Mixed-Integer Constrained Grey-Box Optimization based on Dynamic Surrogate Models and Approximated Interval Analysis

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Abstract: In this paper an algorithmic framework, called GreyOpt, is proposed for the heuristic global optimization of simulations over general constrained mixed-integer sets, where simulations are expressed as a grey-box, i.e. computations using a mix of (1) closed-form analytical expressions, and (2) evaluations of numerical black-box functions that may be non-differentiable and computationally expensive. GreyOpt leverages the partially analytical structure of such problems to dynamically construct differentiable surrogate problems for multiple regions of the search space. These surrogate problems are then used in conjunction with a derivative-based method to locally improve sample points in each region. GreyOpt extends Moore interval arithmetic for approximating the intervals of grey-box objective and constraint functions by fitting quadric surfaces that attempt to roughly underestimate and overestimate embedded black-box functions. This serves as the foundation of a recursive partitioning technique that GreyOpt uses to refine the best points found in each region. An experimental study of GreyOpt's performance is conducted on a set of grey-box optimization problems derived from MINLPLib, where the ratio of black-box function evaluations to analytical expressions is small. The results of the study show that GreyOpt significantly outperforms three derivative-free optimization algorithms on these problems.

1 INTRODUCTION

This paper considers the problem of *mixed-integer constrained grey-box* (MICGB) optimization, namely, of a real objective $f(x,y)$ subject to a box-constrained, vector-valued constraint function $g(x,y)$, where vectors x and y represent real and integer decision variables, respectively, as formally defined in Section 2. This is under the assumption that both $f(x,y)$ and $g(x,y)$ are provided as a *grey-box simulation*, i.e. a computation using a mix of (1) closed-form analytical expressions, and (2) evaluations of numerical black-box functions that can be non-differentiable and computationally expensive. This class of problems can be viewed as a continuum between *white-box* optimization, where f and g are completely defined in closed analytical form, and *black-box* optimization, where f and g are provided as black-box functions.

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MICGB optimization has a wide-range of real-world applications across diverse commercial and industrial domains, such as logistics, manufacturing and supply chain management. This class of optimization problems also arise from the analysis of multi-disciplinary performance models that combine computationally expensive and/or data-driven simulations of continuous physical processes with metrics and constraints involving discrete and finite domain decision variables stemming from business processes ranging from product design to production planning and scheduling (Brodsky et al., 2019). Accurate and efficient analysis of these models is crucial for implementing effective decision guidance (DG) systems that support model-driven decision-making in these domains. DG systems are a special class of decision support systems (DSS) that process large amounts of data and analyze mathematical models to provide an iterative process of ranking, prioritizing, and suggesting actionable recommendations to and collecting feedback from decision-makers, with the goal of arriving at the best course of action (Brodsky and Wang,

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2008; Nachawati et al., 2017).

Despite a growing body of literature on grey-box optimization, today only black-box optimization algorithms are generally available for optimizing MICGB problems. Depending on the complexity of the problem, meta-heuristic black-box algorithms can provide adequate quality solutions with a reasonable level of computational effort Talbi (2013). For problems involving computationally expensive simulations, surrogate-based black-box algorithms, such as EGO (Jones et al., 1998), can find high quality solutions with significantly fewer costly objective and constraint function evaluations than non-surrogate black-box algorithms. However, these methods alone do not scale well for high-dimensional problems (Gilboa et al., 2013).

Although significant progress has been made on the development of black-box optimization algorithms, as their name implies they make little to no use of the partially-analytical structure of MICGB problems. In some cases it may be possible to reformulate grey- and black-box problems, ahead of time, into highly accurate analytical surrogate problems. This approach can take considerably more effort and can result in highly specialized surrogate models that are difficult to reuse and dynamically update (Mazumdar et al., 2019). However, for tightly-constrained and non-convex MICGB problems, the reformulated surrogate can then be optimized using efficient and globally convergent global optimization algorithms that otherwise would not be applicable to the original MICGB problem.

To ensure global convergence without degenerating into a brute-force search, efficient global optimization algorithms rely on the ability to efficiently fathom large areas of the search space with the aim of quickly finding areas that are likely to contain global optima and avoiding areas that do not. Several fathoming techniques have been proposed in the literature, including those based on: (1) interval arithmetic (Moore, 1966), (2) McCormick relaxations (McCormick, 1976), (3) α-convexification (Androulakis et al., 1995), and (4) Lipschitz continuity (Pintér, 1997). However, because of the significant limitations of the structure and behavior of problems that can be fathomed, none of the techniques above are generally applicable to MICGB optimization.

In recent years, researchers have attempted to enhance surrogate-based methods by exploiting the partially analytical structure of grey-box optimization problems. ARGONAUT, proposed by Boukouvala and Floudas (2017), supports the classification of individual objective and constraint functions as either white- or black-box. The black-box functions from the original problem are then replaced with approximations to generate a surrogate problem, which is repeatedly calibrated and then optimized using ANTIGONE, a global optimization solver originally developed by Misener and Floudas (2014). DEFT-FUNNEL, proposed by Sampaio (2019), follows a similar approach to ARGONAUT for classifying white- and black-box objective and constraint functions, but uses a sequential quadratic programming (SQP) method paired with a multi-level single linkage (MLSL) method instead of performing global optimization on the surrogate.

However, there are some significant limitations to those approaches. The authors of ARGONAUT report a significant computational overhead for model calibration. This problem is perhaps exacerbated by ARGONAUT's coarse-grain classification of objective and constraint functions as either white- or black-box. Specifically, ARGONAUT treats expressions that are largely analytical, but involve a nested black-box function evaluation as completely black-box. Also, the use of ANTIGONE—a global optimization solver—on every iteration against the surrogate problem is not cheap and may be of little use if the surrogate is not accurate. Finally, DEFT-FUNNEL does not support mixed-integer grey-box optimization, and, like ARGONAUT, it is also limited in its coarse-grain classification of objective and constraint functions.

Addressing these limitations is precisely the focus of this paper. Specifically, we make two main contributions. First, we propose GREYOPT, an algorithmic framework for the heuristic global optimization of MICGB problems. GREYOPT supports a more precise expression of grey-box problems than ARGONAUT and DEFT-FUNNEL, where the analytical structure, if any, of each objective and constraint functions is preserved. GREYOPT leverages the partially analytical structure of such problems to dynamically construct differentiable surrogate problems for multiple regions of the search space. These surrogate problems are then used in conjunction with a derivative-based method to locally improve sample points in each region. GREYOPT extends Moore interval arithmetic (Moore, 1966) for approximating the intervals of grey-box objective and constraint functions. This serves as the foundation of a recursive partitioning technique that GREYOPT uses to refine the best points found in each region.

Second, we conduct an experimental study of GREYOPT's performance on a set of 25 MICGB optimization problems, where the ratio of black-box function evaluations to analytical expressions is small.

The test problems are derived from MINLPLib[1] by replacing some nonlinear terms of the object and constraint functions with calls to otherwise equivalent black-box functions. We adopt an evaluation methodology based on performance profiles (Dolan and Moré, 2002) and data profiles (Moré and Wild, 2009). The results of the study show that GREYOPT significantly outperforms three derivative-free optimization algorithms on these problems.

The rest of this paper is organized as follows. In Section 2 we formally describe the MICGB class of optimization problems that GREYOPT is designed to handle. In Section 3 we describe the GREYOPT algorithmic framework for the heuristic global optimization of MICGB problems. In Section 4 we present an experimental study of GREYOPT's performance. Finally, in Section 5 we conclude the paper with some brief remarks on directions for future work.

2 PROBLEM FORMULATION

Without loss of generality, this paper considers MICGB optimization problems of the following form:

$$\underset{x\in\mathbb{R}^n,\ y\in\mathbb{R}^m}{\text{minimize}} \quad f(x,y) \tag{1a}$$

$$\text{subject to} \quad g_L \leq g(x,y) \leq g_U \tag{1b}$$

$$x_L \leq x \leq x_U \tag{1c}$$

$$y_L \leq y \leq y_U \tag{1d}$$

$$y \in \mathbb{Z}^m \tag{1e}$$

where $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ is the objective function to be minimized, and where $g : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^q$ is the vector-valued function of constraints, bounded below by $g_L \in \mathbb{R}^q$ and above by $g_U \in \mathbb{R}^q$, and where $x \in \mathbb{R}^n$ are the real decision variables bounded below by $x_L \in \mathbb{R}^n$ and above by $x_U \in \mathbb{R}^n$, and where $y \in \mathbb{R}^m$ are the integer decision variables bounded below by $y_L \in \mathbb{R}^m$ and above by $y_U \in \mathbb{R}^m$, and lastly where $n,m,q \in \mathbb{N}_0$.

Stochastic optimization problems can be handled using the formulation above through the use of expected values and chance constraints (Charnes and Cooper, 1959). A stochastic objective $\tilde{f}(x,y,\xi)$, where ξ is the vector of uncertainty, can be transformed into the objective function $f(x,y) \triangleq E(\tilde{f}(x,y,\xi))$, i.e. its expected value. Stochastic constraints $\tilde{g}_L \leq \tilde{g}(x,y,\xi) \leq \tilde{g}_U$ can be transformed into the constraints $g_L \leq g(x,y) \leq g_U$, where $g(x,y) \triangleq P(\tilde{g}_L \leq \tilde{g}(x,y,\xi) \leq \tilde{g}_U)$, and where g_L and g_U are the lower and upper bounds of the vector of probabilities that the stochastic constraints hold.

[1]URL: http://www.minlplib.org/

It is assumed that $f(x,y)$ and $g(x,y)$ are provided as a factorized grey-box simulation over input vectors x and y, formally expressed as a Wengert list (Wengert, 1964) of $K \in \mathbb{N}$ assignments:

$$(e_i \triangleq E_i(a_i))_{i=1}^{K} \tag{2}$$

where the computed values of $f(x,y)$ and $g(x,y)$ correspond to values e_F and e_G, respectively, given $F,G \in [1,K]$, and where e_i is a tensor of real-valued elements, and where input a_i is a sequence of zero or more values, in any order, from the sequence $(e_1,...,e_{i-1})$, and lastly where E_i is one of the following:

- a constant tensor of real-valued elements
- a tensor of real-valued elements composed of any of the components of variables x and y or any of the elements of tensors $e_1,...,e_{i-1}$
- a closed-form analytical expression in terms of the elements of input a_i
- an evaluation of a black-box function $\mathbb{R}^N \to \mathbb{R}^M$ on input a_i

3 GREY-BOX OPTIMIZATION

This section describes the GREYOPT algorithmic framework for the heuristic global optimization of MICGB problems. The main idea behind GREYOPT is two-fold. First, the partially analytical structure of MICGB optimization problems is leveraged to dynamically construct differentiable surrogate problems for different regions of the search space. These surrogate problems are then used in conjunction with a derivative-based method to locally improve sample points in each region. Second, a recursive partitioning technique with a fathoming heuristic based on an approximated interval analysis is used to refine the best points in each region.

Assuming the compact interval notation of $[x] \triangleq [\underline{x},\overline{x}]$, where $\underline{x}$ and $\overline{x}$ are the lower and upper bounds of interval $[x]$, respectively, given a function $f : \mathbb{R}^n \to \mathbb{R}^m$, its *interval extension* (Moore, 1966) is a function $[f] : [\mathbb{R}]^n \to [\mathbb{R}]^m$ such that for any input interval $[x] \in [\mathbb{R}^n]$ the resulting interval $[f]([x])$ bounds all the points in the set $\{f(y) : \forall y \in [x]\}$. Moore interval arithmetic provides interval extensions of many standard arithmetic operations and functions that are generally admitted in closed-form expressions. For example, the addition of intervals $[x]$ and $[y]$ is defined as $[x]+[y] \triangleq [x_L+y_L, x_L+y_L]$. For a general function $f : \mathbb{R}^n \to \mathbb{R}^m$ that can be defined in such closed analytical form, its interval extension can be obtained by the recursive substitution of each operation and function with their respective interval extension. This is known as the *natural interval extension* (Moore, 1966). GREYOPT extends Moore interval arithmetic for approximating the natural interval extension of grey-box objective and constraint functions by fitting quadric surfaces (see Equation 6 and Figure 1) that roughly underestimate and overestimate each embedded black-box function call.

The high-level pseudocode for GREYOPT is given in Algorithm 1. For input, GREYOPT expects a tuple p that fully describes the MICGB optimization problem:

$$p \triangleq \langle e, F, G, x_0, y_0, x_L, x_U, y_L, y_U, g_L, g_U \rangle \quad (3)$$

where e is a Wengret list representing the factorized grey-box simulation (see Equation 2), and where F and G are indexes of e that correspond to the objective function $f(x,y)$ value and constraint function $g(x,y)$ value, respectively, and where x_0 and y_0 are the initial values for the decision variables, and where x_L, x_U, y_L, and y_U are the upper and lower bounds of the decision variables, and finally where g_L and g_U are the upper and lower bounds of the constraint function $g(x,y)$.

The parameters of GREYOPT are denoted in this section by `MONOSPACED` text. GREYOPT expects to be provided a configuration of parameter values that define its run-time behavior. As an algorithmic framework, each parameterization can be considered as a particular algorithm of GREYOPT to run. Upon termination, GREYOPT returns the best point (x^*, y^*) found during the search. As a heuristic algorithm, GREYOPT makes no guarantee that the point it returns is either optimal or feasible, even if such a solution is known to exist. The rest of this section describes the essential steps of the GREYOPT in more detail.

LINE 1 of Algorithm 1—*Initialization.* For problem p, GREYOPT begins by calling the Initialize routine, which returns (1) an initial champion point (x^*, y^*) using the initial values (x_0, y_0) for the decision variables of problem p, and (2) a priority queue R of regions. In the implementation of GREYOPT, if an initial value is not provided for a real-valued decision variable x_i, the midpoint of its bounds $\frac{x_{L_i}+x_{U_i}}{2}$ is used. For an integer-valued decision variable y_i, the closest integer to the midpoint within the bounds of the decision variable is used, i.e. $\lfloor \frac{y_{L_i}+y_{U_i}}{2} \rfloor$ or $\lceil \frac{y_{L_i}+y_{U_i}}{2} \rceil$.

During the evaluation of the objective and constraint functions for initial values (x_0, y_0), GREYOPT records the execution time for each black-box function call to determine whether a surrogate function should be used. If the execution time, in seconds, of a black-box function does not exceed `BLACKBOX_TIME_THRESHOLD`, then GREYOPT

Algorithm 1: GREYOPT.

```
Input: $p$
Output: $x^* \in \mathbb{R}^n, y^* \in \mathbb{R}^m$
Method:
1  $(x^*, y^*, R) \leftarrow \mathsf{Initialize}(p)$
2  $i \leftarrow 0$
3  do
4      $r \leftarrow \mathsf{SelectRegion}(R, i)$
5      $(x_r^*, y_r^*) \leftarrow \mathsf{Champion}(\{r\})$
6      if $x_L(r) = x_U(r) \wedge y_L(r) = y_U(r)$ then
7          goto LINE 25 of Algorithm 1
8      $S_0 \leftarrow \mathsf{Sample}(r)$
9      $r \leftarrow \mathsf{Calibrate}(r, S_0)$
10     $S_1 \leftarrow \{\}$
11     foreach $(x_0, y_0) \in S_0$ do
12         $(\tilde{x}, \tilde{y}) \leftarrow \mathsf{Improve}(r, x_0, y_0)$
13         if $\mathsf{SurrogateCompare}(r, \tilde{x}, \tilde{y}, x_r^*, y_r^*)$
            then
14             if $\tilde{y} \notin \mathbb{Z}^m$ where $m \triangleq |\tilde{y}|$ then
15                 $(\tilde{x}, \tilde{y}) \leftarrow \mathsf{Repair}(r, \tilde{x}, \tilde{y})$
16             if $p$ is separable then
17                 $(\tilde{x}, \tilde{y}) \leftarrow \mathsf{FixedImprove}(p, \tilde{x}, \tilde{y})$
18             if $\mathsf{Compare}(p, \tilde{x}, \tilde{y}, x_r^*, y_r^*)$ then
19                 $S_1 \leftarrow S_1 \cup (\tilde{x}, \tilde{y})$
20                 $r \leftarrow \mathsf{UpdateChampion}(r, \tilde{x}, \tilde{y})$
21     end
22     if $|S_1| > 0$ then
23         $R \leftarrow R \cup \mathsf{Cluster}(r, S_1)$
24     else
25         $R \leftarrow R \cup \mathsf{Refine}(r, R)$
26     while $|R| >$ MAX_REGION_QUEUE_SIZE do
27         $R \leftarrow R \setminus \{\mathsf{WorstRegion}(R)\}$
28     end
29     $i \leftarrow i + 1$
30     $(x^*, y^*) \leftarrow \mathsf{Champion}(R)$
31 while $\neg\mathsf{Converged}(R, i)$
32 return $(x^*, y^*)$
```

will not generate surrogates for that function and its derivatives will be approximated by finite differences. In the implementation of GREYOPT, this feature can be disabled by the user on a per-function basis. For the rest of this section, we use the term black-box function to refer exclusively to those whose derivatives will not be approximated by finite differences, unless otherwise noted. After initialization, GREYOPT iterates through lines 4-30 of Algorithm 1 until at least one of the convergence criteria has been fulfilled (see the description for LINE 31 of Algorithm 1).

The region queue R is initialized with the global region object r_g corresponding to the entire search space of problem p. Region objects are used as an intensification mechanism by GREYOPT to restrict sampling and surrogate calibration to a specific area of a problem's search space. Formally, a region object r is defined by a tuple:

$$r \triangleq \langle \tilde{p}, i, x^*, y^*, x_L, x_U, y_L, y_U \rangle \tag{4}$$

where $\tilde{p}$ is the region's surrogate problem, and where i is the region's iteration count, and where (x^*, y^*) is the region's champion point (i.e. the best point found in that region), and where x_L, x_U, y_L, and y_U are the upper and lower bounds of the decision variables for the region. The surrogate problem $\tilde{p}$ is obtained by replacing all the black-box functions of the original problem p with surrogate functions that are calibrated using all the sample points that fall within the bounds of the region (see the description for LINE 9 of Algorithm 1).

LINE 4 of Algorithm 1—*Region Selection*. At the start of each iteration, GREYOPT selects and removes a region r from the front of region queue R, and increments the iteration count i of region r. To balance exploration versus exploitation, regions within R are first ordered by the iteration count i, and then by the fitness of its champion point (x^*, y^*). GREYOPT uses the comparison function in Algorithm 2 to compare the fitnesses of two points (x_0, y_0) and (x_1, y_1), where the Evaluate function computes the objective value f, the constraint values vector g, and the constraint violation vector v for a point (x, y) in the search space of problem p.

Algorithm 2: Comparison.

```
1  function Compare($p, x_0, y_0, x_1, y_1$)
2      $m \leftarrow |y_0|$
3      $(f_0, g_0, v_0) \leftarrow$ Evaluate($p, x_0, y_0$)
4      $(f_1, g_1, v_1) \leftarrow$ Evaluate($p, x_1, y_1$)
5      if $\|v_0\|_2 = 0$ then
6          if $\|v_1\|_2 > 0$ then
7              return true
8          if $y_0 \in \mathbb{Z}^m$ then
9              if $y_1 \notin \mathbb{Z}^m$ then
10                 return true
11         else if $y_1 \in \mathbb{Z}^m$ then
12             return false
13         return $f_0 < f_1$
14     if $\|v_1\|_2 = 0$ then
15         return false
16     return $\|v_0\|_2 < \|v_1\|_2$
17 end
```

LINE 8 of Algorithm 1—*Sampling*. For each iteration, GREYOPT randomly samples a set S_0 of points within the bounds of the selected region r. If the problem has no black-box functions then only one point is randomly sampled per iteration, otherwise the total number of points to sample is determined by the MAXIMUM_SAMPLES_PER_ITERATION parameter.

Samples are drawn by alternating between two different sampling distributions: (1) a uniform distribution $U(a,b)$, where $a \triangleq (x_L, y_L)$ and $b \triangleq (x_U, y_U)$, and (2) a modified-PERT distribution $MPERT(a,b,c,\gamma)$, where $a \triangleq (x_L, y_L)$, $b \triangleq (x^*, y^*)$, $c \triangleq (x_U, y_U)$, and $\gamma \triangleq (x_U - x_L, y_U - y_L)$. For integer-valued decision variables, the closest integer to the sampled value within the bounds of the decision variable is selected. The rationale behind the use of the two distributions is to balance between sample point diversity that is provided by the uniform distribution, and sample point intensification around the current champion point (x^*, y^*) of region r that is provided by the modified-PERT distribution.

Definition 3.1 (White-box Constraint)**.** Let p be a MICGB problem with vector-valued constraint function $g(x,y)$. We say that a component $g_i \in g(x,y)$ is a *white-box constraint* if and only if its computation does not entail any call to a black-box function.

Definition 3.2 (Restorable Problem)**.** Let p be a MICGB problem with vector-valued constraint function $g(x,y)$. We say that p is a *restorable problem* if and only if there exists a component $g_i \in g(x,y)$ that is a white-box constraint.

For highly constrained problems, it is unlikely that any sample point (x_0, y_0) will be feasible. If the problem is restorable, GREYOPT tries to find the closest point (x,y) that satisfies all white-box constraints $g_i \in g(x,y)$ by solving the following restoration problem:

$$\underset{x \in \mathbb{R}^n,\, y \in \mathbb{R}^m}{\text{minimize}} \quad \|x_0 - x\|_2 + \|y_0 - y\|_2 \tag{5a}$$

$$\text{subject to} \quad w_L \le w(x,y) \le w_U \tag{5b}$$

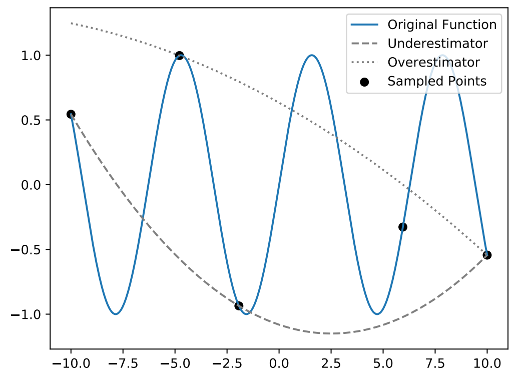
$$x_L \le x \le x_U \tag{5c}$$

$$y_L \le y \le y_U \tag{5d}$$

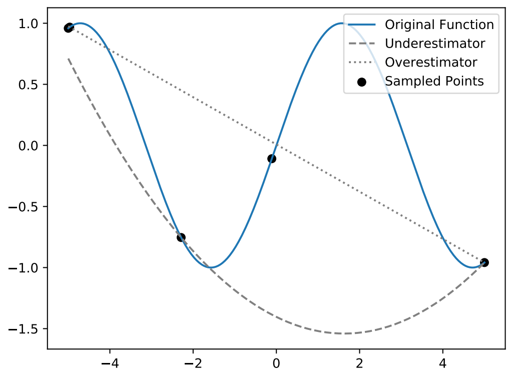
$$y \in \mathbb{Z}^m \tag{5e}$$

where (x_0, y_0) is the sample point to restore, and where (x,y) are the decision variables representing the restored point, and where $w : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^q$ is the vector-valued function of white-box constraints that is obtained from $g(x,y)$ of the original problem by removing all components $g_i \in g(x,y)$ that are not a white-box constraint, and where $w(x,y)$ is bounded below by $w_L \in \mathbb{R}^q$ and above by $w_U \in \mathbb{R}^q$. If successful, the original sample point (x_0, y_0) is replaced by the restored point (x,y).

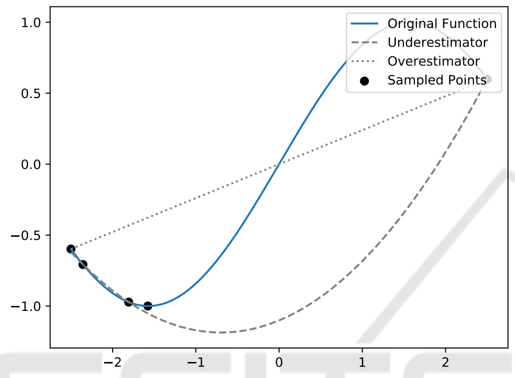
LINE 9 of Algorithm 1—*Calibration*. The Calibrate routine constructs and calibrates a surrogate problem $\tilde{p}$ for region r by replacing each call



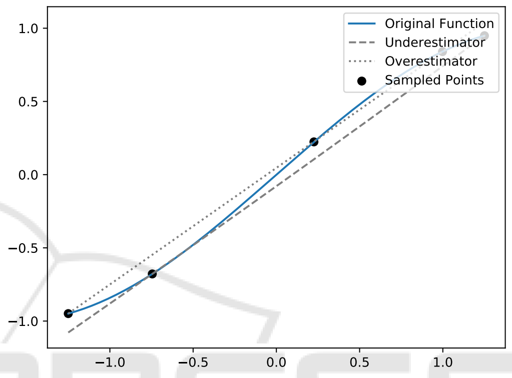
(a) Interval [-10, 10].



(b) Interval [-5, 5].



(c) Interval [-2.5, 2.5].



(d) Interval [-1.25, 1.25].

Figure 1: Plots of $sin(x)$ versus quadric surrogates used as a rough underestimator and overestimator that is fitted based on three randomly sampled points, plus the limit points, over increasingly smaller intervals.

to a black-box function $\mathcal{B}$ in the original problem with a call to a corresponding surrogate function. For each black-box function $\mathcal{B}$, the upper and lower bounds of region r are projected onto the domain of the $\mathcal{B}$ using the approximated interval arithmetic described at the beginning of this section. The projected upper and lower bounds of the domain of $\mathcal{B}$ in region r are used to select a subset $S_{\mathcal{B}}$ of previously evaluated input and output values for $\mathcal{B}$ from a cache that is maintained for each black-box function. The size of this cache is controlled by the `MAXIMUM_CACHED_SAMPLES_PER_FUNCTION` parameter. If a surrogate function has already been constructed and calibrated for $\mathcal{B}$ in region r, the coefficient of determination, i.e. R^2 score, is computed using set $S_{\mathcal{B}}$. If the R^2 score of the surrogate function falls below `CALIBRATION_SCORE_THRESHOLD`, it is replaced by a new surrogate function that is calibrated using set $S_{\mathcal{B}}$. Otherwise, the previously calibrated surrogate function is reused for the remainder of the current iteration.

A simple model selection method on an ordered set of candidate surrogate models is used to automatically choose a surrogate function for black-box function $\mathcal{B}$. In the implementation of GREYOPT the following two regression models, provided by scikit-learn (Pedregosa et al., 2011), are considered for model selection: (1) a polynomial regression model using a combination of polynomial features, where the maximum degree is controlled by the `MAXIMUM_POLYNOMIAL_SURROGATE_DEGREE` parameter, and (2) a Gaussian process regression (GPR) model with a radial basis function (RBF) kernel. The polynomial model is first calibrated and scored using set $S_{\mathcal{B}}$ of input and output values. If its R^2 score is greater than or equal to `CALIBRATION_SCORE_THRESHOLD`, then the calibrated polynomial model is chosen. Otherwise the GPR model is calibrated and scored using $S_{\mathcal{B}}$, and the model with the best R^2 is chosen.

To calibrate the quadric surface used to approximately underestimate a black-box function $\mathcal{B} : \mathbb{R}^n \rightarrow \mathbb{R}^m$, the following constrained regression problem is

Algorithm 3: Refinement.

```
function Refine($(r,R)$)
    $(x^*,y^*) \leftarrow$ Champion($R$)
    $R^* \leftarrow \{\}$
    $c \leftarrow 0$
    $R_c \leftarrow \{$ExpandChampion$(r,c)\}$
    while $|R_c| > 0$ do
        $r_c \leftarrow$ RefinementRegion($R_c$)
        $x_\Delta \leftarrow \|x_U(r_c) - x_L(r_c)\|_\infty$
        $y_\Delta \leftarrow \|y_U(r_c) - y_L(r_c)\|_\infty$
        $\sigma \leftarrow \min\{\varepsilon, \frac{\text{MINIMUM\_PARTITION\_SIZE}}{10^c}\}$
        if $x_\Delta \le \sigma \wedge y_\Delta \le \sigma$ then
            $R^* \leftarrow R^* \cup \{r_c\}$
            if $|R^*| \ge$ MAX_REFINES then
                break
        else
            $x_m \leftarrow \frac{x_L(r_c)+x_U(r_c)}{2}$
            $y_m \leftarrow \frac{y_L(r_c)+y_U(r_c)}{2}$
            $(f_c,g_c) \leftarrow$ Evaluate($p,x_m,y_m$)
            if $\neg$Validate($r_c,f_c,g_c$) then
                $r_c \leftarrow$ CalibrateQuadric($r_c$)
            $(r_0,r_1) \leftarrow$ Partition($r_c$)
            if RegionCompare($r_0,x^*,y^*$) then
                $R_c \leftarrow R_c \cup \{r_0\}$
            if RegionCompare($r_1,x^*,y^*$) then
                $R_c \leftarrow R_c \cup \{r_1\}$
        while $|R_c| >$ CACHED_REGIONS do
            $R_c \leftarrow R_c \setminus \{$WorstRegion$(R_c)\}$
        end
        $c \leftarrow c+1$
        if $c >=$ ITERATION_LIMIT then
            break
    end
    if $r$ is the global region then
        $R^* \leftarrow R^* \cup \{r\}$
    else if $|R^*| = 0$ then
        if RegionCompare($r,x^*,y^*$) then
            $R^* \leftarrow R^* \cup \{r\}$
    return $R^*$
end
```

solved:

$$\underset{A,B,C}{\text{minimize}} \quad \|Y - (AX^{\circ 2} + BX + CJ)\|_2 \tag{6a}$$

$$\text{subject to} \quad Y - (AX^{\circ 2} + BX + CJ) \ge \varepsilon \tag{6b}$$

$$\forall i\, \forall j, A_{ij} \ge \varepsilon \tag{6c}$$

where $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times n}$, $C \in \mathbb{R}^{m\times 1}$ are the coefficients of the quadric surface, where $J \in \{1\}^{1\times s}$ is a unit matrix, where $X \in \mathbb{R}^{n\times s}$ and $Y \in \mathbb{R}^{m\times s}$ are the input and output values of S_b in matrix form, where s is the number of samples in $S_{\mathcal{B}}$, and where $\circ$ is used to denote element-wise exponentiation. A small positive number constant, ε, is used (1) to ensure that the quadric surface is never greater than any of the output values contained in $S_{\mathcal{B}}$ (Equation 6b), and (2) to ensure the convexity of the quadric surface (Equation 6c).

The quadric surface for approximately overestimating a black-box function $\mathcal{B}$ is calibrated in a similar fashion, except the inequalities in Equation 6 are reversed. Figure 1 shows some plots of $sin(x)$ versus quadric surrogates used as a rough underestimator and overestimator that is fitted based on three randomly sampled points, plus the limit points, over increasingly smaller intervals.

LINES 10-21 of Algorithm 1—*Improvement.* With the surrogate problem $\tilde{p}$ of region r constructed, GREYOPT tries to locally improve each sample point $(x_0,y_0) \in S_0$. The Improve routine runs a derivative-based convex nonlinear optimization solver on $\tilde{p}$ with a starting point of (x_0,y_0). In the implementation of GREYOPT, the open-source solver IPOPT (Wächter and Biegler, 2006) is used with a `max_cpu_time` of

$$\text{IMPROVE\_TIME\_LIMIT\_FACTOR} \times (n+m+q) \tag{7}$$

where n, m, and q are the number of variables (real- and integer-valued) and constraints of the problem p (see the MICGB formulation in Equation 1).

On Line 13 of Algorithm 1, the call to the SurrogateCompare function compares the surrogate fitnesses of points $(\tilde{x},\tilde{y})$ and (x_r^*,y_r^*) using the surrogate problem of region r, and returns `true` if $(\tilde{x},\tilde{y})$ is better than (x_r^*,y_r^*), and `false` otherwise. The SurrogateCompare function is similar to the comparison function in Algorithm 2), except that it uses the surrogate problem of region r to evaluate the objective value f and constraint violations vector v, and it relaxes the requirement for integer feasibility.

On Lines 14-15 of Algorithm 1, if the point $(\tilde{x},\tilde{y})$ is not integer feasible, the Repair routine runs a derivative-based, mixed-integer convex nonlinear optimization solver on $\tilde{p}$ with a starting point of $(\tilde{x},\tilde{y})$ to try to achieve integer feasibility. In the implementation of GREYOPT, the open-source solver BONMIN (Bonami et al., 2008) is used with a `time_limit` of

$$\text{REPAIR\_TIME\_LIMIT\_FACTOR} \times (n+m+q) \tag{8}$$

where n, m, and q are the number of variables (real- and integer-valued) and constraints of the problem p (see the MICGB formulation in Equation 1).

Definition 3.3 (White-box Decision Variable)**.** Let p be a MICGB problem with decision variables (x,y). We say that a real-valued decision variable $x_i \in x$ or an integer-valued decision variable $y_i \in y$ is a *white-box decision variable* if and only if that variable does not contribute to the input of any black-box function called for the computation of the objective and constraint functions of p.

Definition 3.4 (Separable Problem)**.** Let p be a MICGB problem with decision variables (x,y). We say that p is a *separable problem* if and only if there exists a real-valued decision variable $x_i \in x$ or an integer-valued decision variable $y_i \in y$ that is white-box.

On Lines 16-17 of Algorithm 1, if problem p is separable, the FixedImprove routine runs a derivative-based, mixed-integer convex nonlinear optimization solver on the original problem p with a starting point of $(\tilde{x},\tilde{y})$. Unlike with the Improve routine, which uses the original decision variable bounds of the problem p, the FixedImprove routine fixes the bounds of all decision variables that are not white-box to the values of the champion point (x_r^*,y_r^*). To prevent costly re-evaluations of black-box functions, GREYOPT caches and recalls the last evaluated point for each black-box function call while running FixedImprove.

On Line 18 of Algorithm 1, the call to the Compare function compares the fitnesses of points $(\tilde{x},\tilde{y})$ and (x_r^*,y_r^*), using the original problem p, and returns `true` if $(\tilde{x},\tilde{y})$ is better than (x_r^*,y_r^*), and `false` otherwise (see Algorithm 2). If Compare returns `true`, the point $(\tilde{x},\tilde{y})$ is added to set S_1 and the champion point of r is updated (as appropriate).

LINES 22-23 of Algorithm 1—*Clustering*. If the improvement step finds points that are better than the current champion point of region r, i.e. $|S_1| > 0$, GREYOPT calls the Cluster routine to construct a set of new regions around those points. For each point $(x_j,y_j) \in S_1$ a new region r_j is constructed, in the form of Equation 4, by reusing the previously calibrated surrogate problem $\tilde{p}_r$ from region r and initially setting its upper and lower bounds to (x_j,y_j), as shown below:

$$r_i \triangleq \langle \tilde{p}_r, 0, x_i, y_i, x_i, x_i, y_i, y_i \rangle \tag{9}$$

The set of new regions, R_i, constructed from the points $(x_j,y_j) \in S_1$ are then iteratively clustered so that the infinity norm of the difference between the midpoints of any two regions $(r_0,r_1) \in R_i \times R_i$ is greater than the `MAXIMUM_CLUSTERING_DISTANCE` parameter. Clustering two regions r_0 and r_1 involves replacing them with a new larger region having a champion point as the better champion point of regions r_0 and r_1 and having an upper and lower bounds as the union of the upper and lower bounds of regions r_0 and r_1.

These new regions are then added to the region queue R, replacing the current region r. An exception is made if the current region r happens to be the global region r_g. In this case, the global region r_g is appended to the set of regions returned by the Cluster routine to ensure that it remains a candidate in the region queue R for selection at the start of each iteration.

LINES 24-25 of Algorithm 1—*Refinement*. At the end of each iteration, if a new champion point has not been found for region r, i.e. $|S_1| = 0$, then a refinement of current champion point of region r is performed. The Refine function takes in a region r and region queue R and returns a new set of tightly bounded regions that (1) have an approximated constraint interval that intersects the constraint bounds of the problem, $[g_L, g_U]$, and (2) have an approximated objective interval with a lower bound less than the objective value of the champion point of every region in the region queue R. The approximation of the objective and constraint intervals of region r is performed according to the approximated interval arithmetic described at the beginning of this section. Like with the clustering step, these new regions are then added to the region queue R, replacing the current region r with a set of regions that more tightly constrain the search space for sampling and surrogate construction.

The pseudocode of the Refine function is given in Algorithm 3. The ExpandChampion function, called on Line 5 of Algorithm 3, constructs a new region around the champion point of region r such that the approximated intervals of the objective and constraints of region r satisfies conditions (1) and (2) from the previous paragraph. This is done by iteratively expanding the bounds of randomly chosen decision variables until these conditions have been satisfied. The RefinementRegion function, called on Line 7 of Algorithm 3, selects and removes a region r_c from R_c that has an approximated objective interval with a lower bound that is less than or equal to all other regions $r \in R_c$. The Validate function, called on Line 19 of Algorithm 3, returns a value of `true` if f_c and g_c are contained in the approximated intervals of the objective and constraints, respectively, otherwise it returns a value of `false`.

The CalibrateQuadric function, called on Line 20 of Algorithm 3, updates the coefficients of the quadric surfaces used as rough underestimators and overestimators of region r_c using the known values for the midpoint (x_m,y_m) and the limit points of the region r_c by solving the constrained regression problem in Equation 6. The Partition function, called on Line 21 of Algorithm 3, takes a region r and returns two new regions $r0$ and r_1 by bisecting the bounds of region r on a single decision variable with largest, or one of the largest, difference between its lower and upper bound. The RegionCompare function, called on lines 22, 24, and 36 of Algorithm 3, takes in a region r and a point

(x,y) returns a value of `true` if (1) the approximated constraint interval of region r intersects the constraint bounds of the problem, $[g_L, g_U]$ and (2) when point (x,y) is feasible the approximated objective interval of region r has a lower bound that is strictly less than the objective value for point (x,y).

LINES 26-28 of Algorithm 1—*Truncation*. While the clustering and refinement steps add new regions to the region queue R, at the end of each iteration, the truncation step ensures that the size of R does not grow unwieldy large. This is done by removing the region $\mathsf{WorstRegion}(R)$ from R until its size does not exceed `MAXIMUM_REGION_QUEUE_SIZE`. The WorstRegion function accepts a set of regions R and returns a region $r_w \in R$ whose champion point is not better than any other region $r \in R$.

LINE 31 of Algorithm 1—*Convergence*. After finding an initial solution, GREYOPT, like other iteration-based optimization algorithms, produces a monotonically decreasing sequence of objective function values as better solutions are found. Short of an exhaustive search, there is generally no indication that any particular point of a MICGB problem is indeed a globally optimal solution. Thus, for the practical use of GREYOPT, it is necessary to impose convergence criteria to ensure that it terminates within a finite number of iterations. GREYOPT converges when any of the following thresholds are reached: (1) maximum CPU time, (2) maximum number of black-box function evaluations, (3) maximum number of iterations with no improvement, or (4) when a feasible point has been found at or below a target objective value. Upon convergence, GREYOPT halts the main iteration and returns the best point (x^*, y^*) found among all regions in R.

4 EXPERIMENTAL STUDY

This section presents an experimental study of GREYOPT's performance against three derivative-free optimization algorithms on a set of 25 MICGB optimization problems derived from MINLPLib.

4.1 Test Problems

Despite a growing body of literature, we were unable to find a standard collection of MICGB problems, similar in scope to what exists for other classes of problems, such as MINLPLib for mixed-integer nonlinear programming (MINLP), and BBOB (Hansen et al., 2010) for black-box optimization. To evaluate ARGONAUT, Boukouvala and Floudas (2017) construct a set of grey-box problems from GlobalLib and CUTEr by making some of the objective or constraint functions a black-box. A similar approach is adopted for this study, but rather than making the entire objective or constraint a black-box, only some of its nonlinear terms are replaced with calls to otherwise equivalent black-box functions that compute those terms.

For this study, we developed a tool using an open-source AMPL parser library, available on GitHub[2], to automatically translate problems from MINLPLib into MICGB optimization problems. The tool works by replacing three nonlinear terms in the objective and constraints with calls to, otherwise equivalent, black-box functions. The resulting MICGB problems are expressed in Python using a light-weight expression library that we developed on top of CasADi and NumPy. To illustrate how MICGB problems can be implemented with GREYOPT in Python, an example that was derived from the *trigx* problem of MINLPLib is provided in Figure 3, where the `n.call` function is used to wrap calls to black-box functions.

From all 1704 problems in MINLPLib at the time we conducted this study, we focused only on the 636 problems that had an AMPL .mod file size less than 10 kilobytes. Then from these 636 problems, 310 problems were successfully translated by our tool. Finally, from these 310 translated problems, a set of 25 problems were randomly selected for the study, which are listed in Table 1 of the Appendix. There were three reasons why our tool failed to translate the other 326 problems: (1) the problem had less than three nonlinear terms in the objective and constraints, considering only one nonlinear term per objective or constraint, (2) a limitation[3] of the CPython parser that causes a stack overflow when parsing deeply nested expression, and (3) the AMPL model was too complex for our tool to parse.

4.2 Test Algorithms

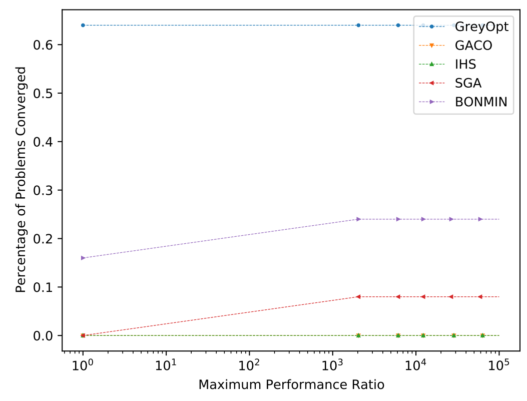
This study compares the performance of GREYOPT against the following derivative-free optimization algorithms: (1) *GACO*[4] – Extended Ant Colony Optimization (Schlüter et al., 2009), (2) *IHS*[4] – Improved Harmony Search (Mahdavi et al., 2007), and (3) *SGA*[4,5] – Simple Genetic Algorithm (Oliveto et al., 2007). The implementation of these algorithms is provided by Pygmo2 (Biscani and Izzo, 2020). The criteria we used to select these algorithms for this study was simply to include all derivative-free algo-

[2]URL: https://github.com/danielvatov/ampl

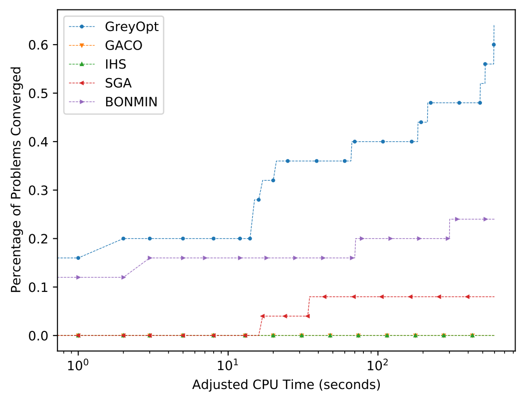
[3]URL: https://bugs.python.org/issue3971

[4]As implemented in Pygmo2, Version 2.16.0

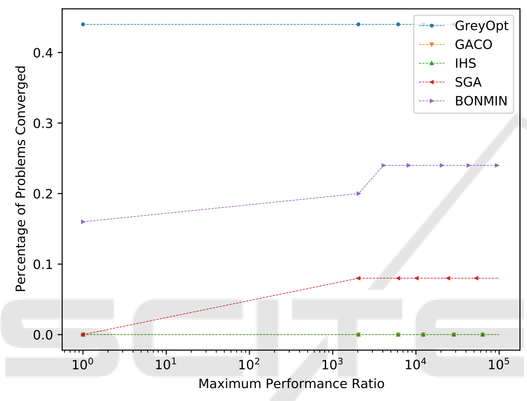
[5] With Pygmo2's self-adaptive constraint handling algorithm based on the work of Farmani and Wright (2003)



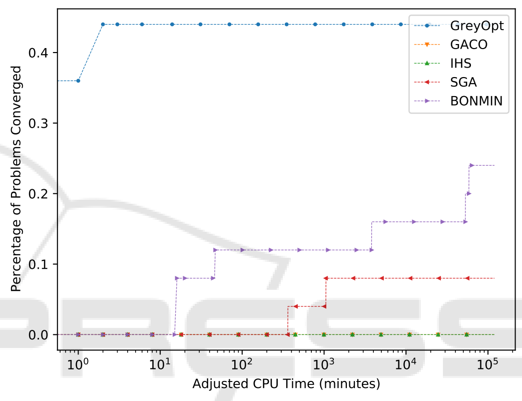
(a) Performance Profile
BBT = 0 seconds (per call).



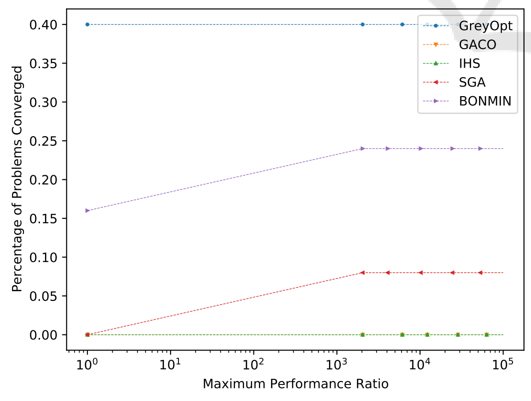
(b) Data Profile
BBT = 0 seconds (per call).



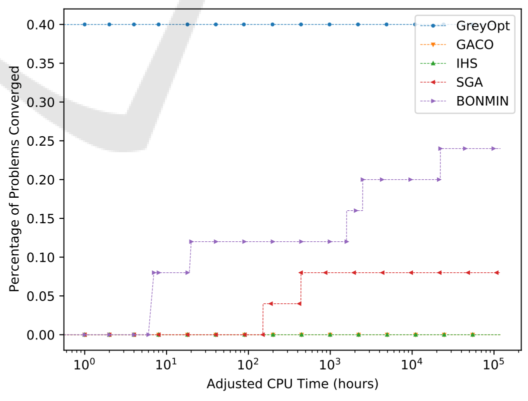
(c) Performance Profile
BBT = 1 second (per call).



(d) Data Profile
BBT = 1 second (per call).



(e) Performance Profile
BBT = 10 seconds (per call).



(f) Data Profile
BBT = 10 seconds (per call).

Figure 2: Performance and data profiles using the median of multiple runs of each algorithm for different levels of black-box function computation times (BBT).

rithms in Pygmo2 that support mixed-integer optimization. We were unable to find any available implementation of a grey-box optimization algorithm that supports MICGB problems. Although an open-source implementation in MATLAB of DEFT-FUNNEL is available on GitHub[6], it does not support MICGB

[6]https://github.com/phrsampaio/deft-funnel

```
import greyopt.numerics as n

def trigx_model(input, options={}):
  bbt = options.get("bbt", None)
  x2 = input["x2"]
  x3 = input["x3"]
  return {
    "obj": n.call(lambda x2: x2 * x2, x2, bbt=bbt)
        + x3 * x3,
    "constraints": {
      "e2": x2 - n.call(lambda x2, x3: n.sin(
        2.0 * x2 + 3.0 * x3), x2, x3, bbt=bbt)
        - n.cos(3.0 * x2 - 5.0 * x3) == 0.0,
      "e3": x3 - n.call(lambda x2, x3: n.sin(
        x2 - 2.0 * x3), x2, x3, bbt=bbt)
        + n.cos(x2 + 3.0 * x3) == 0.0
    }
  }

def trigx(options={}):
  output = trigx_model({
    "x2": n.variable(name="x2", value=None,
      bounds=[float("-inf"), float("inf")]),
    "x3": n.variable(name="x3", value=None,
      bounds=[float("-inf"), float("inf")])
    }, options)
  return n.problem(name="trigx",
    objectives=[output["obj"]],
    constraints=output["constraints"],
    options=options)
```

Figure 3: Python code for MIGCB problem derived from the trigx problem of MINLPLib.

problems.

In addition to these derivative-free algorithms, we also report results for BONMIN, a mixed-integer convex nonlinear solver, where the first order derivatives are computed using a combination of automatic differentiation for analytical expressions and finite-differences for embedded black-box function calls. All algorithms were configured with their default options selected.

4.3 Experimental Setup

The prototype of GREYOPT used for this study has been implemented in Python and depends on six open-source Python packages: (1) CasADi[7] v3.5.5, (2) NumPy[8] v1.19.4, (3) PyInterval[9] v1.2.0, (4) Scikit-Learn[10] v0.23.2, (5) SciPy[11] v1.5.4, and (5) SortedContainers[12] v2.3.0. CasADi (Andersson et al., 2019) is a software framework for nonlinear optimization and optimal control that GREYOPT uses for symbolic computation, automatic differentiation, and interfaces for derivative-based optimization solvers. Specifically, GREYOPT uses the convex nonlinear solvers IPOPT (Biegler and Zavala, 2009) and BONMIN (Bonami et al., 2008) for the optimization of the surrogate problems. GREYOPT uses PyInterval (Taschini, 2008) for computing the intervals of analytical expressions. GREYOPT uses Scikit-Learn (Pedregosa et al., 2011) for polynomial and Gaussian process regression.

We extend each black-box function to accept a parameter, BBT, that controls how much additional CPU time, in seconds, to consume for each call to that function. Instead of wasting CPU cycles for the duration of BBT, in this study the actual CPU time that is measured and reported is adjusted by $c \times \texttt{BBT}$, where c is the total number of calls to black-box functions. This can be used to make an otherwise inexpensive black-box function appear more expensive to both the algorithm and the experimental study, without having to modify the structure of the problem. In this study, three different levels of BBT are considered: 0 seconds, 1 second, and 10 seconds.

All experiments were run on ARGO-1, a research computing cluster provided by the Office of Research Computing[13] at George Mason University. We adopt the same CPU time budget as used by Rios and Sahinidis (2009), where each algorithm is allocated a budget of 10 CPU minutes to optimize each problem. Although the measured and reported CPU time is adjusted by the BBT parameter, we do not adjust the CPU time budget. Each trial of this study involved running an algorithm on a problem for the duration of the CPU time budget and recording the convergence trace of the objective value of the best feasible point found over a BBT-adjusted CPU time horizon. If a feasible point has not yet been found, a value of ∞ is assumed for the objective.

While the problems considered in this study are all deterministic, some of the algorithms tested are stochastic, where multiple runs of the same algorithm on the same problem with the same starting point can return different results. To account for this, we conducted 15 trials for each experiment that consumed over 312 hours of CPU time on the cluster. We report the median objective value, which is robust to outliers, instead of the mean since we use a value of ∞ for the objective of infeasible points.

[7]URL: https://github.com/casadi/casadi
[8]URL: https://github.com/numpy/numpy
[9]URL: https://github.com/taschini/pyinterval
[10]URL: https://github.com/scikit-learn/scikit-learn
[11]URL: https://github.com/scipy/scipy
[12]URL: https://github.com/grantjenks/python-sortedcontainers
[13]URL: https://orc.gmu.edu

4.4 Evaluation Methodology

The evaluation methodology of this study is based on the *performance profile* of Dolan and Moré (2002) and the *data profile* of Moré and Wild (2009). In this section we denote the set of algorithms listed in Section 4.2 by $\mathcal{A}$, and the set of problems listed in Table 1 by $\mathcal{P}$. Because none of the algorithms for MICGB optimization tested in this study are globally convergent to a global optima in finite time, we use the following test of relative convergence for an algorithm $a \in \mathcal{A}$ on a problem $p \in \mathcal{P}$:

$$f_* - f_a >= (1 - \tau)(f_* - f^*) \tag{10}$$

where f_* is the worst (i.e. highest) objective value among the set containing the first feasible point found, if any, by each algorithm $a \in \mathcal{A}$ for problem p, where f^* is the best (i.e. lowest) objective value among the feasible points found by any algorithm $a \in \mathcal{A}$ on problem p, where f_a is the objective value of the best point found, feasible or otherwise, by algorithm a on problem p, and where τ is the tolerance parameter. We use the same tolerance used by Costa and Nannicini (2018) of $\tau \triangleq 10^{-3}$.

The *performance ratio* $r_{p,a}$ for a problem $p \in \mathcal{P}$ and an algorithm $a \in \mathcal{A}$ is defined by Dolan and Moré (2002) as:

$$r_{p,a} \triangleq \frac{t_{p,a}}{min\{t_{p,a} : a \in \mathcal{A}\}} \tag{11}$$

where t is the *performance measure* of interest. In this study, we define $t_{p,a}$ as the minimum median BBT-adjusted CPU time, in seconds, that algorithm a needed to converge for problem p, based on the convergence test in Equation 10. If algorithm a failed to converge for problem p, then we assign $t_{p,a}$ the value of ∞.

The performance profile of Dolan and Moré (2002) is defined in this study as follows:

$$\rho_a(x) \triangleq \frac{|\{p \in \mathcal{P} : r_{p,a} \leq x\}|}{|\mathcal{P}|} \tag{12}$$

where $\rho_a(x)$ for algorithm a is the percentage of problems $\mathcal{P}$ where the performance ratio $r_{p,a}$ is less than or equal to x. The lowest value that parameter x can be is equal to the best possible performance ratio (i.e. 1).

Finally, the data profile of Moré and Wild (2009) is defined in this study as follows:

$$d_a(x) \triangleq \frac{|\{p \in \mathcal{P} : t_{p,a} \leq x\}|}{|\mathcal{P}|} \tag{13}$$

where $d_a(x)$ is the percentage of problems $\mathcal{P}$ that algorithm a converges for within x BBT-adjusted CPU seconds.

4.5 Results

The results of this study are shown in Figure 2, where plots of the data and performance profile for each BBT level tested are provided. Starting with the performance profile for BBT = 0 seconds (per call), GREYOPT converges on over 60% of the problems tested when the performance ratio is equal to 1 (i.e. the best possible case). The data profile for BBT = 0 seconds (per call) shows that the number of problems that GREYOPT converges on steadily increases over the CPU time horizon. Moving on to the performance profile for BBT = 1 second (per call), the percentage of problems that GREYOPT converges on drops to about 43%, but is still considerably more than the next best algorithm, multi-start BONMIN. To account for the large increase in computational effort required by the other solvers, the data profile for BBT = 1 second (per call) switches the units of the horizontal axis from adjusted CPU seconds to adjusted CPU minutes. Similarly is the case for both the performance and data profile for BBT = 10 seconds (per call), where the units of the horizontal axis jumps from adjusted CPU minutes to adjusted CPU hours. Both the performance profile and data profile show that GREYOPT significantly outperforms all of other algorithms evaluated in this study, even outperforming the multi-start BONMIN algorithm when the black-box functions are cheap.

5 CONCLUSIONS

The GREYOPT algorithmic framework has been proposed for the heuristic global optimization of MICGB problems. We have shown how the partially analytical structure of such problems can be leveraged to guide the exploration of the search space using dynamically constructed surrogate problems and approximations of the intervals of grey-box objective and constraint functions. We have conducted an experimental study of GREYOPT's performance on a set of 25 MICGB optimization problems derived from MINLPLib where the ratio of black-box function evaluations to analytical expressions is small. The results of the study show that GREYOPT significantly outperforms the three derivative-free optimization algorithms evaluated on these problems, as well as a random restart version of the open-source convex nonlinear optimization solver BONMIN.

The development of GREYOPT is an ongoing effort. Possible directions for future work include: (1) extending GREYOPT to support multi-objective optimization, (2) direct support for the optimization of problems containing calls to noisy black-box functions, and (3) incorporating meta-optimization techniques for the automatic, problem-specific configuration of GREYOPT's parameters.

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APPENDIX

Tables 1 lists the MICGB problems tested in the experimental study presented in Section 4. For each problem, we list its name, which corresponds to the original problem from MINLPLib, the number of variables, and the number of constraints.

Table 1: MICGB problems derived from MINLPLib.

Problem	**Variables**	**Constraints**
cvxnonsep_psig20r	42	22
eniplac	141	189
ex1266a	48	53
ex14_2_3	6	9
ex14_2_5	4	5
ex8_4_8_bnd	42	30
ex8_5_3	5	4
feedtray2	88	284
glider100	1315	1209
inscribedsquare01	8	8
inscribedsquare02	8	8
kall_circlesrectangles_c1r12	49	52
kall_circlesrectangles_c6r1	184	192
nous2	50	43
pooling_foulds2pq	36	34
sfacloc1_2_90	199	348
st_e03	10	7
super3t	1056	1343
syn30h	228	345
wastepaper5	104	46
wastewater05m2	133	151
wastewater13m1	382	83
waterno2_01	166	204
waterund01	40	38
waterund18	60	64