.

The master performs the following tasks:

- *The initialization step*: normalizes the domain (D) and evaluates the objective and constraint functions at the center point. Here, only the optimization problem and the information about the domain D are shared with slaves $lab_i, i = 2, \ldots, \rho$.
- *At each iteration*:
  - checks the stopping conditions and informs the slaves if any of them have been met.
  - finds the full set of POHs by performing a selection step considering the combined set of local POHs.
  - splits the full set of POHs among all slaves and itself equally.
  - gives instructions to the slaves having an excess of POHs (in their local memory) to share them with those who have a deficit, including itself.
  - sends or receives POHs according to its instructions.
  - performs the sampling, subdivision, and local selection steps as the slave.
  - receives from slaves the information about their local POHs sets.

The slaves perform the following tasks:

- *At each iteration*:
  - Send or receive POHs, according to the master's instructions.
  - Perform the sampling and subdivision steps sequentially.
  - Perform the selection using the information in their local memory and send local POHs to the master.
  - Terminate when such an instruction from the master is received.

The master lab decides which hyper-rectangles will be sampled and subdivided and how these tasks will be distributed among all available slave labs. Additionally, the master lab is responsible for stopping the algorithm. The master lab also performs load balancing by distributing the selected hyper-rectangles to the rest of the slave labs. When the slave labs ($lab_i, i = 1, \ldots, \rho$) receive tasks from the master lab, each sequentially performs the sampling and subdivision steps. Then finds a local set of POHs and sends local data back to the master lab for the further global selection step. After this, each slave becomes idle until further instructions are received. Suppose any of the termination conditions are satisfied. In that case, all slave labs receive the notification that the master lab has become inactive, and the slave labs will terminate themselves without further messaging. We refer to [93] for a more detailed description and analysis of parallel schemes.

We should note that not all DIRECT-type implementations can use the latter scheme of parallelism. For example, implementations using the *conhull* function, which returns all the points on a convex hull, cannot. To preserve the determinism, only the master should select POHs and have all data stored in its memory. The framework shown in Fig. 5 is inappropriate, and a new one should be developed. The DIRECT-NAS algorithm has an additional expensive constraint handling step not addressed in the proposed parallel scheme. As summarized in Table 1, currently, 17 DIRECT-type algorithms are implemented in parallel within the DIRECTGO toolbox.

3 DIRECTGO TOOLBOX

The sequential and parallel implementation of DIRECT-type algorithms presented in the previous sections forms the basis for our DIRECTGO toolbox. The toolbox consists of two main parts:

- **DIRECTGO.mltbx** - MATLAB toolbox package containing implementations of DIRECT-type algorithms (from Table 1), including an extensive DIRECTGOLib v1.0 library of the box and generally constrained test and practical engineering global optimization problems, often used for benchmarking DIRECT-type algorithms.
- **DIRECTGO.mlappinstall** - A single MATLAB app installer containing everything necessary to install and run the DIRECTGO toolbox, including a graphical user interface (GUI).

3.1 Graphical user interface

After installation (using **DIRECTGO.mlappinstall**), DIRECTGO can be launched from MATLAB **APPS**, located in the toolbar. The graphical interface of the main DIRECTGO toolbox window is shown in Fig. 6. Application is divided into three main parts: i) selection of the problem's type from DIRECTGOLib v1.0; ii) setting up an optimization problem and algorithmic options; iii) selection of DIRECT-type algorithm, his implementation, and convergence plot of obtained results.

The first step is to specify the objective and constraint functions, loading them from the integrated DIRECTGOLib v1.0 library or selecting them from other sources. Examples of the structure needed are present. All test problems from the DIRECTGOLib v1.0 library have up to three key features: i) known globally optimal solutions, ii) a complete

description of the problem, including objective and constraint functions (if any), and iii) problem visualization (only for two-dimensional problems).

After selecting the optimization problem, the second step is to set up the bound constraints for each variable. First, the user needs to specify the algorithm and the type of implementation. Two implementations are based on different data structures (static and dynamic), and the third is a parallel version of the algorithm. For simplicity, some toolbox options are set to default values and not displayed in the GUI but can be changed in the toolbox settings. After the termination, the **Results** part displays the final solution and performance metrics. Additionally, the convergence process is shown in the **Convergence status** part.

3.2 MATLAB toolbox

After installation of the MATLAB toolbox (using **DIRECTGO.mltbx**), all implemented DIRECT-type algorithms and test problems can be freely accessed in the command window of MATLAB. Unlike using GUI, algorithms from the command line require more programming knowledge, and configurations must be done manually. All algorithms can be run using the same style and syntax:

```
1. f_min = algorithm(P);
2. f_min = algorithm(P, OPTS);
3. f_min = algorithm(P, OPTS, D);
4. [f_min, x_min]  = algorithm(P, OPTS, D);
5. [f_min, x_min, history]  = algorithm(P, OPTS, D);
```

The left side of the equations specifies the output parameters. After the termination, the algorithm returns the best objective value (f_min), solution point (x_min), and history of the algorithmic performance during all iterations (history). The information presented here is the iteration number, the total number of objective function evaluations, the current minimum value, and execution time.

The algorithm name (algorithm) and at least one input parameter are needed to specify on the right side. The first one is the problem structure (P) consisting of an objective function:

```
>> P.f = 'objfun';
```

If the problem involves additional constraints, they also must be specified:

```
>> P.constraint = 'confun';
```

The second parameter (OPTS) customizes the default algorithmic settings. The third parameter (D) is used to specify the bound constraints for each variable (see Eq. (1)).

4 EXPERIMENTAL INVESTIGATION OF DIRECT-TYPE ALGORITHMS IN THE DIRECTGO TOOLBOX

This section presents the performance evaluation of DIRECT-type algorithms on test and engineering design problems from the DIRECTGOLib v1.0 [86, 91]. The DIRECTGOLib v1.0 library consists of the box and generally constrained test and practical engineering global optimization problems for various DIRECT-type algorithms benchmarking. Experimental results presented in this section are also available in digital form in the Results/TOMS directory of the Github repository https://github.com/blockchain-group/DIRECTGO [85]). The most recent version of DIRECTGOLib v1.1 [87, 92] has a

Fig. 6. The graphical user interface (GUI) of `DIRECTGO` toolbox.

few additional test functions introduced in other parallel studies but has not been considered in this article. Despite this, our vision is to develop `DIRECTGOLib` further so that all algorithms can use the latest version of `DIRECTGOLib` without any additional preparations.

We distinguish the following classes (types) of global optimization problems:

- **BC** – **B**ox-**C**onstrained problems;
- **LC** – **L**inearly-**C**onstrained problems;
- **GC** – **G**enerally-**C**onstrained problems.

A summary of all optimization problems in `DIRECTGOLib v1.0` and their properties is given in Appendix A, Table 13. We note that some test problems have several variants, e.g., *Bohachevsky*, *Shekel*, and some of them, like *Alpine*, *Csendes*, and *Griewank*, can be used by changing the problem's dimensionality. We used the following dimensions in our experimental setting: $n = 2, 5, 10, 15$. For some test problems, the second dimension ($n = 2$) was skipped because the problem was then too easy to solve, and sometimes we skipped $n = 15$ because the resulting problem was too hard that none of the algorithms were able to solve it. The fourth column in Table 13 indicates the exact dimensions used for all test problems.

All computations were carried out on a 6-core computer with 8th Generation Intel R Core^{TM} i7-8750H @ 2.20GHz Processor, 16 GB of RAM, and `MATLAB R2020b`. Performance analysis was carried out using physical cores only and disabled hyper-threading.

All global minima f^* are known for all test problems. Therefore, the investigated algorithms were stopped when it was generated such the point **x** with whom the percent error

$$pe = 100\% \times \begin{cases} \frac{f(\mathbf{x}) - f^*}{|f^*|}, & f^* \neq 0, \\ f(\mathbf{x}), & f^* = 0, \end{cases} \tag{17}$$

is smaller than the tolerance value ε_{pe}, i.e., $pe \leq \varepsilon_{pe}$. Additionally, we stopped the tested algorithms when the number of function evaluations exceeded the prescribed maximal limit (equal to 2×10^6) or took more than $43,000.00$ seconds.

In any of these situations, the final result is set to 2×10^6 to further process results. Two different values for ε_{pe} were considered: 10^{-2}, 10^{-8}. By default, algorithms were tested using the $\varepsilon_{\text{pe}} = 10^{-2}$ value. Algorithms incorporating additional schemes to speed up the solution's refinement have been tested using the $\varepsilon_{\text{pe}} = 10^{-8}$ value.

Additionally, we analyze and compare the algorithms' performance by applying the data profiles [57] to the convergence test (17). The data profile is a popular and widely used tool for benchmarking and evaluating the performance of several algorithms (solvers) when run on a large problem set. Benchmark results are generated by running a certain algorithm v (from a set of algorithms $\mathcal{V}$ under consideration) for each problem u from a benchmark set $\mathcal{U}$ and recording the performance measure of interest. The performance measure could be, for example, the number of function evaluations, the computation time, the number of iterations, or the memory used. We used a number of function evaluations and the execution (computation) time criteria.

The data profiles provide the percentage of problems that can be solved with a given budget of the desired performance measure. The data profile is defined

$$\lambda_v(\alpha) = \frac{1}{card(\mathcal{U})} \text{size} \left\{ u \in \mathcal{U} : t_{u,v} \leq \alpha \right\}, \tag{18}$$

where $t_{u,v} > 0$ is the number of performance measure required to solve problem u by the algorithm v, and $card(\mathcal{U})$ is the cardinality of $\mathcal{U}$. In our case, the $\lambda_v(\alpha)$ shows the percentage of problems that can be solved within α function evaluations, or seconds.

In the experimental studies, the developed DIRECT-type algorithms (within the DIRECTGO toolbox) were compared among themselves and with three TOMLAB DIRECT-type solvers:

- TOMLAB/glbSolve [35] – implementation of the DIRECT algorithm [39];
- TOMLAB/glcSolve [35] – implementing an extended DIRECT version [37, 39] capable of handling linear and non-linear constrained problems;
- TOMLAB/glcCluster [35] – implementation of the DIRECT algorithm [39], hybridized with local search subroutine and clustering techniques.

We note that the TOMLAB/glcCluster algorithm has a large number and different input parameters that may significantly impact the algorithm's performance. Even a parameter such as the maximum allowed number of function evaluations can significantly impact the algorithm's performance. Our aim was not to find the optimal parameters values, as this is a complex process, but to investigate how these algorithms compare using the default values (provided by TOMLAB software developers). When the algorithm reaches the default limit for the maximum number of function evaluations (M_{max}) set in the default parameters, we restarted the algorithm using the final status from the previous run ("*warm start*" [35]) with doubled $2M_{\text{max}}$. In such a way, sometimes a default M_{max} value was doubled up to our maximal limit of evaluations 2×10^6 was reached.

The Scripts/TOMS directory of the Github repository (https://github.com/blockchain-group/DIRECTGO) provides four different MATLAB scripts for cycling through all different classes of test problems used in this paper. The constructed scripts can be handy for reproducing the results presented here, as well as for comparison and evaluation of newly developed algorithms.

4.1 Comparison of DIRECT-type algorithms for box constrained optimization

Table 3 summarizes experimental results using $\varepsilon_{\text{pe}} = 10^{-2}$. The smallest number of unsolved problems is achieved using DIRECT-GL (3/81). At the same time, the second, third and fourth best algorithms are TOMLAB/glcCluster (4/81),

Table 3. The performance of DIRECT-type algorithms from DIRECTGO and TOMLAB based on the number of function evaluations ($f_{eval.}$), the total execution time in seconds (*time*), and the total number of iterations (*iter.*) criteria on a set of box-constrained problems (from DIRECTGOLib v1.0) using $\varepsilon_{pe} = 10^{-2}$ in (17).

Algorithm	Avg. # local searches	Failed	Average results			Average results ($n \leq 4$)			Average results ($n \geq 5$)			Median results		
			$f_{eval.}$	time	iter.	$f_{eval.}$	time	iter.	$f_{eval.}$	time	iter.	$f_{eval.}$	time	iter.
DIRECT	–	16/81	452,244	263.29	1,645	135,328	220.05	2,535	638,666	183.98	1,121	7,795	0.61	51
DIRECT-restart	–	23/81	608,719	5,518.88	155	268,291	3,088.88	84	808,971	6,948.29	197	12,861	1.05	48
DIRECT-m	–	27/81	745,865	340.83	2,505	123,565	384.15	2,543	1,111,924	315.35	2,482	17,559	2.91	135
DIRECT-l	–	24/81	627,987	4,486.48	65,377	134,552	952.43	22,558	918,243	6,565.33	90,565	7,185	15.44	437
DIRECT-rev*	3	7/81	223,483	1,971.68	27,093	67,176	437.96	4,081	315,429	2,873.87	40,629	545	0.13	13
DIRECT-a	–	41/81	1,019,956	830.72	4,645	203,905	600.68	3,699	1,499,986	966.03	5,201	2,000,000	285.43	176
DIRMIN*	748	5/81	155,384	18.45	72	67,178	22.73	91	207,271	15.94	61	361	0.04	1
PLOR	–	31/81	775,748	2,584.88	57,574	275,890	2,162.11	39,006	1,069,782	2,833.57	68,496	3,311	1.12	437
glbSolve	–	23/81	624,411	472.42	2,326	135,726	335.40	2,627	911,873	314.68	2,149	20,823	1.16	54
glbSolve-sym	–	36/81	923,592	4,152.72	10,128	467,654	1,288.24	10,426	1,191,790	5,837.70	9,953	199,533	446.61	470
glbSolve-sym2	–	35/81	899,684	5,283.04	10,388	603,737	1,594.43	10,931	1,073,771	7,452.82	10,069	124,961	594.60	355
MrDIRECT	–	18/81	502,032	178.35	2,689	73,156	9.05	373	754,313	277.93	4,051	9,721	0.52	93
MrDIRECT075	–	16/81	477,176	241.40	3,605	69,755	18.71	520	716,835	372.40	5,420	8,547	0.83	103
BIRECT	–	9/81	255,671	1,914.41	6,829	68,112	914.36	2,729	366,000	2,502.68	9,241	2,112	1.28	71
GB-DISIMPL-C	–	46/81	1,156,420	3,903.78	11,887	224,138	1,945.78	16,156	1,704,821	5,055.54	9,376	2,000,000	138.44	24
GB-DISIMPL-V	–	36/81	898,336	19,858.76	2,109	73,335	1,623.49	1,934	1,383,631	30,585.39	2,211	66,257	4,298.97	39
Gb-BIRECT	–	13/81	367,464	2,451.11	20,203	70,721	789.93	7,937	542,019	3,428.28	27,419	5,782	1.56	153
BIRMIN*	1	5/81	125,541	2,575.78	13,106	66,982	1,433.43	6,628	159,987	3,247.76	16,917	322	0.07	21
Gb-glbSolve	–	25/81	671,030	668.70	8,092	137,164	1059.04	15,501	985,069	439.08	3,733	22,541	2.40	69
DISIMPL-C	–	46/81	1,149,469	4,257.54	11,952	215,702	1,979.85	13,649	1,698,744	5,593.43	10,953	2,000,000	126.36	22
DISIMPL-V	–	34/81	844,074	18,265.14	709	67,988	1,436.35	431	1,300,595	28,164.43	872	21,828	667.34	25
ADC	–	30/81	753,474	16,537.93	20,962	74,665	1,768.67	8,999	1,152,774	25,225.73	28,000	8,868	43.91	603
Aggressive DIRECT	–	14/81	475,318	20.71	95	172,708	11.37	88	653,324	26.21	99	65,253	2.34	44
DIRECT-G	–	10/81	310,535	32.85	348	84,905	16.21	309	443,259	42.64	371	9,835	0.45	51
DIRECT-L	–	16/81	430,885	99.07	622	68,918	39.97	362	643,807	133.84	775	9,601	0.52	46
DIRECT-GL	–	3/81	152,505	11.78	99	9,469	0.68	47	236,645	18.30	130	7,737	0.33	36
TOMLAB/glbSolve	–	20/81	534,930	1,421.26	1,676	201,103	1,214.37	2,576	731,298	1,542.98	1,147	13,991	1.89	49
TOMLAB/glcCluster*	21	4/81	116,281	2,202.07	2	68,612	1,390.14	2	148,607	2,760.65	2	10,043	1.31	1

* – a hybrid version of the algorithm, enriched with the local search subroutine

BIRMIN (5/81) and DIRMIN (5/81), hybrid versions enriched with the local search subroutines. In column '**Avg. # local searches**' we report the average number of local searches performed by each hybridized algorithm. Hybridization of the BIRMIN algorithm allows solving more problems compared to, e.g., the globally biased version Gb-BIRECT (12/81). Among traditional DIRECT-type algorithms, the second and third best algorithms are BIRECT and DIRECT-G. Both methods failed to solve (9/81) and (10/81) test problems accordingly.

Furthermore, hybridization significantly reduces the total number of function evaluations (see **Average results** and **Median results** columns). The BIRECT and PLOR were the most effective algorithms among the traditional algorithms based on the median number of function evaluations (see **Median results** column). However, for PLOR, such performance needs to be interpreted correctly. As PLOR restricts POH set to only two hyper-rectangles per iteration, a lower number of function evaluations are required to get closer to the solution for simpler (low-dimensional) problems. However, looking at the average number of function evaluations, even restricted to the simplest subset of problems (see **Average results** ($n \leq 4$)), PLOR performance is among the worst. PLOR has failed on a larger number of simpler test problems than other approaches. In contrast, DIRECT-GL is only in eight place based on the median number of function evaluation criteria but is the only algorithm that solves all simpler ($n \leq 4$) problems and is the best performing algorithm, including hybridized

Fig. 7. Data profiles of DIRECT-type algorithms from DIRECTGO and TOMLAB on the whole set of box-constrained optimization problems from DIRECTGOLib v1.0 using $\varepsilon_{pe} = 10^{-2}$ in (17).

versions. Moreover, on average, DIRECT-GL required approximately 35% percent fewer evaluations of the objective function than the second-best, BIRECT algorithm, among all traditional DIRECT-type algorithms on a class of more challenging problems (see **Average results** ($n \geq 5$)). Not surprisingly, the hybridized TOMLAB/glcCluster and BIRMIN algorithms within this class deliver the best average performance. Compared with the best traditional DIRECT-type algorithm, DIRECT-GL, TOMLAB/glcCluster, and BIRMIN require approximately 37% and 32% fewer evaluations.

Based on the execution time (*time*), DIRECT-GL and Aggressive DIRECT are the best among all traditional algorithms. Aggressive DIRECT does not have a traditional POH selection procedure. Instead, the algorithm selects at least one candidate from each group of different measures. Therefore, the number of selected hyper-rectangles per iteration is larger, especially for higher dimensionality test problems. Consequently, the number of iterations (*iter.*) using Aggressive DIRECT is among the smallest. Overall, DIRECT-GL showed the most promising performance among all tested traditional DIRECT-type algorithms.

The data profiles of all algorithms are shown in Fig. 7. Again, the data profiles confirm that the hybridized algorithms (enriched with fmincon procedure) are more efficient than traditional DIRECT-type approaches. All three versions (DIRECT-rev, DIRMIN, and BIRMIN) can solve about 60% of problems in less than 1, 000 function evaluations (see the left panel of Fig. 7). However, by increasing the maximal budget of function evaluations, which is needed for more challenging problems, the TOMLAB/glcCluster, and traditional DIRECT-GL algorithm outperformed all others, including

Table 4. The performance of selected DIRECT-type algorithms from DIRECTGO and TOMLAB based on the number of function evaluations ($f_{eval.}$), the total execution time in seconds ($time$), and the total number of iterations ($iter.$) criteria on a set of box-constrained problems (from DIRECTGOLib v1.0) using $\varepsilon_{pe} = 10^{-8}$ in (17)

Algorithm	Avg. # local searches	Failed	Average results			Average results ($n \leq 4$)			Average results ($n \geq 5$)			Median results		
			$f_{eval.}$	$time$	$iter.$	$f_{eval.}$	$time$	$iter.$	$f_{eval.}$	$time$	$iter.$	$f_{eval.}$	$time$	$iter.$
DIRECT	−	40/81	1,066,171	918.13	7,823	809,880	1,483.54	17,456	1,216,930	585.54	2,157	1,297,025	268.16	224
DIRECT-restart	−	29/81	778,771	7,840.37	200	333,394	4,377.27	114	1,035,618	10,191.29	252	53,629	6.00	91
DIRECT-rev*	3	15/81	396,246	1,095.13	19,360	200,403	1,145.29	9,595	511,449	1,065.63	25,104	844	0.16	21
DIRMIN*	1,001	12/81	345,763	43.52	164	135,323	33.49	106	469,551	49.41	198	501	0.09	2
glbSolve	−	55/81	1,423,737	1,027.22	9,609	825,086	1,720.33	19,061	1,775,885	619.51	4,050	2,000,000	340.86	1,201
MrDIRECT	−	38/81	996,523	2,021.44	11,177	706,737	1,733.35	21,678	1,166,986	2,190.90	5,001	542,125	66.20	406
MrDIRECT$_{075}$	−	39/81	1,036,760	473.40	6,438	207,944	104.02	2,539	1,524,299	690.68	8,732	1,125,661	141.77	806
BIRMIN*	4	12/81	298,791	4,827.15	18,742	136,309	2,867.45	11,448	394,369	5,979.91	23,033	379	0.06	21
DIRECT-L	−	21/81	572,082	151.41	952	136,742	86.78	695	828,164	189.42	1,104	23,069	1.45	87
DIRECT-GL	−	6/81	277,242	29.66	241	85,123	26.84	252	390,254	31.32	235	28,211	1.17	60
TOMLAB/glcCluster*	76	29/81	753,378	16,307.54	4	338,957	6,959.64	3	990,121	22,553.22	5	66,391	54.86	3

* – a hybrid version of the algorithm, enriched with the local search subroutine

hybridized ones. While DIRECT-GL delivers the best overall performance (based on function evaluations), data profiles in Fig. 7 reveal that other DIRECT-type extensions (PLOR, DIRECT-l, BIRECT, Gb-BIRECT) perform better when the maximal budget of function evaluations is $\leq 10^5$. Moreover, they can solve about 70% of problems (mainly lower dimensionality) quicker. The two-step-based selection strategy in DIRECT-GL selects a more extensive set of POH. While for more straightforward problems, this is detrimental, it often helps to locate a global solution with higher accuracy faster. In terms of execution time (see the right panel in Fig. 7), DIRECT-GL is the fastest among the traditional DIRECT-type algorithms (excluding hybridized).

Some algorithms have integrated schemes helping speed up the refinement of solutions. Therefore, we tested them with a much higher precision solution ($\varepsilon_{pe} = 10^{-8}$). In Table 4, we summarize our experimental findings. First, the number of failed problems is much higher when higher accuracy is needed (see the **Failed** column in Tables 3 and 4). The smallest number of unsolved problems is achieved using DIRECT-GL (6/81), where all failed test problems belong to the ($n \geq 5$) class. The DIRECT-GL algorithm turns out to be more efficient even than hybrid methods. Overall, DIRECT-GL required approximately 7% fewer function evaluations and took 32% less time than the second and third best algorithms, BIRMIN and DIRMIN, accordingly (see **Average results** column in Table 4). However, the BIRMIN algorithm has the best median value (see **Median results** column), solving at least half of the problems with the best performance. Finally, let us stress the inefficiency of the original DIRECT algorithm (DIRECT and glbSolve implementations). As the median value is more than 2,000,000, glbSolve failed more than half of the test problems to solve. The performance of the TOMLAB/glcCluster algorithm, which showed the best average results in the previous study, has also decreased significantly (see the **Average results** column in Tables 3 and 4). It turns out that the use of fmincon with default parameters in hybridized methods (DIRECT-rev, DIRMIN, and BIRMIN) is much more effective in finding a solution with higher accuracy than the TOMLAB/glcCluster. Furthermore, TOMLAB/glcCluster turned out to be the slowest algorithm among all involved in this study.

Finally, the data profiles of the selected algorithms are shown in Fig. 8. Once again, the date profiles confirm that the hybridized algorithms are more efficient than traditional DIRECT-type approaches. However, by increasing the maximal budget of function evaluations, the traditional DIRECT-GL algorithm starts outperforming all algorithms, including hybridized ones.
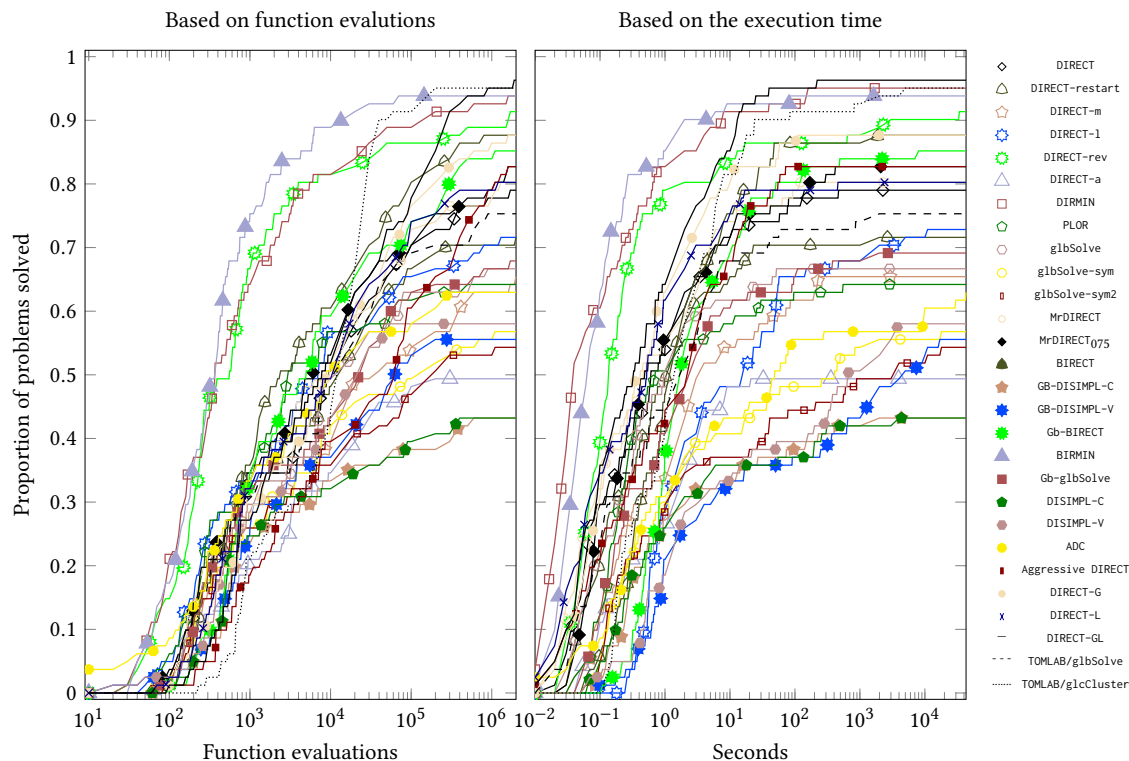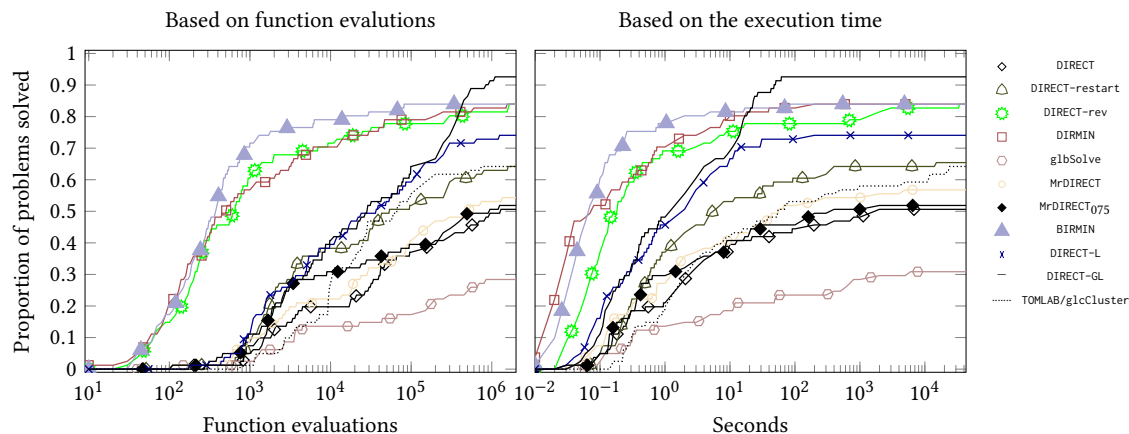
Fig. 8. Data profiles of selected DIRECT-type algorithms from DIRECTGO and TOMLAB on the whole set of box-constrained optimization problems from DIRECTGOLib v1.0 using $\varepsilon_{\mathrm{pe}} = 10^{-8}$ in (17).

4.2 Comparison of DIRECT-type algorithms for constrained global optimization

The comparison presented in this section was carried out using 80 global optimization test problems with various constraints. In DIRECTGOLib v1.0, 35 test problems contain linear constraints, 39 problems have non-linear constraints where 5 include equality constraints. All necessary details about the test problems are given in Appendix A, Table 13. We used the same stopping condition in these experimental investigations as in the previous ones, and the value $\varepsilon_{\mathrm{pe}} = 10^{-2}$.

Let us stress that 5 of the test problems contain equality constraints, which we transform into inequality constraints as follows:

$$\mathbf{h}(\mathbf{x}) = 0 \rightarrow |\mathbf{h}(\mathbf{x}) - \varepsilon_{\mathrm{h}}| \leq 0, \tag{19}$$

where $\varepsilon_{\mathrm{h}} > 0$ is a small tolerance for equality constraints. In our experiments, it was set to 10^{-8}.

4.2.1   Test results on problems with hidden constraints. In the first part, we compared DIRECT-type versions devoted to problems with hidden constraints. We have used all constrained test problems but assumed that any information about the constraints is unavailable. In the experimental investigation, the hidden search area (D^{hidden}) was defined as

$$D^{\mathrm{hidden}} = \{\mathbf{x} \in D : \mathbf{g}(\mathbf{x}) \leq 0, \mathbf{h}(\mathbf{x}) = 0\} \tag{20}$$

Still, this information is unavailable for the tested algorithms and used only to determine whether a certain point is feasible or not. Obtained experimental results are summarized in the upper part of Table 5 (see 'Performance of DIRECT-type algorithms for problems with hidden constraints'). First, let us note that 13 out of the 80 test problems contain complex constraints leading to a tiny feasible region. As the algorithms within this class do not use any information about constraint functions, none of the tested algorithms could find a single feasible point for these 13 test problems.

The best among all DIRECT-type algorithms for problems with hidden constraints is DIRECT-GLh (failed to solve (18/80)), while the second-best is DIRECT-NAS (failed to solve (29/80)). The median number of function evaluations (see f_{eval} in **Median results**) is similar for both. Still, DIRECT-GLh is the best, primarily based on the number of iterations (*iter.*) and the execution *time*: DIRECT-GLh took around 4.5 times fewer iterations and approximately 33

Table 5. The performance of `DIRECT`-type algorithms from `DIRECTGO` and `TOMLAB` based on the number of function evaluations ($f_{eval.}$), the total execution time in seconds ($time$), and the total number of iterations ($iter.$) criteria on a set of constrained (hidden, general, and linear) optimization problems

Algorithm	Parameter	Failed	Average results			Average results (Non-lin. constr.)			Average results (Lin. constr.)			Median results		
			$f_{eval.}$	$time$	$iter.$	$f_{eval.}$	$time$	$iter.$	$f_{eval.}$	$time$	$iter.$	$f_{eval.}$	$time$	$iter.$
Performance of DIRECT-type algorithms for problems with hidden constraints														
`DIRECT-NAS`	–	29/80	711,720	15,372.02	20,049	943,276	20,453.13	31,129	414,006	8,839.17	5,802	9,124	18.68	144
`DIRECT-Barrier`	–	46/80	1,192,521	2,908.88	38,069	1,260,510	3,821.84	51,635	1,105,106	1,735.09	20,627	2,000,000	723.03	2596
`subDIRECT-Barrier`	$sub = 2$	53/80	1,364,353	860.50	6,896	1,316,302	886.75	6,042	1,426,132	826.76	7,994	2,000,000	295.60	65
`subDIRECT-Barrier`	$sub = 3$	48/80	1,240,771	773.74	3,623	1,270,693	773.81	902	1,202,301	773.65	7,121	2,000,000	286.48	251
`subDIRECT-Barrier`	$sub = 5$	47/80	1,229,037	1,359.66	11,199	1,367,032	1,526.87	10,660	1,051,614	1,144.67	11,892	2,000,000	559.34	1,294
`DIRECT-GLh`	–	18/80	470,807	312.40	104	648,370	491.81	92	242,513	81.74	119	7,068	0.57	32
Performance of DIRECT-type algorithms for generally constrained optimization problems														
`DIRECT-GLc`	–	11/80	330,659	67.46	352	480,785	106.79	542	137,639	16.90	108	3,759	0.34	37
`DIRECT-GLce`	–	7/80	258,462	40.02	270	380,598	62.13	368	101,430	11.59	143	9,768	0.86	75
`DIRECT-GLce-min`*	–	2/80	62,233	10.72	45	109,975	18.99	77	852	0.09	4	124	0.04	1
`DIRECT-L1`	$\gamma = 10$	43/80	1,087,528	228.17	1,688	1,206,763	363.14	2,617	934,227	54.63	494	2,000,000	0.19	49
`DIRECT-L1`	$\gamma = 10^2$	41/80	1,051,478	870.98	3,369	1,181,710	1,425.34	3,974	884,038	158.24	2,591	2,000,000	2.49	64
`DIRECT-L1`	$\gamma = 10^3$	40/80	1,042,671	1,144.35	8,203	1,151,444	1,249.36	5,178	902,820	1,009.33	12,093	1,564,860	62.27	241
`TOMLAB/glcSolve`	–	24/80	607,397	11,031.02	13,568	801,828	14,550.11	20,288	357,415	6,506.48	4,927	3,013	2.75	145
`TOMLAB/glcCluster`*	–	8/80	207,226	3,780.92	2	364,484	6,718.99	2	5,038	3.40	1	2,734	1.40	1
Performance of DIRECT-type algorithms devoted for problems with linear constraints only														
`Lc-DISIMPL-C`	–	5/35	N/A	N/A	N/A	N/A	N/A	N/A	290,402	6,424.68	387	443	0.12	27
`Lc-DISIMPL-V`	–	3/35	N/A	N/A	N/A	N/A	N/A	N/A	171,738	3,686.81	24	16	0.01	1

* – a hybrid version of the algorithm, enriched with the local search subroutine
N/A – not available

times less execution time than the second-best `DIRECT-NAS`, algorithm. The speed is the essential factor differentiating `DIRECT-GLh` from `DIRECT-NAS`.

For an extra subdividing step-based `subDIRECT-Barrier`, the user must define how often this step is activated. Unfortunately, the authors in [58] did not make any sensitivity analysis and guidance. In our experiments, we start the subdividing step at $sub^k, k = 1, 2, \ldots$ iterations. We tested three different values for the variable sub, i.e., $sub = 2, 3$, and 5. Our experience showed that an extra subdividing step combined with a traditional barrier approach based on `subDIRECT-Barrier` did not significantly improve performance (based on the number of **Failed** problems and the **Average results**) over the original `DIRECT-Barrier`. The most obvious difference is that, on average, `subDIRECT-Barrier` subdivides much more POH per iteration because of an extra subdividing step, leading to a smaller number of iterations ($iter.$) and the execution $time$. `subDIRECT-Barrier` algorithm suffers solving larger dimensionality and problems where D^{hidden} contains non-linear constraints (see **Average results (Non-lin. constr.)** column). Therefore, this limits `subDIRECT-Barrier` applicability primarily to low-dimensional problems.

Finally, in Fig. 9, the comparative performance of algorithms using the data profiles is demonstrated. They confirm that the `DIRECT-GLh` is the most effective optimizer in this class and has the highest efficiency based on the function evaluations and execution time.

4.2.2 Test results on problems with general constraints. Better performance of `DIRECT`-type algorithms can be expected when the constraint function information is known. Let us note that all `DIRECT`-type algorithms considered in the previous section are included in this analysis. The new experimental results are added in the middle part of Table 5 (see 'Performance of `DIRECT`-type algorithms for generally constrained optimization problems). First, let us note that the recently proposed `DIRECT-GLc` and `DIRECT-GLce` algorithms can be much more successful (compared to the algorithms for problems with hidden) in solving problems containing complex and tiny feasible regions. The best average results among traditional `DIRECT`-type algorithms for constrained optimization were obtained using the `DIRECT-GLce` (failed
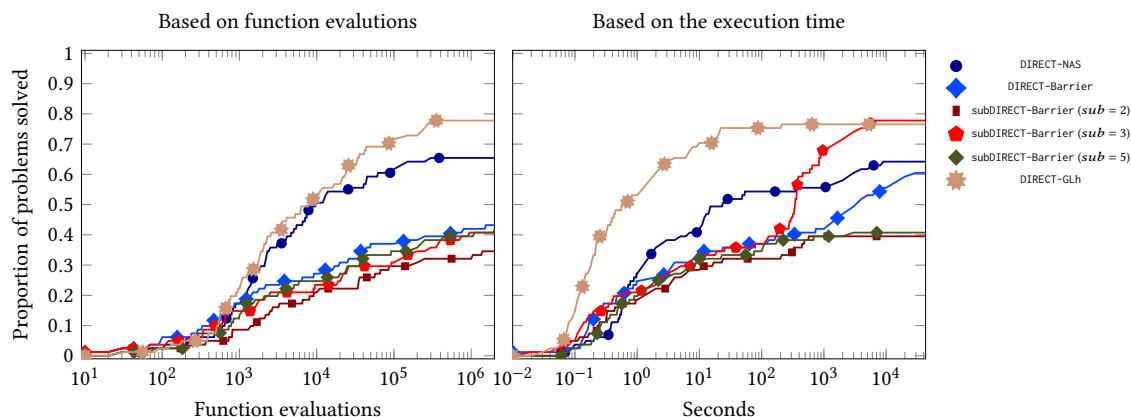
Fig. 9. Data profiles of `DIRECT`-type algorithms for problems with hidden constraints on the whole set of constrained optimization test problems. Explicit information about the constraints for all these algorithms was unknown.

to solve 7/80). Interestingly, the performance based on the number of failed problems using `DIRECT-GLc` is worse, but based on the median results, it outperforms `DIRECT-GLce` quite clearly. It looks that `DIRECT-GLc` is effective on simpler problems, but the effectiveness drops in solving more complicated problems, e.g., higher dimensionality with non-linear constraints. We also note that the solution point is often located on the feasible region's boundaries for optimization problems with general constraints. The common problem of some `DIRECT`-type algorithms in this class (`DIRECT-Barrier`, `subDIRECT-Barrier`) is that hyper-rectangles with infeasible midpoints situated closely to the edges of feasibility are penalized with large values, resulting in a low probability of being elected as POH. In such situations, these algorithms converge very slowly.

The best traditional `DIRECT`-type algorithm based on the median value was the `TOMLAB/glcSolve` method (see **Median results** column in Table 5). However, this is the only category where this algorithm showed the best results. Overall, the `TOMLAB/glcSolve` algorithm required 57% times more objective function evaluations than `DIRECT-GLce`. Furthermore, the `TOMLAB/glcSolve` appears to be the slowest algorithm in this class.

Hybridized `DIRECT-GLce-min` and `TOMLAB/glcCluster` are the only two candidates among all approaches within this class. Again, incorporating the local minimization procedure into `DIRECT-GLce` improves the performance significantly, e.g., it reduces the overall number of function evaluations approximately seven times. Moreover, `DIRECT-GLce-min` fails to solve only two test problems. `TOMLAB/glcCluster` fails to solve eight test instances and, on average, is around 353 times slower than the `DIRECT-GLce-min` method.

Finally, in Fig. 10, the comparative performance using the data profiles tool is demonstrated. Data profiles confirm the same trends, i.e., the hybridized versions are the best performing, and the overall advantage of methods that incorporate constrained information versus designed explicitly for problems with hidden constraints (see also Fig. 9).

4.2.3   Test results on problems with linear constraints. In the final part, we test the performance of `DIRECT`-type algorithms on problems with linear constraints. We consider all previously tested algorithms and two specifically designed simplicial partitions-based `Lc-DISIMPL-V` and `Lc-DISIMPL-C` [67]. The main advantage of simplices is that they can cover a feasible region defined by linear constraints. Thus any infeasible areas are not involved in the search. Moreover, for most problems from `DIRECTGOLib v1.0`, the solution is located at the intersection of linear constraints.

Based on function evalutions   Based on the execution time

Fig. 10. Data profiles of `DIRECT`-type algorithms from `DIRECTGO` and `TOMLAB` on the whole set of constrained optimization test problems.

Based on function evalutions   Based on the execution time

Fig. 11. Data profiles of `DIRECT`-type algorithms for problems with constraints on the subset of constrained optimization test problems containing linear constraints.

Therefore `Lc-DISIMPL-V` finds it in the early or even in the first iteration. The data profiles (see Fig. 11) reveal the overall effectiveness of the `Lc-DISIMPL-V` algorithm for such problems with linear constraints. The latter algorithm even outperformed the hybridized `DIRECT-GLce-min` method, which is surprisingly enough. Nevertheless, the efficiency of simplicial partition-based algorithms suffers from the problem dimension. Three higher dimensionality linearly constrained problems were unsolved by the `Lc-DISIMPL-V` algorithm (see the bottom part of Table 5, 'Performance of `DIRECT`-type algorithms devoted to problems with linear constraints only'). Moreover, simplicial partition-based implementations are pretty slow. For example, on average, `DIRECT-GLce` is approximately 307 times faster than `Lc-DISIMPL-V`. Moreover, `DIRECT-GLce`, `DIRECT-GLce-min`, and `TOMLAB/glcCluster` solved all test problems with linear constraints.

5 DIRECTGO PERFORMANCE ON ENGINEERING PROBLEMS

In this section, the algorithms from DIRECTGO and TOMLAB were tested on eleven engineering design problems: tension/compression spring, three-bar truss, NASA speed reducer, pressure vessel, welded beam, and six different versions of the general non-linear regression problem. The general non-linear regression problem is box-constrained, while the others involve different constraints. Only the most promising algorithms (based on Section 4) were considered. We used the same stopping rule as the global minimums are known for all these engineering problems. A detailed description of all engineering problems and mathematical formulations is given in Appendix B.

5.1 Tension/compression spring design problem

Here, we consider the tension-compression string design problem. This problem aims to minimize the string weight under the constraints on deflection, shear stress, surge frequency, and limits on the outside diameter. A detailed description of the practical problem can be found in [40], while in Appendix B.1, we give a short description and mathematical formulation.

A comparison of found solutions and performance metrics by the algorithms from DIRECTGO and TOMLAB is shown in Table 6. Four considered algorithms were able to solve this problem. Based on the number of function evaluation criteria, a slightly unexpectedly DIRECT-NAS was significantly better than other algorithms. The surprise is that the algorithm does not use any information about the constraint functions. However, the DIRECT-NAS algorithm was approximate four times slower than the second-best method DIRECT-GLce. Another surprise was that none of the hybridized algorithms performed well on this practical problem. Moreover, the TOMLAB/glcCluster algorithm failed to find a solution within the given time limit.

Table 6. Performance of the DIRECT-type algorithms from DIRECTGO and TOMLAB on a tension/compression design problem

Algorithm (input)	Parameter	Iterations	f_{eval}	Time (s)	f_{min}
DIRECT-NAS	–	297	17, 659	77.46	0.012680
DIRECT-Barrier	–	40, 478	$> 2 \times 10^6$	2, 465.81	0.012867
subDIRECT-Barrier	$sub = 2$	256	$> 2 \times 10^6$	207.89	0.012708
subDIRECT-Barrier	$sub = 3$	2, 187	$> 2 \times 10^6$	198.94	0.012741
subDIRECT-Barrier	$sub = 5$	15, 626	$> 2 \times 10^6$	722.79	0.012867
DIRECT-GLh	–	700	$> 2 \times 10^6$	214.81	0.012683
DIRECT-GLc	–	675	423, 209	47.53	0.012680
DIRECT-GLce	–	624	178, 115	20.45	0.012680
DIRECT-GLce-min*	–	624	178, 115	20.70	0.012680
DIRECT-L1	$\gamma = 10^1$	34, 395	$> 2 \times 10^6$	3, 265.38	0.012755
DIRECT-L1	$\gamma = 10^2$	33, 897	$> 2 \times 10^6$	3, 147.87	0.012867
DIRECT-L1	$\gamma = 10^3$	33, 571	$> 2 \times 10^6$	3, 041.00	0.012867
TOMLAB/glcSolve	–	64	$> 2 \times 10^6$	560.36	0.014669
TOMLAB/glcCluster*	–	12	1, 528, 205	$> 43, 000.00$	0.014669

* – a hybrid version of the algorithm, enriched with the local search subroutine

5.2 Three-bar truss design problem

Here, we consider the three-bar truss design problem. The goal is to minimize the volume subject to stress constraints. A detailed description of the problem is given in [74], while in Appendix B.2, we provide a brief description and mathematical formulation.

A comparison of found solutions and performance metrics is shown in Table 7. Here, hybridized `DIRECT-GLce-min` was the most efficient optimizer. However, none of the algorithms (with the proper input parameters) had any difficulty solving this problem, and they found the solution in less than one-second time.

Table 7. Performance of the `DIRECT`-type algorithms from `DIRECTGO` and `TOMLAB` on a three-bar truss design problem

Algorithm (input)	Parameter	Iterations	f_{eval}	Time (s)	f_{min}
DIRECT-NAS	–	29	339	0.05	263.915790
DIRECT-Barrier	–	13	125	0.02	263.915790
subDIRECT-Barrier	$sub = 2$	512	$> 2 \times 10^6$	141.63	283.223781
subDIRECT-Barrier	$sub = 3$	17	333	0.02	263.915800
subDIRECT-Barrier	$sub = 5$	14	161	0.02	263.915790
DIRECT-GLh	–	12	231	0.03	263.915790
DIRECT-GLc	–	17	727	0.08	263.911750
DIRECT-GLce	–	33	1,055	0.13	263.915790
DIRECT-GLce-min[*]	–	6	93	0.03	263.895850
DIRECT-L1	$\gamma = 10^1$	1	1	0.01	199.705600[a]
DIRECT-L1	$\gamma = 10^2$	2	11	0.01	262.344700[a]
DIRECT-L1	$\gamma = 10^3$	17	179	0.03	263.915790
TOMLAB/glcSolve	–	25	647	0.43	263.910482
TOMLAB/glcCluster[*]	–	1	992	0.55	263.910482

[*] – a hybrid version of the algorithm, enriched with the local search subroutine
a – result is outside the feasible region

5.3 NASA speed reducer design problem

Here we consider the NASA speed reducer design problem. The goal is to minimize the overall weight subject to constraints on the gear teeth' bending stress, surface stress, transverse deflection of the shaft, and stresses in the shafts. A detailed description of the problem can be found in [74], while in Appendix B.3, we provide a short description and mathematical formulation.

A comparison of the found solutions and performance metrics is shown in Table 8. Only three algorithms (`DIRECT-GLce`, `DIRECT-GLce-min`, and `TOMLAB/glcCluster`) were able to tackle this problem. Again, the hybridized `DIRECT-GLce-min` algorithm showed the best performance. Note that the found solutions with `DIRECT-L1` are better than the best-known value f_{min}. However, the reported solution point is outside the feasible region and violates some constraints. The `TOMLAB/glcSolve` was very close to a solution, but could not find it with a required accuracy within the maximum time limit.

Table 8. Performance of the DIRECT-type algorithms from DIRECTGO and TOMLAB on a NASA speed reducer design problem

Algorithm (input)	Parameter	Iterations	f_{eval}	Time (s)	f_{min}
DIRECT-NAS	–	6, 719	325, 691	> 43, 000.00	3, 006.874789
DIRECT-Barrier	–	32, 031	$> 2 \times 10^6$	2, 625.88	3, 006.838136
subDIRECT-Barrier	$sub = 2$	64	$> 2 \times 10^6$	389.49	3, 045.559256
subDIRECT-Barrier	$sub = 3$	243	$> 2 \times 10^6$	85.07	3, 040.464809
subDIRECT-Barrier	$sub = 5$	11, 112	$> 2 \times 10^6$	1, 234.33	3, 006.838136
DIRECT-GLh	–	528	$> 2 \times 10^6$	169.74	3, 003.135167
DIRECT-GLc	–	1, 623	$> 2 \times 10^6$	373.40	3, 002.869474
DIRECT-GLce	–	254	123, 175	9.70	2, 996.572800
DIRECT-GLce-min*	–	55	10, 229	0.93	2, 996.348212
DIRECT-L1	$\gamma = 10^1$	4	67	0.01	2, 943.869936[a]
DIRECT-L1	$\gamma = 10^2$	4	67	0.02	2, 982.462161[a]
DIRECT-L1	$\gamma = 10^3$	661	26, 667	3.01	2, 995.382568[a]
TOMLAB/glcSolve	–	66, 305	1, 504, 889	> 43, 000.00	2, 996.659779
TOMLAB/glcCluster*	–	1	12, 736	7.35	2, 996.347954

* – a hybrid version of the algorithm, enriched with the local search subroutine
a – result is outside the feasible region

5.4 Pressure vessel design problem

In this subsection, we consider a pressure vessel design problem, and the goal is to minimize the total cost of the material, form, and weld a cylindrical vessel. A detailed description of the problem can be found in [40], while in Appendix B.4, we provide a short description and mathematical formulation.

A comparison of the found solutions and performance metrics is shown in Table 9. Five algorithms solved this problem: DIRECT-NAS, DIRECT-GLh, DIRECT-GLce, TOMLAB/glcCluster, and DIRECT-GLce-min was the most efficient optimizer again. DIRECT-NAS is the best performing and outperformed the second-best by approximately 1.8 times, among traditional DIRECT-type algorithms. However, the DIRECT-NAS algorithm was about 26 times slower than the second-best method (DIRECT-GLh). As in the previous case, the DIRECT-L1 returned a better than the best-know value f_{min}, but the solution points lay outside the feasible region.

5.5 Welded beam design problem

The fifth engineering problem is the welded beam design. The goal is to minimize a welded beam for a minimum cost, subject to seven constraints. The detailed description is presented in [54, 55], while in Appendix B.5, we provide a short description and mathematical formulation.

A comparison of the algorithms is shown in Table 10. In total, six algorithms were able to solve the problem, and once again, the DIRECT-GLce-min was the most efficient one. Again, the DIRECT-NAS algorithm showed the best performance (based on the total number of function evaluations) among traditional DIRECT-type algorithms but significantly suffered based on the execution time.

5.6 General non-linear regression problem

In the final part, a general non-linear regression design problem is considered in the form of fitting a sum of damped sinusoids to a series of observations. The detailed description of the problem can be found in [26, 61, 80], while in

Table 9. Performance of the `DIRECT`-type algorithms from `DIRECTGO` and `TOMLAB` on a pressure vessel design problem

Algorithm (input)	Parameter	Iterations	f_{eval}	Time (s)	f_{min}
`DIRECT-NAS`	–	273	31, 081	126.64	7, 164.437307
`DIRECT-Barrier`	–	26, 379	$> 2 \times 10^6$	1, 600.15	7, 234.041903
`subDIRECT-Barrier`	$sub = 2$	128	$> 2 \times 10^6$	190.11	7, 234.402264
`subDIRECT-Barrier`	$sub = 3$	729	$> 2 \times 10^6$	99.05	7, 234.222516
`subDIRECT-Barrier`	$sub = 5$	15, 626	$> 2 \times 10^6$	1, 328.98	7, 234.041903
`DIRECT-GLh`	–	252	55, 837	4.80	7, 164.437300
`DIRECT-GLc`	–	2, 358	$> 2 \times 10^6$	433.87	7, 224.704257
`DIRECT-GLce`	–	322	88, 585	8.52	7, 164.437301
`DIRECT-GLce-min`[*]	–	1	134	0.24	7, 163.739570
`DIRECT-L1`	$\gamma = 10^1$	86	2, 117	0.34	7, 025.940549[a]
`DIRECT-L1`	$\gamma = 10^2$	86	2, 099	0.33	7, 037.428049[a]
`DIRECT-L1`	$\gamma = 10^3$	87	2, 295	0.23	7, 152.303079[a]
`TOMLAB/glcSolve`	–	123	$> 2 \times 10^6$	529.69	8, 260.982616
`TOMLAB/glcCluster`[*]	–	1	10, 026	5.74	7163.739569

[*] – a hybrid version of the algorithm, enriched with the local search subroutine
a – result is outside the feasible region

Table 10. Performance of the `DIRECT`-type algorithms from `DIRECTGO` and `TOMLAB` on a welded beam design problem

Algorithm (input)	Parameter	Iterations	f_{eval}	Time (s)	f_{min}
`DIRECT-NAS`	–	698	86, 863	4, 692.00	1.724970
`DIRECT-Barrier`	–	22, 934	$> 2 \times 10^6$	1, 363.24	1.728488
`subDIRECT-Barrier`	$sub = 2$	128	$> 2 \times 10^6$	152.58	1.728060
`subDIRECT-Barrier`	$sub = 3$	729	$> 2 \times 10^6$	128.37	1.728043
`subDIRECT-Barrier`	$sub = 5$	10, 954	$> 2 \times 10^6$	860.06	1.728037
`DIRECT-GLh`	–	189	158, 747	11.70	1.724970
`DIRECT-GLc`	–	211	108, 683	9.19	1.724970
`DIRECT-GLce`	–	366	104, 191	9.80	1.724970
`DIRECT-GLce-min`[*]	–	3	163	0.06	1.724884
`DIRECT-L1`	$\gamma = 10^1$	21, 143	$> 2 \times 10^6$	1, 995.01	1.728491
`DIRECT-L1`	$\gamma = 10^2$	20, 879	$> 2 \times 10^6$	1, 814.33	1.728491
`DIRECT-L1`	$\gamma = 10^3$	20, 767	$> 2 \times 10^6$	1, 679.76	1.728488
`TOMLAB/glcSolve`	–	86	$> 2 \times 10^6$	526.06	2.473711
`TOMLAB/glcCluster`[*]	–	1	9, 884	5.85	1.724852

[*] – a hybrid version of the algorithm, enriched with the local search subroutine

Appendix B.6, we provide a short description and mathematical formulation. The problem is multi-modal and is considered challenging, especially with the increase in the number of samples (T). The higher number of sinusoids (ς) leads to a more accurate but, at the same time, more challenging optimization problem.

Our experiments have used three different values for $\varsigma = 1, 2,$ and 3 (correspond to 3, 6, and 9-dimensional problems) and two different values, $T = 10$ and $T = 100$ for each dimension n as was done in [61].

The obtained results are summarized in Tables 11 and 12. Solving the lowest dimension ($n = 3$) cases (corresponding to $\varsigma = 1, T = 10$ and $\varsigma = 1, T = 100$) all algorithms located solution correctly (the success rate is 100%). Among the

Table 11. Performance of the DIRECT-type algorithms from DIRECTGO and TOMLAB on a non-linear regression design problem

Algorithm	Iter.	f_{eval}	Time(s)	f_{min}	Iter.	f_{eval}	Time(s)	f_{min}	Iter.	f_{eval}	Time(s)	f_{min}
		$\varsigma = 1, T = 10$				$\varsigma = 2, T = 10$				$\varsigma = 3, T = 10$		
DIRECT	31	501	0.03	0.000021	9,328	$> 2 \times 10^6$	362.84	0.001228	3,186	$> 2 \times 10^6$	215.58	0.007295
DIRECT-restart	31	501	0.03	0.000021	327	$> 2 \times 10^6$	24,247.41	0.018320	1,690	1,945,435	$> 43,000.00$	0.034164
DIRECT-m	31	501	0.08	0.000021	10,174	$> 2 \times 10^6$	692.12	0.001229	3,254	$> 2 \times 10^6$	233.60	0.007284
DIRECT-l	121	1,329	3.38	0.000021	103,675	$> 2 \times 10^6$	2,761.66	0.004189	122,325	$> 2 \times 10^6$	4,207.92	0.097183
DIRECT-rev*	1	103	0.13	9.29×10^{-14}	1	343	0.12	1.68×10^{-12}	2	2,218	0.52	8.37×10^{-9}
DIRECT-a	31	501	0.06	0.000021	11,505	$> 2 \times 10^6$	799.78	0.000691	3,585	$> 2 \times 10^6$	338.38	0.007331
DIRMIN*	3	415	0.18	4.36×10^{-13}	1	395	0.07	1.67×10^{-12}	2	2,567	0.33	8.37×10^{-12}
PLOR	35	305	0.04	0.000021	203,119	$> 2 \times 10^6$	6,746.14	0.018320	93,457	$> 2 \times 10^6$	2,287.23	0.009475
glbSolve	31	517	0.17	0.000021	2,805	1,978,935	190.77	0.000097	1,415	$> 2 \times 10^6$	134.80	0.021190
glbSolve-sym	27	369	0.22	0.000021	13,177	$> 2 \times 10^6$	859.96	0.283888	9,085	$> 2 \times 10^6$	1,572.94	0.144776
glbSolve-sym2	25	331	0.23	0.000021	13,180	$> 2 \times 10^6$	901.01	0.283888	9,086	$> 2 \times 10^6$	1,661.46	0.144776
MrDIRECT	106	1,615	0.48	0.000021	15,563	$> 2 \times 10^6$	558.19	0.000289	8,796	$> 2 \times 10^6$	391.51	0.021800
MrDIRECT$_{075}$	106	1,493	0.57	0.000021	17,801	$> 2 \times 10^6$	649.95	0.000665	15,189	$> 2 \times 10^6$	604.55	0.021733
BIRECT	58	616	0.43	0.000094	8,729	471,930	438.66	0.000096	36,981	$> 2 \times 10^6$	5,185.32	0.004731
GB-DISIMPL-C	240	4,504	3.56	0.000084	11,407	871,606	11,908.40	0.000099	124,966	$> 2 \times 10^6$	18,480.38	0.022092
GB-DISIMPL-V	223	2,563	2.61	0.000093	13,021	204,286	$> 43,000.00$	0.004809	14	5,676	18,021.63	0.470434^{β}
Gb-BIRECT	57	616	0.29	0.000095	12,546	356,724	293.07	0.000097	45,716	$> 2 \times 10^6$	9,055.27	0.003564
BIRMIN*	5	101	0.03	1.04×10^{-13}	15	316	0.03	3.82×10^{-7}	85,458	722,243	5,438.98	8.40×10^{-9}
Gb-glbSolve	31	501	0.25	0.000021	16,421	$> 2 \times 10^6$	1,384.93	0.000353	9,656	$> 2 \times 10^6$	489.68	0.009475
DISIMPL-C	223	4,856	5.88	0.000084	7,417	664,424	36,619.83	0.000099	6,620	1,296,672	$> 43,000.00$	0.011085
DISIMPL-V	150	2,344	2.18	0.000091	7,506	188,518	$> 43,000.00$	0.004860	6	5,447	13,480.53	0.474346^{β}
ADC	549	2,459	1.81	0.000089	126,297	398,856	$> 43,000.00$	0.004755	97,369	213,600	$> 43,000.00$	0.096970
Aggressive DIRECT	31	5,061	0.41	0.000087	311	$> 2 \times 10^6$	68.24	0.005848	213	$> 2 \times 10^6$	64.41	0.099088
DIRECT-G	36	863	0.14	0.000088	2,604	$> 2 \times 10^6$	124.51	0.000289	1,974	$> 2 \times 10^6$	110.58	0.075381
DIRECT-L	71	3,087	0.32	0.000085	1,576	427,475	43.53	0.000098	3,294	$> 2 \times 10^6$	333.59	0.000158
DIRECT-GL	27	1,617	0.29	0.000021	184	62,965	3.32	0.000099	652	543,207	36.50	0.000086
TOMLAB/glbSolve	32	501	0.05	0.000021	2,768	1,993,523	3,282.31	0.000098	1,209	$> 2 \times 10^6$	1,566.85	0.031797
TOMLAB/glcCluster*	1	5,688	0.51	9.77×10^{-10}	1	12,065	1.53	2.11×10^{-9}	2	47,903	259.97	0.000001
Success rate (%)		100.00				42.86				17.86		

β – algorithm crash, lack of memory
* – a hybrid version of the algorithm, enriched with the local search subroutine
N/A – not available

hybridized methods, the BIRMIN and DIRECT-rev proved the most effective. Among the traditional algorithms, the PLOR algorithm is the most efficient in solving the first problem (with $\varsigma = 1, T = 10$ parameters). However, by increasing the number of samples T, PLOR performed worst among all DIRECT-type algorithms. The most efficient algorithm for the case with $\varsigma = 1$ and $T = 100$ was glbSolve.

For the higher dimensionality case ($n = 6$), more than half of the algorithms failed to find the correct solution. The success rates for these two cases are 42.86% and 39.28%, respectively. The DIRECT-GL algorithm has shown a significant advantage among the traditional DIRECT-type algorithms. The best two performing hybridized methods were the BIRMIN and DIRECT-rev.

Finally, most DIRECT-type methods have faced significant challenges in solving two variants of the highest dimensional ($n = 9$) case. The success rates on these two cases are only 17.86% and 17.86%, respectively. While hybridized methods had no significant difficulties, among the traditional, only the DIRECT-GL algorithm solved both variants.

6 CONCLUSION

This paper has introduced a new open-source DIRECT-type MATLAB toolbox (DIRECTGO) for derivative-free global optimization. The new toolbox combines various state-of-the-art DIRECT-type algorithms for the global solution of box-constrained, generally-constrained, and optimization problems with hidden constraints. All algorithms were implemented using two different data structures: static and dynamic. Additionally, several parallel schemes were adopted

Table 12. Performance of the DIRECT-type algorithms from DIRECTGO and TOMLAB on a non-linear regression design problem

Algorithm	Iter.	f_{eval}	Time(s)	f_{min}	Iter.	f_{eval}	Time(s)	f_{min}	Iter.	f_{eval}	Time(s)	f_{min}
		$\varsigma=1, T=100$				$\varsigma=2, T=100$				$\varsigma=3, T=100$		
DIRECT	89	1,923	0.15	0.000025	9,191	$>2\times10^6$	367.06	0.001696	3,722	$>2\times10^6$	309.91	0.034532
DIRECT-restart	88	1,839	0.15	0.000026	379	916,449	$>43,000.00$	0.018320	1,153	$>2\times10^6$	4,625.37	0.059241
DIRECT-m	88	1,807	0.28	0.000026	9,596	$>2\times10^6$	627.22	0.001697	3,736	$>2\times10^6$	330.63	0.034538
DIRECT-l	167	2,037	4.81	0.000026	106,353	$>2\times10^6$	2,543.40	0.006783	125,804	$>2\times10^6$	4,253.70	0.114946
DIRECT-rev*	1	95	0.13	9.30×10^{-14}	1	318	0.09	1.13×10^{-12}	7	3,677	0.54	5.65×10^{-11}
DIRECT-a	88	1,799	0.22	0.000026	11,545	$>2\times10^6$	821.49	0.001255	3,809	$>2\times10^6$	501.22	0.034546
DIRMIN*	3	416	0.19	1.15×10^{-13}	1	415	0.08	5.83×10^{-10}	3	3,653	0.53	6.12×10^{-11}
PLOR	6,811	45,423	10.90	0.000025	203,159	$>2\times10^6$	8,147.64	0.020558	91,574	$>2\times10^6$	2,395.47	0.041690
glbSolve	37	669	0.07	0.000026	2,602	1,713,841	195.49	0.000096	1,165	$>2\times10^6$	169.23	0.041937
glbSolve-sym	62	1,239	0.29	0.000026	13,098	$>2\times10^6$	873.50	0.298576	9,235	$>2\times10^6$	1,579.90	0.161607
glbSolve-sym2	59	1,149	0.26	0.000026	13,098	$>2\times10^6$	894.10	0.298576	9,225	$>2\times10^6$	1,633.59	0.161607
MrDIRECT	124	1,991	0.60	0.000026	15,324	$>2\times10^6$	547.68	0.001146	9,328	$>2\times10^6$	436.52	0.043663
MrDIRECT$_{075}$	124	1,857	0.56	0.000026	17,627	$>2\times10^6$	680.61	0.001247	15,660	$>2\times10^6$	670.92	0.034531
BIRECT	86	1,042	0.22	0.000096	13,028	675,332	238.64	0.000097	36,473	$>2\times10^6$	6,874.16	0.019857
GB-DISIMPL-C	226	4,098	2.90	0.000098	27,508	$>2\times10^6$	5,240.49	0.003371	121,510	$>2\times10^6$	21,508.76	0.044617
GB-DISIMPL-V	227	2,353	2.04	0.000004	11,838	168,651	$>43,000.00$	0.008066	14	5,676	19,133.02	0.488079^β
Gb-BIRECT	85	1,042	0.26	0.000097	15,029	414,268	370.36	0.000091	48,312	$>2\times10^6$	10,437.74	0.014167
BIRMIN*	5	105	0.02	1.15×10^{-13}	15	292	0.06	2.23×10^{-7}	89,360	730,887	6,871.27	2.30×10^{-9}
Gb-glbSolve	86	1,691	0.44	0.000026	16,218	$>2\times10^6$	1,316.70	0.000712	13,339	$>2\times10^6$	599.68	0.041748
DISIMPL-C	214	4,556	5.31	0.000098	7,518	650,936	32,115.01	0.000088	7,148	1,309,272	$>43,000.00$	0.014357
DISIMPL-V	179	3,024	2.76	0.000087	10,124	244,502	$>43,000.00$	0.008066	6	5,447	11,406.93	0.488079^β
ADC	644	2,848	2.46	0.000088	127,872	355,695	$>43,000.00$	0.007043	73,097	190,302	$>43,000.00$	0.115773
Aggressive DIRECT	36	6,921	0.52	0.000091	311	$>2\times10^6$	91.84	0.006979	213	$>2\times10^6$	98.15	0.117012
DIRECT-G	40	1,045	0.11	0.000045	2,361	$>2\times10^6$	151.77	0.000786	2,031	$>2\times10^6$	147.34	0.094152
DIRECT-L	67	2,833	0.30	0.000093	689	294,415	23.61	0.000099	3,617	$>2\times10^6$	382.54	0.000248
DIRECT-GL	29	1,829	0.18	0.000025	188	65,645	3.93	0.000097	251	158,989	9.99	0.000099
TOMLAB/glbSolve	89	1,997	0.21	0.000026	2,495	1,666,955	2,160.47	0.000097	1,162	$>2\times10^6$	1,557.18	0.041937
TOMLAB/glcCluster*	1	6,092	0.57	1.28×10^{-9}	1	12,034	1.18	4.47×10^{-10}	1	18,008	4.91	0.000008
Success rate (%)		100.00				39.28				17.86		

β – algorithm crash, lack of memory
* – a hybrid version of the algorithm, enriched with the local search subroutine
N/A – not available

to promising algorithms. Furthermore, an online test library DIRECTGOLib v1.0, containing 119 global optimization test and engineering problems, has been presented.

The performance of various algorithms within DIRECTGO has been investigated via a detailed numerical study using the test problems from DIRECTGOLib v1.0. A further 11 examples of using the DIRECTGO for engineering design optimization have been investigated. The results demonstrate the promising performance of DIRECTGO in tackling these challenging problems. We also gave guidance on which algorithms to use for specific optimization problems.

Motivated by the promising performance, we plan to extend this work to facilitate the broader adoption of DIRECTGO. We plan to include newly appearing promising DIRECT-type algorithms within this toolbox continuously. Another direction is extending the developed algorithms using a hybrid CPU-GPU scheme. Finally, we will consider advanced data structures for better organization and reduced communication overhead.

SOURCE CODE STATEMENT

All implemented DIRECT-type algorithms (DIRECTGO toolbox) are available at the GitHub repository: https://github.com/blockchain-group/DIRECTGO and can be used under the MIT license. We welcome contributions and corrections to it.

DATA STATEMENT

`DIRECTGOLib` - `DIRECT` **G**lobal **O**ptimization test problems **Lib**rary is designed as a *continuously-growing* open-source GitHub repository (https://github.com/blockchain-group/DIRECTGOLib) to which anyone can easily contribute. Therefore, the most recent version is slightly different from the one used in these studies. The exact data underlying this article (`DIRECTGOLib v1.0`) can be accessed either on GitHub or at Zenodo (connected with GitHub):

- at GitHub: https://github.com/blockchain-group/DIRECTGOLib/tree/v1.0,
- at Zenodo: https://doi.org/10.5281/zenodo.6491863,

and used under the MIT license.

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A summary of all optimization problems in DIRECTGOLib v1.0 [86, 91] and their properties are given in Table 13. The first column denotes the problem type, and the second contains the problem name. The third column contains the source of the problem. The fourth column specifies the dimension (n) of the used problems. When problems are of various dimensionality, all considered dimensions are listed. The fifth through eighth columns ($\mathbf{g}$, $\mathbf{h}$, a, D) specify the number of inequality ($\mathbf{g}$) and equality ($\mathbf{h}$) constraints, the number of active constraints (a), and two versions of optimization domains, default (D) and perturbed ($\tilde{D}$), respectively. The default domains are taken from the literature. However, whenever the global minimum point lay for at least one algorithm from DIRECTGO at the initial sampling point, the default feasible region (D) was perturbed and used in the experimental analysis. Here the sign "-" means that $\tilde{D}$ is the same as D. Finally, the last column contains the best-known optimal solution value (f^*).

Table 13. Key characteristics of the `DIRECTGOLib v1.0` [86, 91] test problems for global optimization

Problem		Source	Problem properties						f^*
Type	Name		n	g	h	a	D	$\tilde{D}$	
BC	Ackley	[32, 95]	2, 5, 10	0	0	0	$[-15, 30]^n$	$[-15, 35]^n$	0.0000
	Alpine	[12]	5, 10, 15	0	0	0	$[0, 10]^n$	–	-2.8081^n
	Beale	[32, 95]	2	0	0	0	$[-4.5, 4.5]^n$	–	0.0000
	Bohachevsky1	[32, 95]	2	0	0	0	$[-100, 100]^n$	$[-100, 110]^n$	0.0000
	Bohachevsky2	[32, 95]	2	0	0	0	$[-100, 100]^n$	$[-100, 110]^n$	0.0000
	Bohachevsky3	[32, 95]	2	0	0	0	$[-100, 100]^n$	$[-100, 110]^n$	0.0000
	Booth	[32, 95]	2	0	0	0	$[-10, 10]^n$	–	0.0000
	Branin	[18, 32, 95]	2	0	0	0	$[-5, 10] \times [0, 15]$	–	0.3978
	Bukin6	[95]	2	0	0	0	$[-15, 5] \times [-3, 3]$	–	0.0000
	Colville	[32, 95]	4	0	0	0	$[-10, 10]^n$	–	0.0000
	Cross_in_Tray	[95]	2	0	0	0	$[-10, 10]^n$	–	-2.0626
	Csendes	[12]	5, 10, 15	0	0	0	$[-10, 10]^n$	$[-10, 21]^n$	0.0000
	Dixon_and_Price	[32, 95]	2, 5, 10	0	0	0	$[-10, -10]^n$	–	0.0000
	Drop_wave	[95]	2	0	0	0	$[-5.12, -5.12]^n$	$[-5.12, -6.12]^n$	-1.0000
	Easom	[32, 95]	2	0	0	0	$[-100, 100]^n$	–	-1.0000
	Eggholder	[95]	2	0	0	0	$[-512, 512]^n$	–	-959.6406
	Goldstein_and_Price	[18, 32, 95]	2	0	0	0	$[-2, 2]^n$	–	3.0000
	Griewank	[32, 95]	5, 10, 15	0	0	0	$[-600, 600]^n$	$[-600, 700]^n$	0.0000
	Hartman3	[32, 95]	3	0	0	0	$[0, 1]^n$	–	-3.8627
	Hartman6	[32, 95]	6	0	0	0	$[0, 1]^n$	–	-3.3223
	Holder_Table	[95]	2	0	0	0	$[-10, 10]^n$	–	-19.2085
	Hump	[32, 95]	2	0	0	0	$[-5, 5]^n$	–	-1.0316
	Langermann	[95]	2	0	0	0	$[0, 10]^n$	–	-4.1558
	Levy	[32, 95]	5, 10, 15	0	0	0	$[-5, 5]^n$	–	0.0000
	Matyas	[32, 95]	2	0	0	0	$[-10, 10]^n$	$[-10, 15]^n$	0.0000
	McCormick	[95]	2	0	0	0	$[-1.5, 4] \times [-3, 4]$	–	-1.9132
	Michalewicz	[32, 95]	2	0	0	0	$[0, \pi]^n$	–	-1.8013
	Michalewicz	[32, 95]	5	0	0	0	$[0, \pi]^n$	–	-4.6876
	Michalewicz	[32, 95]	10	0	0	0	$[0, \pi]^n$	–	-9.6601
	Perm	[32, 95]	8	0	0	0	$[-i, i]^n$	–	0.0000
	Permdb	[32, 95]	5	0	0	0	$[-i, i]^n$	–	0.0000
	Powell	[32, 95]	4	0	0	0	$[-4, 4]^n$	$[-4, 5]^n$	0.0000
	Power_Sum	[32, 95]	4	0	0	0	$[0, 4]^n$	–	0.0000
	Qing	[12]	5, 10, 15	0	0	0	$[-500, 500]^n$	–	0.0000
	Rastrigin	[32, 95]	2, 5, 10	0	0	0	$[-5.12, 5.12]^n$	$[-6.12, 5.12]^n$	0.0000
	Rosenbrock	[18, 32, 95]	5, 10, 15	0	0	0	$[-5, 10]^n$	–	0.0000
	Rotated_H_Ellip	[95]	5, 10, 15	0	0	0	$[-65.536, 65.536]^n$	$-65.536, 66.536]^n$	0.0000
	Schwefel	[32, 95]	2, 5, 10	0	0	0	$[-500, 500]^n$	–	0.0000
	Shekel5	[32, 95]	4	0	0	0	$[0, 10]^n$	–	-10.1531
	Shekel7	[32, 95]	4	0	0	0	$[0, 10]^n$	–	-10.4029
	Shekel10	[32, 95]	4	0	0	0	$[0, 10]^n$	–	-10.5364
	Shubert	[32, 95]	2	0	0	0	$[-10, 10]^n$	–	-186.7309
	Sphere	[32, 95]	5, 10, 15	0	0	0	$[-5, 5]^n$	$[-5.12, 6.12]^n$	0.0000
	Styblinski_Tang	[12]	5, 10, 15	0	0	0	$[-5, 5]^n$	–	$-39.1661n$
	Sum_of_Powers	[95]	5, 10, 15	0	0	0	$[-1, 1]^n$	$[-1, 2.5]^n$	0.0000
	Sum_Square	[95]	5, 10, 15	0	0	0	$[-10, 10]^n$	$[-10, 15]^n$	0.0000
	Trid6	[32, 95]	6	0	0	0	$[-36, 36]^n$	–	-50.0000
	Trid10	[32, 95]	10	0	0	0	$[-100, 100]^n$	–	-210.0000
	Zakharov	[32, 95]	2, 5, 10	0	0	0	$[-5, 10]^n$	$[-5, 11]^n$	0.0000
LC	Bunnag1	[97]	4	1	0	1	$[0, 3]^n$	–	0.1111
	Bunnag2	[97]	4	2	0	2	$[0, 4]^n$	–	-6.4052
	Bunnag3	[97]	5	3	0	1	$[0, 3] \times [0, 2] \times [0, 4] \times [0, 4] \times [0, 2]$	–	-16.3692
	Bunnag4	[97]	6	2	0	1	$[0, 1]^5 \times [0, 20]$	–	-213.0470
	Bunnag5	[97]	6	5	0	1	$[0, 2] \times [0, 8] \times [0, 2] \times [0, 1]^2 \times [0, 2]$	–	-11.0000

Continued on next page

Table 13 Continued from previous page

Type	Name	Source	n	g	h	a	D (Default)	D (Perturbed)	f^*
	*Bunnag*6	[97]	10	11	0	3	$[0,1]^n$	–	−268.0146
	*Bunnag*7	[97]	10	5	0	0	$[0,1]^n$	–	−39.0000
	*G*01	[43]	13	9	0	6	$[0,10]^9 \times [0,100]^3 \times [0,10]$	–	−15.0000
	*Genocop*9	[97]	3	5	0	2	$[0,10]^n$	–	−2.4714
	*Genocop*10	[97]	4	5	0	0	$[0,3] \times [0,10]^2 \times [0,1]$	–	−4.5280
	*Genocop*11	[97]	6	5	0	0	$[0,5] \times [0,8] \times [0,5] \times [0,1]^2 \times [0,2]$	–	−11.0000
	*Horst*1	[36]	2	3	0	1	$[0,3] \times [0,2]$	–	−1.0625
	*Horst*2	[36]	2	3	0	2	$[0,2.5] \times [0,2]$	–	−6.8995
	*Horst*3	[36]	2	3	0	0	$[0,1] \times [0,1.5]$	–	−0.4444
	*Horst*4	[36]	3	4	0	2	$[0.5,2] \times [0,3] \times [0,2.8]$	–	−6.0858
	*Horst*5	[36]	3	4	0	0	$[0,1.2]^2 \times [0,1.7]$	–	−3.7220
	*Horst*6	[36]	3	7	0	2	$[0,6] \times [0,5.0279] \times [0,2.6]$	–	−32.5784
	*Horst*7	[36]	3	4	0	2	$[0,6] \times [0,3]^2$	–	−52.8769
	*hs*021	[97]	2	1	0	1	$[2,50] \times [−50,10]$	–	−99.9599
	*hs*021*mod*	[97]	7	3	0	1	$[2,50] \times [−50,50] \times [0,50] \times [2,10] \times [−10,10] \times$ $[−10,0] \times [0,10]$	–	4.0400
	*hs*024	[97]	2	3	0	2	$[0,5]^n$	–	−1.0000
	*hs*035	[97]	3	1	0	1	$[0,3]^n$	–	0.1111
	*hs*036	[97]	3	1	0	1	$[0,20] \times [0,11] \times [0,15]$	–	−3300.0000
	*hs*037	[97]	3	2	0	1	$[0,42]^n$	–	−3456.0000
	*hs*038	[97]	4	2	0	0	$[−10,10]^n$	–	0.0000
	*hs*044	[97]	4	6	0	2	$[0,5]^n$	–	−15.0000
	*hs*076	[97]	4	3	0	1	$[0,1] \times [0,3] \times [0,1]^2$	–	−4.6818
	*P*9	[23]	3	9	0	2	$[10^{-5},3] \times [10^{-5},4]^2$	–	−13.4020
	*P*14	[23]	3	4	0	2	$[10^{-5},3] \times [10^{-5},4] \times [0,1]$	–	−4.51420
	*s*224	[97]	2	4	0	1	$[0,6] \times [0,11]$	–	−304.0000
	*s*231	[97]	2	2	0	0	$[−10,10]^n$	–	0.0000
	*s*232	[97]	2	3	0	2	$[0,100]^n$	–	−1.0000
	*s*250	[97]	3	2	0	1	$[0,20] \times [0,11] \times [0,42]$	–	−3300.0000
	*s*251	[97]	3	1	0	1	$[0,42]^n$	–	−3456.0000
	*zecevic*2	[97]	3	2	0	1	$[0,10]^n$	–	−4.1249
GC	*circle*	[97]	3	10	0	3	$[0,10]^n$	–	4.5742
	*G*02	[43]	20	2	0	1	$[0,10]^n$	–	−0.8036
	*G*04	[43]	5	6	0	2	$[78,102] \times [33,45] \times [27,45]^3$	–	−30665.5386
	*G*06	[43]	2	2	0	2	$[13,100] \times [0,100]$	–	−6961.8138
	*G*07	[43]	10	8	0	6	$[−10,10]^n$	–	24.3062
	*G*08	[43]	2	2	0	0	$[0,10]^n$	–	−0.0958
	*G*09	[43]	7	4	0	2	$[−10,10]^n$	–	680.6300
	*G*10	[43]	8	6	0	6	$[100,10,000] \times [1,000,10,000]^2 \times [10,1,000]^5$	–	7049.2480
	*G*12	[43]	3	1	0	0	$[0.2,10]^n$	–	−1.0000
	*G*16	[43]	5	38	0	4	$[704.4148,906.3855] \times [68.6,288.88] \times$ $[0,134.75] \times [193,287.0966] \times [25,84.1988]$	–	−1.9051
	*G*18	[43]	9	13	0	6	$[0,10]^n$	–	−0.8660
	*G*19	[43]	15	5	0	0	$[0,10]^n$	–	32.6555
	*G*24	[43]	2	2	0	2	$[0,3] \times [0,4]$	–	−5.5080
	Goldstein_and_PriceC	[58]	2	2	0	1	$[−2,2]^n$	–	3.5389
	Gomez	[5]	2	1	0	1	$[−1,1]^n$	–	−0.9711
	Himmelblau	[8]	5	5	0	2	$[78,102] \times [33,45] \times [27,45]^3$	–	−31025.5602
	*P*1	[23]	5	0	3	3	$[−5,5]^n$	–	0.0293
	*P*2a	[23]	5	10	0	5	$[0,500]^5$	–	−400.0000
	*P*2b	[23]	5	10	0	5	$[0,500]^5$	–	−600.0000
	*P*2c	[23]	5	10	0	4	$[0,500]^5$	–	−750.0000
	*P*2d	[23]	5	12	0	5	$[0,100] \times [0,200] \times [0,100] \times [0,200] \times [1,3]$	–	−400.0000
	*P*3a	[23]	6	1	4	5	$[0,1]^4 \times [10^{-5},16]^2$	–	0.3888
	*P*3b	[23]	2	1	0	1	$[10^{-5},16]^n$	–	0.3888
	*P*4	[23]	2	1	0	1	$[0,6] \times [0,4]$	–	−6.6666
	*P*5	[23]	3	2	0	2	$[0,9.422] \times [0,5.903] \times [0,267.42]$	–	201.1600

<div align="center">Table 13 Continued from previous page</div>

Problem		Source	Problem properties						f^*
Type	Name		n	g	h	a	D (Default)	D (Perturbed)	
	P6	[23]	2	1	0	1	$[0, 115.8] \times [10^{-5}, 30]$	–	376.2900
	P7	[23]	2	4	0	1	$[-2, 2]^n$	–	−2.8284
	P8	[23]	2	2	0	1	$[-8, 10] \times [0, 10]$	–	−118.7000
	P10	[23]	2	2	0	2	$[0, 1]^n$	–	0.7417
	P11	[23]	2	1	0	1	$[0, 1]^n$	–	−0.5000
	P12	[23]	1	2	0	0	$[0, 2]$	–	−16.7390
	P13	[23]	3	0	2	2	$[10^{-5}, 34] \times [10^{-5}, 17] \times [100, 300]$	–	189.3500
	P15	[23]	3	0	3	3	$[10^{-5}, 12.5] \times [10^{-5}, 37.5] \times [0, 50]$	–	0.0000
	P16	[23]	2	6	0	0	$[1, 3] \times [1, 4]$	–	0.7049
	s365mod	[97]	7	9	0	5	$[0, 19]^n$	–	52.1399
	Tproblem	[21]	2, 3, 4, 5, 6, 7, 8	1	0	1	$[-4, 4]^n$	–	$-n$
	zy2	[97]	2	3	0	1	$[0, 10]^n$	–	2.0000
	zecevic3	[97]	2	2	0	1	$[0, 10]^n$	–	97.3094
	zecevic4	[97]	4	2	0	1	$[0, 10]^n$	–	7.5575

<div align="center">Concluded</div>

B THE MATHEMATICAL FORMULATION OF ENGINEERING PROBLEMS

B.1 Tension/compression spring design problem

The design variables of the tension/compression spring design problem [40] are the number of the wire diameter x_1, the winding diameter x_2, and active coils of the spring x_3. The objective function and the mechanical constraints are given by:

$$\min f(\mathbf{x}) = x_1^2 x_2 (x_3 + 2)$$

$$\text{s.t. } g_1(\mathbf{x}) = 1 - \frac{x_2^3 x_3}{71875 x_1^4} \le 0, \ g_2(\mathbf{x}) = \frac{x_2(4x_2 - x_1)}{12566 x_1^3 (x_2 - x_1)} + \frac{2.46}{12566 x_1^2} - 1 \le 0, \ g_3(\mathbf{x}) = 1 - \frac{140.54 x_1}{x_3 x_2^2} \le 0,$$

$$g_4(\mathbf{x}) = \frac{x_1 + x_2}{1.5} - 1 \le 0$$

where $0.05 \le x_1 \le 0.2$, $0.25 \le x_2 \le 1.3$, $2 \le x_3 \le 15$. The best known solution $\mathbf{x}^* = (0.05169591, 0.35688327, 11.29337893)$, where $f(\mathbf{x}^*) = 0.01267867$. Two of the constraint functions are active (g_1 and g_2).

B.2 Three-bar truss design problem

The three-bar truss design problem [74] has two design variables and three constraints. The optimization problem is formulated as follows:

$$\min f(\mathbf{x}) = 100(2\sqrt{2}x_1 + x_2)$$

$$\text{s.t. } g_1(\mathbf{x}) = \frac{\sqrt{2}x_1 + x_2}{\sqrt{2}x_1^2 + 2x_1 x_2} 2 - 2 \le 0, \ g_2(\mathbf{x}) = \frac{x_2}{\sqrt{2}x_1^2 + 2x_1 x_2} 2 - 2 \le 0, \ g_3(\mathbf{x}) = \frac{1}{x_1 + \sqrt{2}x_2} 2 - 2 \le 0$$

where $0 \le x_1 \le 1$, $0 \le x_2 \le 1$. The best known solution $\mathbf{x}^* = (0.78867531, 0.40824778)$, where $f(\mathbf{x}^*) = 263.89584337$. One of the constraint functions is active (g_1).

B.3 NASA speed reducer design problem

The design variables of the NASA speed reducer design problem [74] are the face width x_1, the module of teeth x_2, the number of teeth on the pinion x_3, the length of the first shaft between the bearings x_4, the distance of the second shaft between the bearings x_5, the diameter of the first shaft x_6, and, finally, the width of the second shaft x_7. The optimization problem is formulated as follows:

$$\min f(\mathbf{x}) = 0.7854x_1x_2^2(3.3333x_3^2 + 14.9334x_3 - 43.0934) - 1.508x_1(x_6^2 + x_7^2) + 7.4777(x_6^3 + x_7^3)$$
$$+ 0.7854(x_4x_6^2 + x_5x_7^2)$$

$$\text{s.t. } g_1(\mathbf{x}) = \frac{27}{x_1x_2^2x_3} - 1 \le 0, \; g_2(\mathbf{x}) = \frac{397.5}{x_1x_2^2x_3^2} - 1 \le 0, \; g_3(\mathbf{x}) = \frac{1.93x_4^3}{x_2x_3x_6^4} - 1 \le 0, \; g_4(\mathbf{x}) = \frac{1.93x_5^3}{x_2x_3x_7^4} - 1 \le 0,$$

$$g_5(\mathbf{x}) = \frac{((\frac{745x_4}{x_2x_3})^2 + 16.9 \times 10^6)^{0.5}}{110x_6^3} - 1 \le 0, \; g_6(\mathbf{x}) = \frac{((\frac{745x_5}{x_2x_3})^2 + 157.5 \times 10^6)^{0.5}}{85x_7^3} - 1 \le 0,$$

$$g_7(\mathbf{x}) = \frac{x_2x_3}{40} - 1 \le 0, \; g_8(\mathbf{x}) = \frac{5x_2}{x_1} - 1 \le 0, \; g_9(\mathbf{x}) = \frac{x_1}{12x_2} - 1 \le 0, \; g_{10}(\mathbf{x}) = \frac{1.5x_6 + 1.9}{x_4} - 1 \le 0,$$

$$g_{11}(\mathbf{x}) = \frac{1.1x_7 + 1.9}{x_5} - 1 \le 0$$

where $2.6 \le x_1 \le 3.6$, $0.7 \le x_2 \le 0.8$, $17 \le x_3 \le 28$, $7.3 \le x_4 \le 8.3$, $7.8 \le x_5 \le 8.3$, $2.9 \le x_6 \le 3.9$, $5 \le x_7 \le 5.5$. The best known solution $\mathbf{x}^* = (3.5, 0.7, 17, 7.3, 7.8, 3.35021467, 5.28668323)$, where $f(\mathbf{x}^*) = 2996.34816924$. Three constraints are active (g_5, g_6 and g_8).

B.4 Pressure vessel design problem

There are four design variables in the pressure vessel design problem [40](in inches): the thickness of the pressure vessel x_1, the thickness of the head x_2, the inner radius of the vessel x_3, and the length of the cylindrical component x_4. The optimization problem is formulated as follows:

$$\min f(\mathbf{x}) = 0.6224x_1x_3x_4 + 1.7781x_2x_3^2 + 3.1661x_1^2x_4 + 19.84x_1^2x_3$$

$$\text{s.t. } g_1(\mathbf{x}) = -x_1 + 0.0193x_3 \le 0, \; g_2(\mathbf{x}) = -x_2 + 0.00954x_3 \le 0, \; g_3(\mathbf{x}) = -\pi x_3^2x_4 - \frac{4}{3}\pi x_3^3 + 1296000 \le 0,$$

$$g_4(\mathbf{x}) = x_4 - 240 \le 0, \; g_5(\mathbf{x}) = 1.1 - x_1 \le 0, \; g_6(\mathbf{x}) = 0.6 - x_2 \le 0$$

where $1 \le x_1 \le 1.375$, $0.625 \le x_2 \le 1$, $25 \le x_3 \le 150$, $25 \le x_4 \le 240$. The best known solution $\mathbf{x}^* = (1.1, 0.625, 56.99481865, 51.00125173)$, where $f(\mathbf{x}^*) = 7163.73956887$. Three constraints are active (g_1, g_3 and g_5).

B.5 Welded beam design problem

The welded beam design problem [54, 55] is to design a welded beam at minimum cost, subject to some constraints [54, 55]. The objective is to find a minimum fabrication cost. Considering the four design variables and constraints of shear stress τ, bending stress in the beam σ, buckling load on the bar P_c, and end deflection on the beam δ. The optimization model is summarized in the following equation:

$$\min f(\mathbf{x}) = 1.10471x_1^2 x_2 + 0.04811x_3 x_4(14 + x_2)$$

s.t. $g_1(\mathbf{x}) = \tau(\mathbf{x}) - 13600 \leq 0,\ g_2(\mathbf{x}) = \sigma(\mathbf{x}) - 3 \times 10^4 \leq 0,\ g_3(\mathbf{x}) = x_1 - x_4 \leq 0,\ g_4(\mathbf{x}) = P - P_c(\mathbf{x}) \leq 0$

$g_5(\mathbf{x}) = 0.10471x_1^2 + 0.04811x_3 x_4(14 + x_2) - 5 \leq 0,\ g_6(\mathbf{x}) = \delta(\mathbf{x}) - 0.25 \leq 0,\ g_7(\mathbf{x}) = 0.125 - x_1 \leq 0,$

with:

$$\tau(\mathbf{x}) = \sqrt{(\tau^1)^2 + (\tau^1)(\tau^2)x_2/R + (\tau^2)^2},\ P_c = \frac{4.013E\sqrt{x_3^2 x_4"6/36}}{L^2}(1 - \frac{x_3}{2L}\sqrt{\frac{E}{4G}}),\ R = \sqrt{\frac{x_2^2)}{4} + (\frac{x_1 + x_3}{2})^2},$$

$$\tau^1 = \frac{P}{\sqrt{2}x_1 x_"},\ \tau^2 = \frac{MR}{J},\ \sigma(\mathbf{x}) = \frac{6PL}{x_4 x_3^2},\ J = 2(\sqrt{2}x_1 x_2(\frac{x_2^2}{12} + \frac{1}{4}(x_1 x_3)^2)),\ \delta(\mathbf{x}) = \frac{4PL^3}{Ex_4 x_3^3},\ M = P\backslash L + \frac{x_2}{2}J,$$

$$P = 6000, L = 14,\ E = 3 \times 10^7,\ G = 12 \times 10^6,$$

where $0.1 \leq x_1 \leq 2,\ 0.1 \leq x_2 \leq 10,\ 0.1 \leq x_3 \leq 10,\ 0.1 \leq x_3 \leq 2$. The best known solution $\mathbf{x}^* = (0.20572963, 3.47048893, 9.03662399, 0.20572964)$, where $f(\mathbf{x}^*) = 1.72485237$. One of the constraint functions is active (g_3).

B.6 General non-linear regression problem

Parameter estimation in the general non-linear regression model [26, 61, 80] can be reduced to solving the minimization problem:

$$\min f(\mathbf{x}) = \sum_{t=1}^{T}(\kappa(t) - \phi(\mathbf{x}, t))^2$$

with:

$$\sum_{q=1}^{\varsigma}\kappa(t) = e^{td_q}\sin(2\pi t\omega_q + \theta_q),\ \sum_{q=1}^{\varsigma}\phi(\mathbf{x}, t) = e^{(x_{3(q-1)+1}t)}\sin(2\pi tx_{3(q-1)+2} + x_{3(q-1)+3})$$

where $-1 \leq x_{3(q-1)+1} \leq 0,\ 0 \leq x_{3(q-1)+2,3(q-1)+2} \leq 1, q = 1...\varsigma$. $\mathbf{d}$ is non-positive damping coefficients, $\boldsymbol{\omega}$ is frequencies, and $\boldsymbol{\theta}$ is phases of the sinusoids (ς) (hereafter, $d_q \in [-1, 0]$, $\omega_q \in [0, 1]$, $\theta_q \in [0, 1]$, $q = 1...\varsigma$). For signal approximation, the parameter $\mathbf{x}$ of the problem is determined to fit best the real-valued signal values observed in the uniformly distributed time moments $t = 1, 2, ..., T$. The general non-linear regression problem is multi-modal, especially with the increase in the number of samples T. The increase of the sinusoid number ς leads to a more accurate but at the same time more challenging optimization problem. In our experimental study, six versions of the problem were considered. The sinusoid number was fixed to $\varsigma = 1, 2$, and 3 (corresponding to 3, 6, and 9-dimensional cases), while the value of T to 10 and 100. The best known solutions: i) $f(\mathbf{x}^*) = 0$ and $\mathbf{x}^* = (-0.2, 0.4, 0.3)$ for $n = 3$; ii) $f(\mathbf{x}^*) = 0$ and $\mathbf{x}^* = (-0.3, 0.3, 0.1, -0.2, 0.4, 0.3)$ for $n = 6$; iii) $f(\mathbf{x}^*) = 0$ and $\mathbf{x}^* = (-0.4, 0.6, 0.2, -0.3, 0.3, 0.1, -0.2, 0.4, 0.3)$ for $n = 9$.

C QUICK DIRECTGO USER GUIDE

This section provides a brief user guide on how to use DIRECTGO software. The following subsections provide examples of using algorithms (their implementations) to solve box constrained and problems with various constraints, including the parallel usage of the algorithms.

C.1   Example of box constrained global optimization algorithm usage

Any `DIRECT`-type algorithmic implementation from the `DIRECTGO MATLAB` toolbox for box constrained global optimization can be called using the same style and syntax introduced in Section 3.2. In this example we use the `PLOR` algorithm and solve *Bukin6* test problem (see Table 13).

The *Bukin6* test problem is defined in `MATLAB` in the following way:

```matlab
function y = Bukin6(x)
    if nargin == 0                      % Extract info from the function
        y.nx = 2;                       % Dimension of the problem
        xl = [-15; -3];
        y.xl = @(i) xl(i);              % Lower bounds for each variable
        xu = [5; 3];
        y.xu = @(i) xu(i);              % Upper bounds for each variable
        y.fmin = @(nx) get_fmin(nx);    % Known solution value
        y.xmin = @(nx) get_xmin(nx);    % Known solution point
        return
    end
    term1 = 100*sqrt(abs(x(2) - 0.01*x(1)^2));
    term2 = 0.01*abs(x(1) + 10);
    y = term1 + term2;                  % Return function value at x
end

function fmin = get_fmin(~)
    fmin = 0;
end

function xmin = get_xmin(~)
    xmin = [-10; 1];
end
```

Each test problem in the `DIRECTGOLib v1.0` stores the information about the problem structure together with the objective function. In this case, in the `Bukin6.m` file, the following information is stored: i) the dimensionality of the problem; ii) the lower and upper bounds for each variable; iii) the objective function value of the known solution; iv) the solution point. For some problems, the optimum might depend on the number of variables, therefore the solution values and points are returned as a functions for all test problems in `DIRECTGOLib v1.0`.

The optimization problem is passed to the algorithm as part of a `P` structure. For a box-constrained problem, only one field of the `P` structure is needed:

```matlab
>> P.f = 'Bukin6';
```

When a user wants to change the default algorithmic settings, the `OPTS` structure should be used:

```
>> opts.maxevals = 50; % Maximal number of function evaluations
>> opts.maxits = 100;  % Maximal number of iterations
>> opts.testflag = 1;  % 1 if global minima is known, 0 otherwise
>> opts.tol = 0.01;    % Tolerance for termination if testflag = 1
```

Now we are ready to call the dynamic data structure based PLOR implementation (dPlor.m) to solve this problem:

```
>> [f_min, x_min, history] = dPlor(P, OPTS);
```

The iterative output stored in the history parameter contains the following information:

```
>> history

history =

    1.0000     5.0000    16.7833    0.0023
    2.0000     7.0000    16.7833    0.0030
    3.0000    13.0000     5.6500    0.0039
    4.0000    19.0000     5.6500    0.0046
    5.0000    27.0000     1.9537    0.0053
    6.0000    33.0000     1.9537    0.0060
    7.0000    41.0000     0.7167    0.0070
    8.0000    47.0000     0.7167    0.0077
    9.0000    55.0000     0.3060    0.0086
```

Here, the first column shows the iteration number, while the second is the total number of function evaluations. The third column shows how the best objective function value improves at each iteration, while the last column shows the execution time in seconds. In this example, the PLOR algorithm was terminated when the maximum number of function evaluations (opts.maxevals = 50) exceeded.

The convergence plot is shown on the right panel of Fig. 12, while the left panel illustrates the *Bukin6* test function over its domain.

C.2 Example of constrained global optimization algorithm usage

Any DIRECT-type algorithmic implementation for constrained global optimization problems can be used the same way as box-constrained problems. However, for constrained problems, implemented algorithms extract additional information from the function's definition, such as the number of inequality constraints, the number of equality constraints, and the constraint functions. Let us take the *G06* problem (see Table 13) as an example, defined in the following way:

```
function y = G06(x)
    if nargin == 0                          % Extract info from the function
        y.nx = 2;                           % Dimension of the problem
        y.ng = 2;                           % Number of g(x) constraints
```

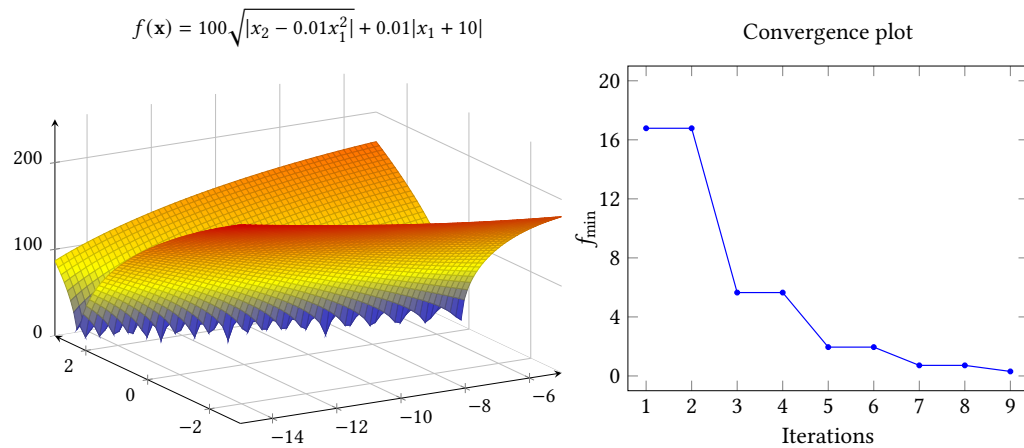$$f(\mathbf{x}) = 100\sqrt{|x_2 - 0.01x_1^2|} + 0.01|x_1 + 10|$$

Fig. 12. The *Bukin6* test function (on the left side) and the convergence plot (on the right side) of the PLOR algorithm in the first 9 iterations.

```matlab
    y.nh = 0;                            % Number of h(x) constraints
    xl = [13, 0];
    y.xl = @(i) xl(i);                   % Lower bounds for each variable
    y.xu = @(i) 100;
    y.fmin = @(nx) get_fmin(nx);         % Known solution value
    y.xmin = @(nx) get_xmin(nx);         % Known solution point
    y.confun = @(i) G06c(i);             % Constraint functions
  return
  end
  y = (x(1) - 10)^3 + (x(2) - 20)^3;     % Return function value at x
end


function [c, ceq] = G06c(x)
    c(1) = -(x(1) - 5)^2 - (x(2) - 5)^2 + 100;
    c(2) = (x(1) - 6)^2 + (x(2) - 5)^2 - 82.81;
    ceq = [];
end


function fmin = get_fmin(~)
    fmin = -6961.8138751273809248;
end


function xmin = get_xmin(~)
```

```
    xmin = [14.0950000002011322; 0.8429607896175201];
end
```

Same as in Appendix C.1, the constrained optimization problem is passed to the algorithm as part of a P structure:

```
>> P.f = 'G06';
```

Next, assume that a user wants to stop the search as soon as the known solution is within a 0.01% error. The OPTS structure should be specified as follows:

```
>> opts.maxevals = 10000;          % Maximal number of function evaluations
>> opts.maxits = 1000;             % Maximal number of iterations
>> opts.testflag = 1;              % 1 if global minima is known, 0 otherwise
>> opts.tol = 0.01;                % Tolerance for termination if testflag = 1
>> opts.showits = 1;               % Print iteration status
```

The desired solver (in this case implementation of the DIRECT-GLc algorithm) is run using:

```
>> [f_min, x_min, history] = dDirect_GLc(P, OPTS);
```

Since opts.showits = 1, the optimization result after the each iteration is printed in the MATLAB command window:

```
Phase_II - searching feasible point:
con viol: 2404.4400000000 fn evals: 5
con viol: 515.5511111111  fn evals: 7
...
con viol: 0.1374240038    fn evals: 123
con viol: 0.0000000000    fn evals: 159  f_min: -5612.1483164940
Phase_I - Improve feasible solution:
Iter: 1   f_min: -5886.5625227848   time(s): 0.05935   fn evals: 197
Iter: 2   f_min: -5931.8554991123   time(s): 0.06473   fn evals: 241
...
Iter: 13  f_min: -6873.0583159376   time(s): 0.13197   fn evals: 947
Iter: 14  f_min: -6901.5099081387   time(s): 0.13869   fn evals: 1027
Minima was found with Tolerance:    1
```

We see that the solution $f_{min} = -6901.5099081387$ (within a 0.01% error) was found after 14 iterations.

C.3   Parallel algorithm usage

This section briefly explains how to use parallel versions of the algorithms. We can see which algorithms are implemented in parallel in Table 1. Assume a user wishes to use parallel code for the PLOR algorithm. First, a parallel implementation of the PLOR algorithm (parallel_dPlor.m) should be chosen. Next, a user should specify the number of workers (computational threads). For parallel PLOR, it is reasonable to select 2, as only two POH are selected per iteration. In

this case, MATLAB parallel pool size should be specified using the `parpool` command, after which the parallel algorithm should be executed:

```
>> parpool(2);
>> [f_min, x_min, history] = parallel_dPlor(P, OPTS);
```

By default, the *parpool* command starts the MATLAB pool on the local machine with one worker per physical CPU core. Using `parpool(2)`, we limit the number of workers to 2. After this, the parallel code is executed using both workers. However, it should be taken into account that creating parallel *parpool* takes some time. Therefore, using the parallel PLOR algorithm is inefficient in solving simple problems. The use of parallel codes should address higher-dimensionality, more expensive optimization problems [93]. When all necessary calculations in parallel mode are finished, the following command:

```
>> delete(gcp);
```

shuts down the parallel pool.