

Efficient Evolutionary Algorithm for Single-Objective Bilevel Optimization

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KanGAL Report Number 2013003

Abstract

Bilevel optimization problems are a class of challenging optimization problems, which contain two levels of optimization tasks. In these problems, the optimal solutions to the lower level problem become possible feasible candidates to the upper level problem. Such a requirement makes the optimization problem difficult to solve, and has kept the researchers busy towards devising methodologies, which can efficiently handle the problem. Despite the efforts, there hardly exists any effective methodology, which is capable of handling a complex bilevel problem. In this paper, we introduce bilevel evolutionary algorithm based on quadratic approximations (BLEAQ) of optimal lower level variables with respect to the upper level variables. The approach is capable of handling bilevel problems with different kinds of complexities in relatively smaller number of function evaluations. Ideas from classical optimization have been hybridized with evolutionary methods to generate an efficient optimization algorithm for generic bilevel problems. The efficacy of the algorithm has been shown on two sets of test problems. The first set is a recently proposed SMD test set, which contains problems with controllable complexities, and the second set contains standard test problems collected from the literature. The proposed method has been evaluated against two benchmarks, and the performance gain is observed to be significant.

1 Introduction

Bilevel optimization is a branch of optimization, which contains a nested optimization problem within the constraints of the outer optimization problem. The outer optimization task is usually referred as the upper level task, and the nested inner optimization task is referred as the lower level task. The lower level problem appears as a constraint, such that only an optimal solution to the lower level optimization problem is a possible feasible candidate to the upper level optimization problem. Such a requirement makes bilevel optimization problems difficult to handle and have kept researchers and practitioners busy alike. In the field of classical optimization, a number of studies have been conducted on bilevel programming [4, 25, 8]. Approximate solution techniques are commonly employed to handle bilevel problems with simplifying assumptions like smoothness, linearity or convexity. Some of the classical approaches commonly used to handle bilevel problems include the Karush-Kuhn-Tucker approach [3, 13], Branch-and-bound techniques [2] and the use of penalty functions [1]. Most of these solution methodologies are rendered inapplicable, as soon as the bilevel optimization problem becomes complex. Heuristic procedures such as evolutionary algorithms have also been developed for handling bilevel problems with higher levels of complexity [28, 26]. Most of the existing evolutionary procedures often involve enormous computational expense, which limit their utility to solving bilevel optimization problems only with smaller number of variables.

There are a number of practical problems which are bilevel in nature. They are often encountered in transportation (network design, optimal pricing), economics (Stackelberg games, principal-agent problem, taxation, policy decisions), management (network facility location, coordination of multi-divisional firms), engineering (optimal design, optimal chemical equilibria) etc [7]. Complex practical problems are usually modified into a simpler single level optimization task, which is solved to arrive at a satisficing solution instead of an optimal solution. For the complex bilevel problems, classical methods fail because of real world difficulties (like non-linearity, discreteness, non-differentiability, non-convexity etc), and evolutionary methods are not very useful because of their enormous computational expense, a hybrid strategy could be solution. In cognizance of the drawbacks associated with the two approaches, we propose a hybrid strategy in this paper, which utilizes principles from classical optimization, within an evolutionary algorithm to quickly approach a bilevel optimum. The proposed method is a bilevel evolutionary algorithm based on quadratic approximations (BLEAQ) of the lower level optimal variables as a function of upper level variables.

To begin with, we provide a review of the past work on bilevel optimization using evolutionary algorithms, followed by description of a general bilevel optimization problem. Thereafter, we provide a supporting evidence that a strategy based on iterative quadratic approximations of the lower level optimal variables with respect to the upper level variables could be used to converge towards the bilevel optimal solution. This is followed by the description of the methodology, which utilizes the proposed quadratic approximation principle within the

evolutionary algorithm. The proposed ideas are further supported by results on a number of test problems. Firstly, BLEAQ is evaluated on recently proposed unconstrained SMD test problems [23], where the method is shown to successfully handle test problems with 10 dimensions. A performance comparison is performed against a nested evolutionary strategy, and the efficiency gain is provided. Secondly, BLEAQ is evaluated on a set of standard test problems chosen from the literature. These are constrained test problems with smaller number of variables. For comparing the results obtained using BLEAQ, we choose the algorithm proposed in [27], which is able to successfully solve all the test problems

2 Past research on Bilevel Optimization using Evolutionary Algorithms

Evolutionary algorithms for bilevel optimization have been proposed as early as in the 1990s. One of the first evolutionary algorithm for handling bilevel optimization problems was proposed by Mathieu et al.[18]. The proposed algorithm was a nested strategy, where the lower level was handled using a linear programming method, and the upper level was solved using a genetic algorithm (GA). Nested strategies could be one of the approaches to handle bilevel problems, where for every upper level vector a lower level optimization task is executed. However, a nested approach is computationally expensive and is not a feasible approach for large scale bilevel problems. Another nested approach was proposed in [28], where the lower level was handled using the Frank-Wolfe algorithm (reduced gradient method). The algorithm was successful in handling non-convex bilevel optimization problems, and the authors claimed it to be better than the classical methods. In 2005, Oduguwa and Roy[19] proposed a co-evolutionary approach for finding optimal solution for bilevel optimization problems. Their approach utilizes two populations. The first population handles upper level vectors, and the second population handles lower level vectors. The two populations interact with each other to converge towards the optimal solution. An extension of this study can be found in [11], where the authors solve a bilevel application problem with linear objectives and constraints.

Wang et al. [27] proposed an evolutionary algorithm based on a constraint handling scheme, where they successfully solve a number of standard test problems. The results produced by their approach finds better solutions for a number of test problems, as compared to what is reported in the literature. The algorithm is able to handle non-differentiability at the upper level objective function. However, the method may not be able to handle non-differentiability in the constraints, or the lower level objective function. Given the robustness of the approach in handling a variety of standard test problems, we choose this algorithm as one of the benchmarks. Another evolutionary algorithm proposed in [17] utilizes particle swarm optimization to handle the bilevel problems. Even this approach is nested as it solves the lower level optimization problem for

each upper level vector. The authors show that the approach is able to handle a number of standard test problems with smaller number of variables. However, they do not report the computational expense of the nested procedure. A hybrid approach proposed in [15], which is also nested, utilizes simplex-based crossover strategy at the upper level, and solves the lower level using one of the classical approaches. This method successfully solves a number of standard test problems, however given the nested nature of the algorithm it is not scalable for large number of variables. The authors report the number of generations and population sizes required by the algorithm, which may be used to compute the function evaluations at the upper level, but they do not explicitly report the total number of function evaluations required at the lower level.

Researchers in the field of evolutionary algorithms have also tried to convert the bilevel optimization problem into a single level optimization problem using the Karush-Kuhn-Tucker (KKT) conditions [26, 14, 16]. However, such conversions are possible only for those bilevel problems, where the lower level is smooth and the KKT conditions can be easily produced.

Recently, there has also been interest in multi-objective bilevel optimization using evolutionary algorithms. Some of the studies in the direction of solving multi-objective bilevel optimization problems using evolutionary algorithms are [12, 21, 6, 22, 20, 29].

3 Single-Objective Bilevel Problem

Bilevel optimization is a nested optimization problem which involves two levels of optimization tasks. The structure of a bilevel optimization problem demands that the optimal solutions to the lower level optimization problem may only be considered as feasible candidates for the upper level optimization problem. The problem contains two classes of variables, the upper level variables $x_u \in X_U \subset \mathbb{R}^n$, and the lower level variables $x_l \in X_L \subset \mathbb{R}^m$. For the lower level problem, the optimization task is performed with respect to variables x_l , and the variables x_u act as parameters. A different x_u leads to a different lower level optimization problem, whose optimal solution needs to be determined. The upper level problem usually involves all variables $x = (x_u, x_l)$, and the optimization is expected to be performed with respect to both the sets of variables. In the following we provide two equivalent definitions of a bilevel optimization problem:

Definition 1 *For the upper-level objective function $F : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$ and lower-level objective function $f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$*

$$\begin{aligned} & \underset{x_u \in X_U, x_l \in X_L}{\text{minimize}} && F_0(x_u, x_l) \\ & \text{subject to} && x_l \in \operatorname{argmin}\{f_0(x_u, x_l) : f_j(x_u, x_l) \leq 0, \\ & && \qquad \qquad \qquad j = 1, \dots, J\} \\ & && F_k(x_u, x_l) \leq 0, k = 1, \dots, K \end{aligned}$$

The above definition can be stated in terms of set-valued mappings as follows:

Definition 2 Let $\Psi : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$ be a set-valued mapping,

$$\Psi(x_u) = \operatorname{argmin}\{f_0(x_u, x_l) : f_j(x_u, x_l) \leq 0, j = 1, \dots, J\},$$

which represents the constraint defined by the lower-level optimization problem, i.e. $\Psi(x_u) \subset X_L$ for every $x_u \in X_U$. Then the bi-level optimization problem can be expressed as a general constrained optimization problem:

$$\begin{aligned} & \underset{x_u \in X_U, x_l \in X_L}{\text{minimize}} && F_0(x_u, x_l) \\ & \text{subject to} && x_l \in \Psi(x_u) \\ & && F_k(x_u, x_l) \leq 0, k = 1, \dots, K \end{aligned}$$

where Ψ can be interpreted as a parameterized range-constraint for the lower-level decision x_l .

The graph of the optimal-decision mapping is interpreted as a subset of $X_U \times X_L$

$$\operatorname{gph} \Psi = \{(x_u, x_l) \in X_U \times X_L \mid x_l \in \Psi(x_u)\},$$

which displays the connections between the upper-level decisions and corresponding optimal lower-level decisions. The domain of Ψ , which is obtained as a projection of $\operatorname{gph} \Psi$ on the upper-level decision space X_U represents all the points $x_u \in X_U$, where the lower-level (follower's) problem has at least one optimal solution, i.e.

$$\operatorname{dom} \Psi = \{x_u \mid \Psi(x_u) \neq \emptyset\}.$$

Similarly, the range is given by

$$\operatorname{rge} \Psi = \{x_l \mid x_l \in \Psi(x_u) \text{ for some } x_u\},$$

which corresponds to the projection of $\operatorname{gph} \Psi$ on the lower-level decision space X_L .

Figure 1 describes the structure of a bilevel problem in terms of two components: (i) $\operatorname{gph} \Psi$, which gives the graph of the optimal decision-mapping Ψ as a subset of $X_U \times X_L$; and (ii) the plot of F_0 evaluated on $\operatorname{gph} \Psi$, which shows the upper level objective function with respect to upper level variables x_u , when the lower level is optimal $x_l \in \Psi(x_u)$. The shaded area of $\operatorname{gph} \Psi$ shows the regions where there are multiple lower level optimal vectors corresponding to any upper level vector. On the other hand, the non-shaded parts of the graph represent the regions where Ψ is a single-valued mapping, i.e. there is a single lower level optimal vector corresponding to any upper level vector. Considering $\operatorname{gph} \Psi$ as the domain of F_0 in the figure, we can interpret F_0 entirely as a function of x_u , i.e. $F_0(x_u, \Psi(x_u))$. Therefore, whenever Ψ is multi-valued, we can also see a shaded region in the plot of F_0 which shows the different upper level function values for any upper level vector with multiple lower level optimal solutions.

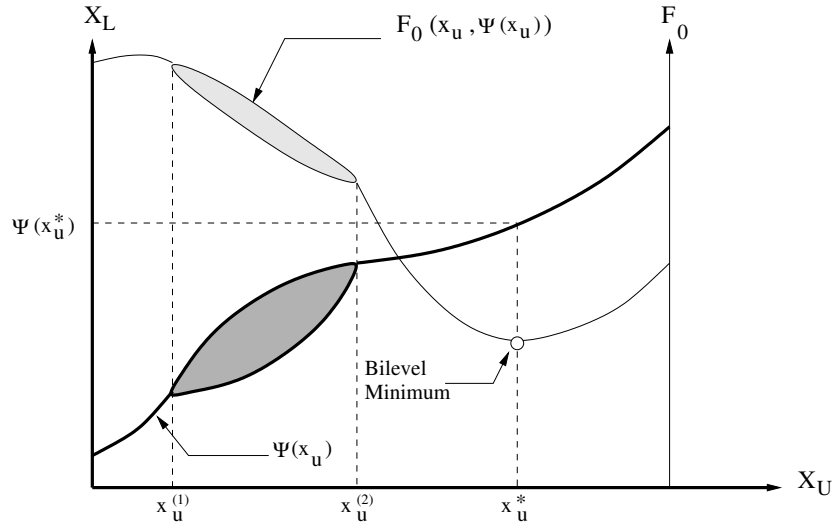


Figure 1: Upper level function with respect to x_u when x_l is optimal.

For instance, in Figure 1, the shaded region of $\text{gph } \Psi$ corresponds to the shaded region of F_0 for the upper level vectors between x_u^1 and x_u^2 .

For a more detailed illustration, see the 3-dimensional graph in Figure 2, where the values of the upper and lower level objective functions F_0 and f_0 are plotted against the decision space $X_U \times X_L$. For simplicity, let us again assume that $\text{gph } \Psi$ is the domain of F_0 . If we now consider the values of F_0 plotted against the plane of decision variables, we obtain the same information as before. However, as an addition to the previous figure, we have also described how the lower level objective function f_0 depends on the upper level decisions. In the figure, the shaded planes marked as A, B and C represent three different lower level optimization problems parameterized by $x_u^{(1)}$, x_u^* and $x_u^{(2)}$, respectively. Once an upper-level decision vector has been fixed, the lower level objective can be interpreted entirely as a function of x_l . Hence each shaded plane shows a single-variable plot of f_0 against X_L given a fixed x_u . Consider, for example, the plane A corresponding to the upper level decision $x_u^{(1)}$. From the shape of the lower level objective function it is easy to see that there are multiple optimal solutions at the lower level. Therefore, also Ψ must be set-valued at this point, and the collection of optimal lower level solutions is given by $\Psi(x_u^{(1)})$. For the other two shaded planes B and C, there is only a single lower level optimal solution for the given x_u , which corresponds to Ψ being single-valued at these points. The optimal upper level solution is indicated by point (x_u^*, x_l^*) , where $\Psi(x_u^*) = \{x_l^*\}$.

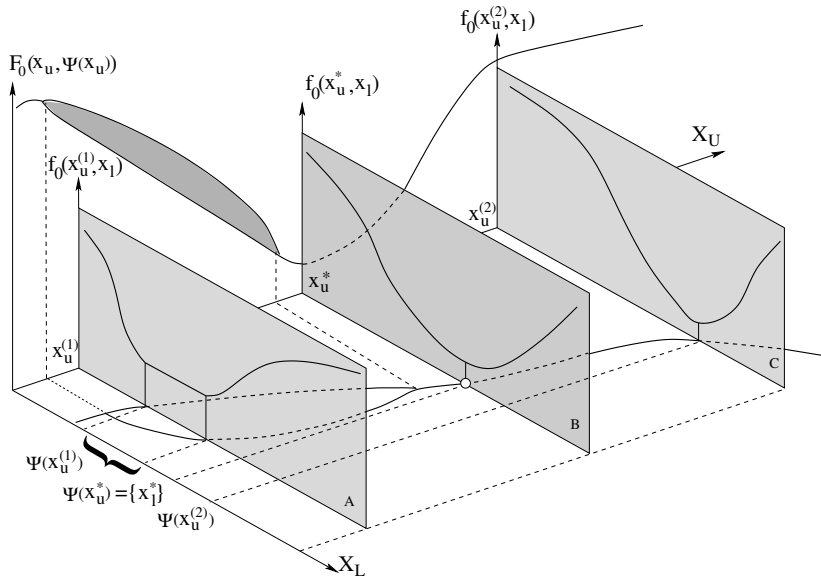


Figure 2: Graphical representation of a simple bilevel optimization problem.

4 Localization of the Follower's Problem

Ideally, the analysis of a bilevel problem would be greatly simplified if the optimal solution mapping Ψ could be treated as if it were an ordinary function. In particular, for the design of an efficient bilevel algorithm, it would be valuable to identify the circumstances under which single-valued functions can be used to construct local approximations for the optimal solution mapping. Given that our study of solution mappings is closely related to sensitivity analysis in parametric optimization, there already exist considerable research on the regularity properties of solution mappings, and especially on the conditions for obtaining single-valued localizations of general set-valued mappings. To formalize the notions of localization and single-valuedness in the context of set-valued mappings, we have adopted the following definition by Dontchev and Rockafellar [10]:

Definition 3 (Localization and single-valuedness) *For a given set-valued mapping $\Psi : X_U \rightrightarrows X_L$ and a pair $(x_u, x_l) \in \text{gph } \Psi$, a graphical localization of Ψ at x_u for x_l is a set-valued mapping Ψ_{loc} such that*

$$\text{gph } \Psi_{\text{loc}} = (U \times L) \cap \text{gph } \Psi$$

for some upper-level neighborhood U of x_u and lower-level neighborhood L of x_l , i.e.

$$\Psi_{\text{loc}}(x_u) = \begin{cases} \Psi(x_u) \cap L & \text{for } x_u \in U, \\ \emptyset & \text{otherwise.} \end{cases}$$

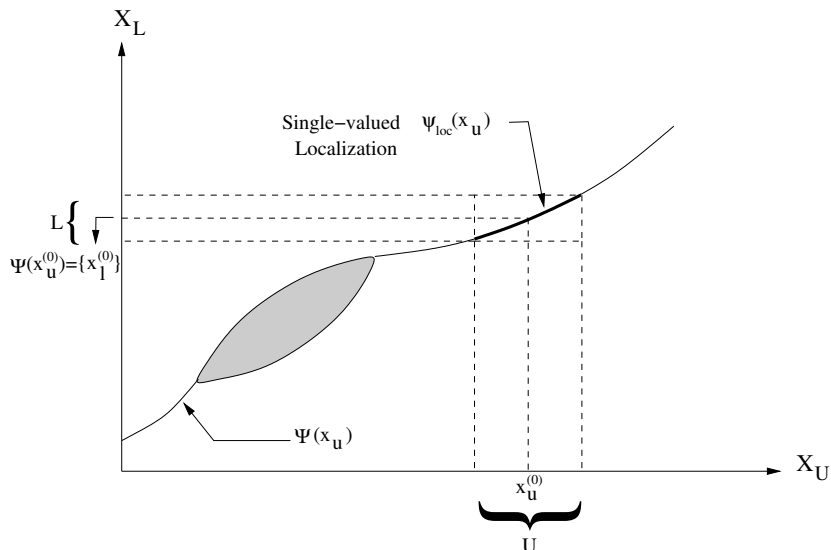


Figure 3: Localization around $x_u^{(0)}$ for $x_l^{(0)}$.

If Ψ_{loc} is actually a function with domain U , it is indicated by referring to a single-valued localization $\psi_{\text{loc}} : U \rightarrow X_L$ around x_u for x_l .

Obviously, graphical localizations of the above type can be defined for any optimal-decision mapping. However, it is more interesting to ask when the localization is not only a single-valued function but also possesses convenient properties such as continuity and certain degree of smoothness. In this section, our plan is to study how the lower-level solution mappings behave under small perturbations, and clarify the regularity conditions in which the solution mapping can be locally characterized by a Lipschitz-continuous single-valued function. We begin the discussion from simple problems with convex set-constraints in section 4.1 and gradually extend the results to problems with general non-linear constraints in section 4.2.

As an example, Figure 3 shows the Ψ mapping and its localization ψ_{loc} around $x_u^{(0)}$ for $x_l^{(0)}$. The notations discussed in the previous definition are shown in the figure to develop a graphical insight for the theory discussed above.

4.1 Localization with Convex Constraints

To motivate the development, suppose that the follower's problem is of form

$$\text{minimize } f_0(x_u, x_l) \text{ over all } x_l \in C, \quad (1)$$

where lower-level decisions are restricted by a simple set-constraint C which is assumed to be non-empty, convex, and closed in X_L .

When the lower-level objective function f_0 is continuously differentiable, the necessary condition for x_l to be a local minimum for the follower's problem is given by the standard variational inequality

$$\nabla_l f_0(x_u, x_l) + N_C(x_l) \ni 0, \quad (2)$$

where

$$N_C(x_l) = \{v | \langle v, x'_l - x_l \rangle \leq 0, \text{ for all } x'_l \in C\} \quad (3)$$

is the normal cone to C at x_l and $\nabla_l f_0$ denotes the gradient of f_0 with respect to the lower-level decision vector. The solutions to the inequality are referred to as *stationary points* with respect to minimizing over C , regardless of whether or not they correspond to local or global minimum. Of course, in the special case when f_0 is also convex, the inequality yields a sufficient condition for x_l to be a global minimum, but in other cases the condition is not sufficient to guarantee lower-level optimality of x_l . Rather the inequality is better interpreted as a tool for identifying quasi-solutions, which can be augmented with additional criteria to ensure optimality. In particular, as discussed by Dontchev and Rockafellar [10], significant efforts have been done to develop tools that help to understand the behavior of solutions under small perturbations which we are planning to utilize while proposing our solution for solving the bilevel problem. With this purpose in mind, we introduce the following definition of a quasi-solution mapping for the follower's problem:

Definition 4 (Quasi-solution mapping) *The solution candidates (stationary points) to the follower's problem of form (1) can be identified by set-valued mapping $\Psi^* : X_U \rightrightarrows X_L$,*

$$\Psi^*(x_u) = \{x_l | \nabla_l f_0(x_u, x_l) + N_C(x_l) \ni 0\},$$

which represents the set of stationary lower-level decisions for the given upper-level decision x_u . When f_0 is convex, Ψ^ coincides to the optimal solution mapping, i.e. $\Psi^* = \Psi$.*

Whereas direct localization of Ψ is difficult, it is easier to obtain a well-behaved localization for the quasi-solution mapping first, and then establish the conditions under which the obtained solutions furnish a lower-level local minimum. The approach is motivated by the fact that for variational inequalities of the above type, there are several variants of implicit function theorem that can be readily applied to obtain localizations with desired properties. Below, we present two localization-theorems for quasi-solution mappings. The first theorem shows the circumstances in which there exists a the single-valued localization of Ψ^* such that it is Lipschitz-continuous around a given pair $(x_u^*, x_l^*) \in \text{gph } \Psi^*$. The second theorem elaborates the result further under the additional assumption that C is polyhedral, which is sufficient to guarantee that for all points in the neighborhood of x_u^* there is a strong local minimum in the follower's problem (1).

Definition 5 (Lipschitz) A single-valued localization $\psi_{\text{loc}} : X_U \rightarrow X_L$ is said to be Lipschitz continuous around an upper-level decision \bar{x}_u when there exists a neighborhood U of \bar{x}_u and a constant $\mu \geq 0$ such that

$$|\psi_{\text{loc}}(x_u) - \psi_{\text{loc}}(x'_u)| \leq \mu |x_u - x'_u| \quad \text{for all } x_u, x'_u \in U.$$

Theorem 6 (Localization of quasi-solution mapping) Suppose in the lower-level optimization problem (1), with $x_l^* \in \Psi^*(x_u^*)$, that

- (i) C is non-empty, convex, and closed in X_L , and
- (ii) f_0 is twice continuously differentiable with respect to x_l , and has a strong convexity property at (x_u^*, x_l^*) , i.e. there exists $\mu > 0$ such that

$$\langle \nabla_U f_0(x_u^*, x_l^*) w, w \rangle \geq \mu |w|^2, \quad \text{for all } w \in C - C.$$

Then the quasi-solution mapping Ψ^* has a Lipschitz continuous single-valued localization ψ around x_u^* for x_l^* .

Proof. When the lower-level objective function f_0 is twice continuously differentiable with the inequality $\langle \nabla_U f_0(x_u^*, x_l^*) w, w \rangle \geq \mu |w|^2$ holding for all $w \in C - C$, then by Proposition 2G.4 and Exercise 2G.5 in [10] the assumptions (a) and (b) in Theorem 2G.2 are satisfied, and this gives the rest. \square

Corollary 7 (Localization with polyhedral constraints) Suppose that in the setup of Theorem (6) C is polyhedral. Then the additional conclusion holds that, for all x_u in some neighborhood of x_u^* , there is a strong local minimum at $x_l = \psi(x_u)$, i.e. for some $\varepsilon > 0$

$$f_0(x_u, x'_l) \geq f_0(x_u, x_l) + \frac{\varepsilon}{2} |x'_l - x_l|^2 \quad \text{for all } x'_l \in C \text{ near } x_l.$$

Proof. See Exercise 2G.5 and Theorem 2G.3 in [10]. \square

It is worthwhile to note that second order conditions to ensure that a quasi-solution corresponds to an actual local minimum exist also for other than polyhedral sets, but the conditions are generally not available in a convenient form.

4.2 Localization with Nonlinear Constraints

Until now, we have considered the simple class of follower's problems where the constraint set is not allowed to depend on the upper-level decisions. In practice, however, the follower's constraints are often dictated by the leader's choices. Therefore, the above discussion needs to be extended to cover the case of general non-linear constraints that are allowed to be functions of both x_l and x_u . Fortunately, this can be done by drawing upon the results available for constrained parametric optimization problems.

Consider the follower's problem of form

$$\begin{aligned} & \underset{x_l \in X_L}{\text{minimize}} && f_0(x_u, x_l) \\ & \text{subject to} && f_j(x_u, x_l) \leq 0, j = 1, \dots, J \end{aligned}$$

where the functions f_0, f_1, \dots, f_J are assumed to be twice continuously differentiable. Let $L(x_u, x_l, y) = f_0(x_u, x_l) + y_1 f_1(x_u, x_l) + \dots + y_J f_J(x_u, x_l)$ denote the Lagrangian function. Then the necessary first-order optimality condition is given by the following variational inequality

$$f(x_u, x_l, y) + N_E(x_l, y) \ni (0, 0),$$

where

$$\begin{cases} f(x_u, x_l, y) = (\nabla_l L(x_u, x_l, y), -\nabla_y L(x_u, x_l, y)), \\ E = X_L \times \mathbb{R}_+^J \end{cases}$$

The pairs (x_l, y) which solve the variational inequality are called the *Karush-Kuhn-Tucker* pairs corresponding to the upper-level decision x_u . Now in the similar fashion as done in Section 4.1, our interest is to establish the conditions for the existence of a mapping ψ_{loc} which can be used to capture the behavior of the x_l component of the Karush-Kuhn-Tucker pairs as a function of the upper-level decisions x_u .

Theorem 8 (Localization with Nonlinear Constraints) *For a given upper-level decision x_u^* , let (x_l^*, y^*) denote a corresponding Karush-Kuhn-Tucker pair. Suppose that the above problem for twice continuously differentiable functions f_i is such that the following regularity conditions hold*

- (i) the gradients $\nabla_l f_i(x_u, x_l)$, $i \in I$ are linearly independent, and
- (ii) $\langle w, \nabla_{ll}^2 L(x_u^*, x_l^*, y^*) w \rangle > 0$ for every $w \neq 0$, $w \in M^+$,

where

$$\begin{cases} I = \{i \in [1, J] \mid f_i(x_u^*, x_l^*) = 0\}, \\ M^+ = \{w \in \mathbb{R}^n \mid w \perp \nabla_l f_i(x_u^*, x_l^*) \text{ for all } i \in I\}. \end{cases}$$

Then the Karush-Kuhn-Tucker mapping $S : X_U \rightrightarrows X_L \times \mathbb{R}^J$,

$$S(x_u) := \{(x_l, y) \mid f(x_u, x_l, y) + N_E(x_l, y) \ni (0, 0)\},$$

has a Lipschitz-continuous single-valued localization s around x_u^* for (x_l^*, y^*) , $s(x_u) = (\psi_{\text{loc}}(x_u), y(x_u))$, where $\psi_{\text{loc}} : X_U \rightarrow X_L$ and $y : X_U \rightarrow \mathbb{R}^J$. Moreover, for every x_u in some neighborhood of x_u^* the lower-level decision component $x_l = \psi_{\text{loc}}(x_u)$ gives a strong local minimum.

Proof. See e.g. Theorem 1 in [9] or Theorem 2G.9 in [10]. \square

Despite the more complicated conditions required to establish the result for general non-linear constraints case, the eventual outcome of the Theorem (8) is essentially similar to Theorems (6) and (7). That is, in the vicinity of the current optimal solution, we can express the locally optimal follower's decisions as a relatively smooth function of the upper-level decisions.

4.3 Approximation with Localizations

The single-valued localizations of solution mappings can be used as effective tools for alleviating computational burden in a greedy evolutionary algorithm. Instead of solving the follower’s problem from scratch for every upper-level decision, we can use localizations to obtain an “educated guess” on the new optimal lower-level decision. The intuition for using the above results is as follows.

Suppose that $(x_u, x_l) \in \text{gph } \Psi$ is a known lower-level optimal pair, i.e. $x_l \in \Psi(x_u)$, and the lower-level problem satisfies the regularity conditions in the previous theorems. Then for some open neighborhoods $U \subset X_U$ of x_u and $L \subset X_L$ of x_l , there exists a uniquely determined μ -Lipschitz continuous function $\psi_{\text{loc}} : U \rightarrow X_L$ such that $x'_l = \psi_{\text{loc}}(x'_u)$ is the unique local optimal solution of the follower’s problem in L for each $x'_u \in U$. The existence of such ψ_{loc} leads to a direct strategy for generating new solution candidates from the existing ones. If the currently known upper level decision x_u is perturbed by a small random vector ε such that $x_u + \varepsilon \in U$, then the newly generated point $(x_u + \varepsilon, \psi_{\text{loc}}(x_u + \varepsilon))$ gives another locally optimal solution where the change in the lower-level optimal decision vector is bounded by $|\psi_{\text{loc}}(x_u + \varepsilon) - x_l| \leq \mu|\varepsilon|$. In theory, this would allow us to reduce the bilevel optimization problem (2) to that of minimizing a locally Lipschitz function $F_0(x_u, \psi_{\text{loc}}(x_u))$; see e.g. Dempe et al. for discussion on implicit function based techniques.

However, an essential difficulty for applying the result in practice follows from the fact that the mapping ψ_{loc} is not known with certainty, except for a few special cases. To resolve this problem in an efficient way, we consider embedding the above results within an evolutionary framework, where estimates of ψ_{loc} are produced by using samples of currently known optimal points. For simplicity, suppose that we want to find an estimate of ψ_{loc} around current best solution $(x_u, x_l) \in \text{gph } \Psi$, and let

$$\mathcal{P} = \{(x_u^{(i)}, x_l^{(i)}) \in X_U \times X_L \mid x_l^{(i)} \in \Psi(x_u^{(i)}), i \in \mathcal{I}\} \subset \text{gph } \Psi$$

be a sample from the neighborhood of (x_u, x_l) . Then the task of finding a good estimator for ψ_{loc} can be viewed as an ordinary supervised learning problem:

Definition 9 (Learning of ψ_{loc}) *Let \mathcal{H} be the hypothesis space, i.e. the set of functions that can be used to predict the optimal lower-level decision from the given upper-level decision. Given the sample \mathcal{P} , our goal is to choose a predictor $\hat{\psi} \in \mathcal{H}$ such that it minimizes the empirical error on the sample data-set, i.e.*

$$\hat{\psi} = \underset{h \in \mathcal{H}}{\text{argmin}} \sum_{i \in \mathcal{I}} L(h(x_u^{(i)}), x_l^{(i)}), \quad (4)$$

where $L : X_L \times X_L \rightarrow \mathbb{R}$ denotes the empirical risk function.

For a graphical illustration, see Figure 4 showing one example of a local approximation $\hat{\psi}$ around $x_u^{(0)}$ for x_l using a quadratic function. When the exact form of the underlying mapping is unknown, the approximation generally leads to an error as one moves away from the point around which the localization is

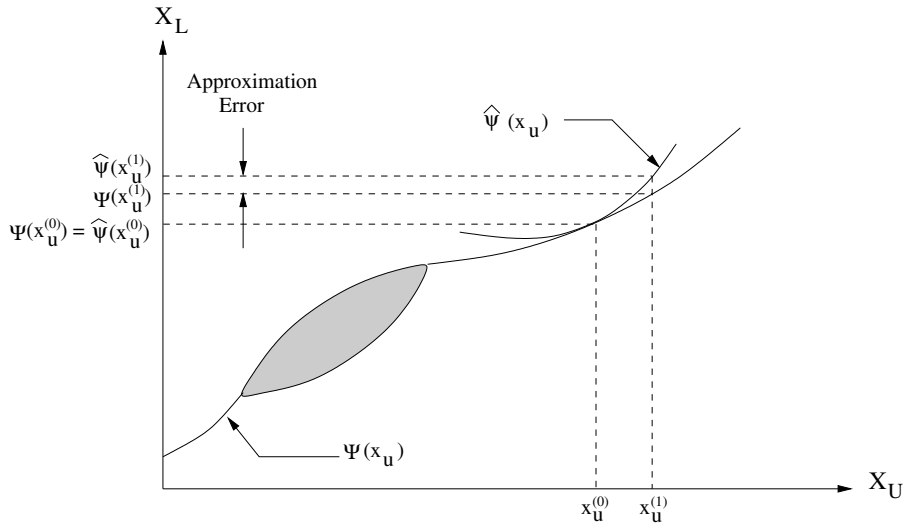


Figure 4: Approximation with localization around $x_u^{(0)}$.

performed. In the figure, the approximation error is shown for a point $x_u^{(1)}$ in the neighborhood of $x_u^{(0)}$. This error may not be significant in the vicinity of $x_u^{(0)}$, and could provide a good guess for the lower-level optimal solution for a new x_u close to $x_u^{(0)}$.

In this paper, we have chosen to use the squared prediction error as the empirical risk function when performing the approximations, i.e.

$$L(h(x_u^{(i)}), x_t^{(i)}) = |x_t^{(i)} - h(x_u^{(i)})|^2,$$

and at the same time we have restricted the hypothesis space \mathcal{H} to consist of second-order polynomials. With these choices the empirical risk minimization problem (4) corresponds to an ordinary quadratic regression problem. Therefore, as long as the estimation problem is kept light enough and the evolutionary framework is such that the solution population can be used to construct a training dataset \mathcal{P} , the use of the estimation approach can be expected to enhance the algorithm's overall performance by reducing the number of times the lower-level optimization problem needs to be solved.

5 Algorithm description

In this section, we provide a description for the bilevel evolutionary algorithm based on quadratic approximations (BLEAQ). The optimization strategy is based on approximation of the lower level optimal variables as a function of upper level variables. To begin with, an initial population of upper level members with random upper level variables is initialized. For each member, the lower

level optimization problem is solved using a lower level optimization scheme, and optimal lower level members are noted. Based on the lower level optimal solutions achieved, a quadratic relationship between the upper level variables and each lower level optimal variable is established. If the approximation is good (in terms of mean squared error) then it can be used to predict the optimal lower level variables for any given set of upper level variables. This eliminates the requirement to solve a lower level optimization problem. However, one needs to be cautious while accepting the optimal solutions from the quadratic approximations as even a single poor solution might lead to a wrong bilevel optimum. At each generation of the algorithm, a new quadratic approximation is generated which goes on improving as the population converges towards the true optima. At the termination of the procedure, the algorithm not only provides the optimal solutions to a bilevel problem, but also acceptably accurate functions representing the relationship between upper and lower variables at the optima. These functions can be useful for strategy developments or making decisions in bilevel problems appearing in fields like game theory, economics, science or engineering. In the following we provide a step-by-step procedure for the algorithm.

- S. 1** Initialization: The algorithm starts with a random population of size N , which is initialized by generating the required number of upper level variables, and then executing the lower level evolutionary optimization procedure to determine the corresponding optimal lower level variables. Fitness is assigned based on upper level function value and constraints.
- S. 2** Tagging: Tag all the upper level members as 1 which have undergone a lower level optimization run, and others as 0.
- S. 3** Selection of upper level parents: Given the current population, we randomly choose $2(\mu - 1)$ number of members from the population and perform a tournament selection based on upper level function value. This produces $\mu - 1$ number of parents.
- S. 4** Evolution at the upper level: Choose the best tag 1 member as the index parent, and the members from the previous step as other parents. Then, create λ number of offsprings from the chosen μ parents, using crossover and polynomial mutation operators.
- S. 5** Quadratic approximation: If the number of tag 1 members in the population is greater than $\frac{(\dim(x_u)+1)(\dim(x_u)+2)}{2} + \dim(x_u)$, then select all the tag 1 upper level members to construct quadratic functions to represent each of the lower level optimal variables as a function of upper level variables. If the number of tag 1 members is less than $\frac{(\dim(x_u)+1)(\dim(x_u)+2)}{2} + \dim(x_u)$ then a quadratic approximation is not performed.
- S. 6** Lower level optimum: If a quadratic approximation was performed in the previous step then find the lower level optima for the offsprings using the quadratic approximation. If the mean squared error e_{mse} is less than

$e_0(1e-3)$, then the quadratic approximation is considered good and the offsprings are tagged as 1, otherwise they are tagged as 0. If a quadratic approximation was not performed in the previous step then execute lower level optimization runs for each of the offsprings. To execute lower level optimization for an offspring member, the closest tag 1 parent is determined. From the closest tag 1 parent, the lower level optimal member ($x_l^{(c)}$) is copied (Refer Section 5.1). Thereafter, a lower level optimization run is performed which first tries to optimize the problem using a quadratic programming approach, and if unsuccessful, it uses an evolutionary optimization algorithm. The copied lower level member from the closest upper level parent is used in the lower level optimization run. Tag the offspring as 1 for which lower level optimization is performed.

- S. 7 Population Update:** After finding the lower level variables for the offsprings, r members are chosen from the parent population. A pool of chosen r members and λ offsprings is formed. The best r members from the pool replace the chosen r members from the population. A termination check is performed and the algorithm moves to the next generation (Step 3) if the termination check is false.

5.1 Property of two close upper level members

For two close upper level members, it is often expected that the lower level optimal solutions will also lie close to each other. This scenario is explained in Figure 5, where $x_u^{(1)}$ and $x_u^{(2)}$ are close to each other, and therefore their corresponding optimal lower level members are also close. On the other hand $x_u^{(3)}$ is far away from $x_u^{(1)}$ and $x_u^{(2)}$. Therefore, its optimal lower level member is not necessarily close to the other two lower level members. This property of the bilevel problems is utilized in the proposed algorithm, such that if a lower level optimization has been performed for one of the upper level members, then the corresponding lower level member is utilized while performing a lower level optimization task for another upper level member in the vicinity of the previous member.

5.2 Lower Level Optimization

At the lower level we first use a quadratic programming approach to find the optima. If the procedure is unsuccessful we use a global optimization procedure using an evolutionary algorithm to find the optimum. The lower level optimization using evolutionary algorithm is able to handle complex optimization problems with multimodality. The fitness assignment at this level is performed based on lower level function value and constraints. Following are the steps for the lower level optimization procedure:

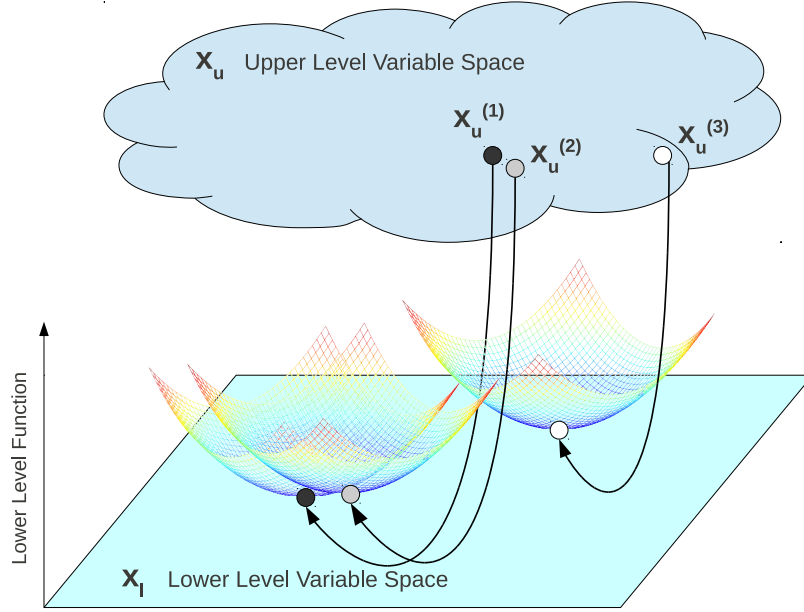


Figure 5: Lower level optimal solutions for three different upper level members.

5.2.1 Lower level quadratic programming

- S. 1 Create $\frac{(\dim(x_l)+1)(\dim(x_l)+2)}{2} + \dim(x_l)$ lower level points about $x_l^{(c)}$ using polynomial mutation.
- S. 2 Construct a quadratic function about $x_l^{(c)}$ using the created points. Construct linear approximations for the constraints.
- S. 3 Optimize the quadratic function with linear constraints using a sequentially quadratic programming approach.
- S. 4 Compute the value of the optimum using the quadratic function and the lower level function. If the absolute difference is less than δ_{min} then accept the solution as lower level optimum, otherwise perform an evolutionary optimization search.

5.2.2 Lower level evolutionary optimization

- S. 1 If lower level evolutionary optimization is executed directly without quadratic programming, then randomly initialize n lower level members. If quadratic programming is executed, then use the solution obtained using quadratic

programming as one of the population members and randomly initialize other $n - 1$ lower level members. The upper level variables are kept fixed for all the population members.

- S. 2** Choose 2μ members randomly from the population, and perform a tournament selection to choose μ parents for crossover.
- S. 3** The best parent among μ parents is chosen as the index parent and λ number of offsprings are produced using the crossover and mutation operators.
- S. 4** A population update is performed by choosing r random members from the population. A pool is formed using r chosen members and λ offsprings, from which the best r members are used to replace the r chosen members from the population.
- S. 5** Next generation (Step 2) is executed if the termination criteria is not satisfied.

5.3 Constraint handling

As we know by now that a bilevel problem has two levels of optimization tasks. There may be constraints at the lower level and also constraints at the upper level. We modify any given bilevel problems such that lower level constraints belong only to the lower level optimization task, however, at the upper level we include both the upper and lower level constraints. This is done to ensure at the upper level that a solution which is not feasible at the lower level cannot be feasible at the upper level, no matter whether the lower level optimization task is performed or not. While computing the overall constraint violation for a solution at the upper level, it is not taken into account whether the lower level variables are optimal or not. We use a separate tagging scheme in the algorithm to account for optimality or non-optimality of lower level variables.

The algorithm uses similar constraint handling scheme at both the levels, where the overall constraint violation for any solution is the summation of the violations of all the equality and inequality constraints. A solution $x^{(i)}$ is said to ‘constraint dominate’ [5] a solution $x^{(j)}$ if any of the following conditions are true:

1. Solution $x^{(i)}$ is feasible and solution $x^{(j)}$ is not.
2. Solution $x^{(i)}$ and $x^{(j)}$ are both infeasible but solution $x^{(i)}$ has a smaller overall constraint violation.
3. Solution $x^{(i)}$ and $x^{(j)}$ are both feasible but the objective value of $x^{(i)}$ is less than that of $x^{(j)}$.

5.4 Crossover Operator

The crossover operator used in Step 2 is similar to the PCX operator proposed in [24]. The operator creates a new solution from 3 parents as follows:

$$c = x^{(p)} + \omega_\xi d + \omega_\eta \frac{p^{(2)} - p^{(1)}}{2} \quad (5)$$

The terms used in the above equation are defined as follows:

- $x^{(p)}$ is the *index* parent
- $d = x^{(p)} - g$, where g is the mean of μ parents
- $p^{(1)}$ and $p^{(2)}$ are the other two parents
- $\omega_\xi = 0.1$ and $\omega_\eta = \frac{\dim(x^{(p)})}{\|x^{(p)} - g\|_1}$ are the two parameters.

The two parameters ω_ξ and ω_η , describe the extent of variations along the respective directions. At the upper level, a crossover is performed only with the upper level variables and the lower level variables are determined from the quadratic function or by lower level optimization call. At the lower level, crossover is performed only with the lower level variables and the upper level variables are kept fixed as parameters.

5.5 Termination Criteria

The algorithm uses a variance based termination criteria at both the levels. At the upper level, when the value of α_u described in the following equation becomes less than α_u^{stop} , the algorithm terminates.

$$\alpha_u = \sum_{i=1}^M \frac{\sigma^2(x_{u_T}^i)}{\sigma^2(x_{u_0}^i)}. \quad (6)$$

From the above equation, α_u is always greater than 0 and should be less than 1 most of the times. M is the number of upper level variables in the bilevel optimization problem, $x_{u_T}^i : i \in \{1, 2, \dots, M\}$ represents the upper level variables in generation number T , and $x_{u_0}^i : i \in \{1, 2, \dots, M\}$ represents the upper level variables in the initial random population. The value of α_u^{stop} should be kept small to ensure a high accuracy.

A similar termination scheme is used for the lower level evolutionary algorithm. The value for α_l is determined as follows.

$$\alpha_l = \sum_{i=1}^m \frac{\sigma^2(x_{l_t}^i)}{\sigma^2(x_{l_0}^i)}. \quad (7)$$

In the above equation, m is the number of variables at the lower level, $x_{l_t}^i : i \in \{1, 2, \dots, m\}$ represents the lower level variables in generation number t , and $x_{l_0}^i : i \in \{1, 2, \dots, m\}$ represents the lower level variables in the initial random population for a particular lower level optimization run. A high accuracy is desired particularly at the lower level, therefore the value for α_l should be kept low. Inaccurate lower level solutions may mislead the algorithm in case of a conflict between the two levels.

Table 1: Overview of test-problem framework components

Panel A: Decomposition of decision variables			
Upper-level variables		Lower-level variables	
Vector	Purpose	Vector	Purpose
x_{u1}	Complexity on upper-level	x_{l1}	Complexity on lower-level
x_{u2}	Interaction with lower-level	x_{l2}	Interaction with upper-level

Panel B: Decomposition of objective functions			
Upper-level objective function		Lower-level objective function	
Component	Purpose	Component	Purpose
$F_0^1(x_{u1})$	Difficulty in convergence	$f_0^1(x_{u1}, x_{u2})$	Functional dependence
$F_0^2(x_{l1})$	Conflict / co-operation	$f_0^2(x_{l1})$	Difficulty in convergence
$F_0^3(x_{u2}, x_{l2})$	Difficulty in interaction	$f_0^3(x_{u2}, x_{l2})$	Difficulty in interaction

5.6 Parameters

The parameters in the algorithm are fixed as $\mu = 3$, $\lambda = 2$ and $r = 2$ at both the level. Crossover probability is fixed at 0.9 and the mutation probability is 0.1. The upper level population size N and the lower level population size n are fixed at 50 for all the problems. The values for α_u^{stop} and α_l^{stop} are fixed as $1e - 5$ at both the upper and the lower levels.

6 SMD problems

A set of test problems (SMD) for single objective bilevel optimization has recently been proposed in [23]. The proposed problems are scalable in terms of number of decision variables. In this section, we discuss about the construction of these test problems in brief and provide a description of the proposed SMD test problems. The construction of the test problem involves splitting the upper and lower level functions into three components. Each of the components is specialized for inducing a certain kind of difficulty into the bilevel test problem. The functions are chosen based on the difficulties required in terms of convergence at the two levels, and interaction between the two level. A generic bilevel test problem is stated as follows:

$$\begin{aligned}
 F_0(x_u, x_l) &= F_0^1(x_{u1}) + F_0^2(x_{l1}) + F_0^3(x_{u2}, x_{l2}) \\
 f_0(x_u, x_l) &= f_0^1(x_{u1}, x_{u2}) + f_0^2(x_{l1}) + f_0^3(x_{u2}, x_{l2})
 \end{aligned} \tag{8}$$

where

$$x_u = (x_{u1}, x_{u2}) \quad \text{and} \quad x_l = (x_{l1}, x_{l2})$$

The above equations contain three terms at both the levels. Table 1 provides a summary for the role played by each term in the equations. The upper level and lower level variables are broken into two smaller vectors (refer Panel A in Table 1), such that, vectors x_{u1} and x_{l1} are used to induce complexities at the upper and lower levels independently, and vectors x_{u2} and x_{l2} are responsible to induce complexities because of interaction. The upper and lower level functions

are decomposed such that each of the components is specialized for a certain purpose only (refer Panel B in Table 1). The term $F_1(x_{u1})$, at the upper level, is responsible for inducing difficulty in convergence solely at the upper level, and the term $f_2(x_{l1})$, at the lower level, is responsible for inducing difficulty in convergence solely at the lower level. The term $F_2(x_{l1})$ decides if there is a conflict or a cooperation between the two levels. The terms $F_3(x_{l2}, x_{u2})$ and $f_3(x_{l2}, x_{u2})$ induce difficulties because of interaction at the two levels, though $F_3(x_{l2}, x_{u2})$ may also be used to induce a cooperation or a conflict. Finally, $f_1(x_{u1}, x_{u1})$ is a fixed term at the lower level which does not induce any difficulties, rather helps to create a functional dependence between lower level optimal solution(s) and the upper level variables.

6.1 SMD1

SMD1 is a test problem with cooperation between the two levels. The lower level optimization problem is a simple convex optimization task. The upper level is convex with respect to upper level variables and optimal lower level variables.

$$\begin{aligned}
F_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
F_0^2 &= \sum_{i=1}^q (x_{l1}^i)^2 \\
F_0^3 &= \sum_{i=1}^r (x_{u2}^i)^2 + \sum_{i=1}^r (x_{u2}^i - \tan x_{l2}^i)^2 \\
f_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
f_0^2 &= \sum_{i=1}^q (x_{l1}^i)^2 \\
f_0^3 &= \sum_{i=1}^r (x_{u2}^i - \tan x_{l2}^i)^2
\end{aligned} \tag{9}$$

The range of variables is as follows,

$$\begin{aligned}
x_{u1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, p\} \\
x_{u2}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, r\} \\
x_{l1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, q\} \\
x_{l2}^i &\in \left(\frac{-\pi}{2}, \frac{\pi}{2}\right), \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{10}$$

Relationship between upper level variables and lower level optimal variables is given as follows,

$$\begin{aligned}
x_{l1}^i &= 0, \quad \forall i \in \{1, 2, \dots, p\} \\
x_{l2}^i &= \tan^{-1} x_{u2}^i, \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{11}$$

The values of the variables at the optima are $x_u = 0$ and x_l is obtained by the relationship given above. Both the upper and lower level functions are equal to 0 at the optima. Figure 6 shows the contours of the upper level function with respect to the upper and lower level variables for a four variable test problem with $\dim(x_{u1}) = \dim(x_{u2}) = \dim(x_{l1}) = \dim(x_{l2}) = 1$. Figure 6 shows the contours of the upper level function at each x_u in Sub-figure P assuming that the lower level variables are optimal. Sub-figure S shows the behavior of the upper level function with respect to x_l at optimal x_u .

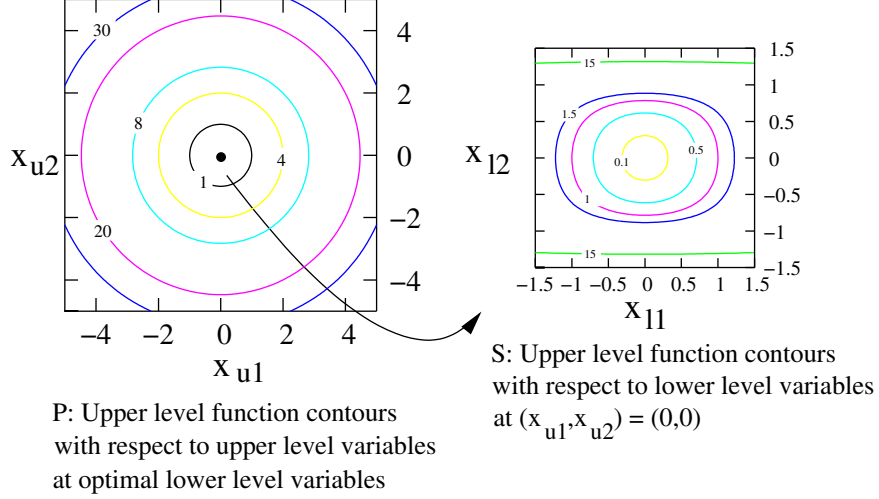


Figure 6: Upper level function contours for a four variable SMD1 test problem.

6.2 SMD2

SMD2 is a test problem with a conflict between the upper level and lower level optimization tasks. The lower level optimization problem is a convex optimization task. An inaccurate lower level optimum may lead to upper level function value better than the true optimum for the bilevel problem. The upper level is convex with respect to upper level variables and optimal lower level variables.

$$\begin{aligned}
F_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
F_0^2 &= -\sum_{i=1}^q (x_{l1}^i)^2 \\
F_0^3 &= \sum_{i=1}^r (x_{u2}^i)^2 - \sum_{i=1}^r (x_{u2}^i - \log x_{l2}^i)^2 \\
f_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
f_0^2 &= \sum_{i=1}^q (x_{l1}^i)^2 \\
f_0^3 &= \sum_{i=1}^r (x_{u2}^i - \log x_{l2}^i)^2
\end{aligned} \tag{12}$$

The range of variables is as follows, The range of variables is as follows,

$$\begin{aligned}
x_{u1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, p\} \\
x_{u2}^i &\in [-5, 1], \quad \forall i \in \{1, 2, \dots, r\} \\
x_{l1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, q\} \\
x_{l2}^i &\in (0, e], \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{13}$$

Relationship between upper level variables and lower level optimal variables is given as follows,

$$\begin{aligned}
x_{l1}^i &= 0, \quad \forall i \in \{1, 2, \dots, q\} \\
x_{l2}^i &= \log^{-1} x_{u2}^i, \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{14}$$

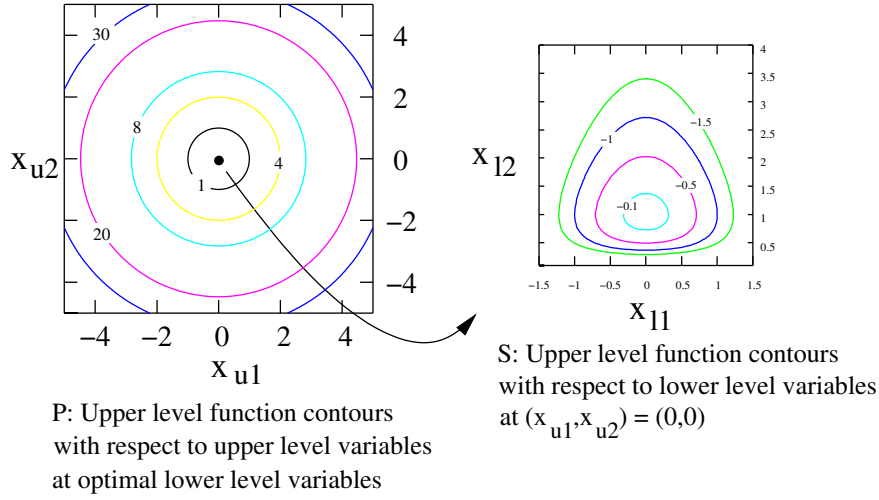


Figure 7: Upper level function contours for a four variable SMD2 test problem.

The values of the variables at the optima are $x_u = 0$ and x_l is obtained by the relationship given above. Both the upper and lower level functions are equal to 0 at the optima. Figure 7 represents the same information as in Figure 6 for a four variable bilevel test problem.

6.3 SMD3

SMD3 is a test problem with a cooperation between the two levels. The difficulty introduced is in terms of multi-modality at the lower level which contains the Rastrigin's function. The upper level is convex with respect to upper level variables and optimal lower level variables.

$$\begin{aligned}
F_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
F_0^2 &= \sum_{i=1}^q (x_{l1}^i)^2 \\
F_0^3 &= \sum_{i=1}^r (x_{u2}^i)^2 + \sum_{i=1}^r ((x_{u2}^i)^2 - \tan x_{l2}^i)^2 \\
f_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
f_0^2 &= q + \sum_{i=1}^q ((x_{l1}^i)^2 - \cos 2\pi x_{l1}^i) \\
f_0^3 &= \sum_{i=1}^r ((x_{u2}^i)^2 - \tan x_{l2}^i)^2
\end{aligned} \tag{15}$$

The range of variables is as follows,

$$\begin{aligned}
x_{u1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, p\} \\
x_{u2}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, r\} \\
x_{l1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, q\} \\
x_{l2}^i &\in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right), \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{16}$$

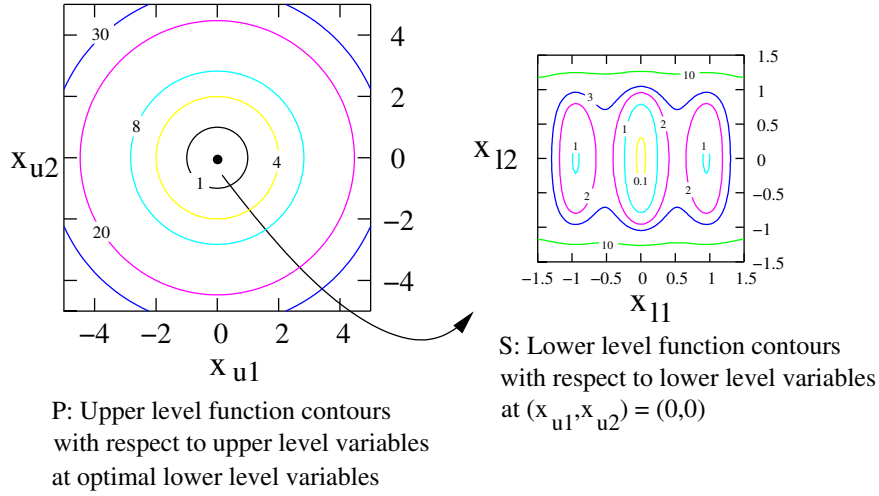


Figure 8: Upper and lower level function contours for a four variable SMD3 test problem.

Relationship between upper level variables and lower level optimal variables is given as follows,

$$\begin{aligned} x_{l1}^i &= 0, \quad \forall i \in \{1, 2, \dots, q\} \\ x_{l2}^i &= \tan^{-1}(x_{u2}^i)^2, \quad \forall i \in \{1, 2, \dots, r\} \end{aligned} \quad (17)$$

The values of the variables at the optima are $x_u = 0$ and x_l is obtained by the relationship given above. Both the upper and lower level functions are equal to 0 at the optima. Figure 8 shows the contours of the upper level function at each x_u in Sub-figure P assuming that the lower level variables are optimal. Sub-figure S shows the behavior of the lower level function at optimal x_u .

6.4 SMD4

SMD4 is a test problem with a conflict between the two levels. The difficulty is in terms of multi-modality at the lower level which contains the Rastrigin's function. The upper level is convex with respect to upper level variables and optimal lower level variables.

$$\begin{aligned} F_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\ F_0^2 &= -\sum_{i=1}^q (x_{l1}^i)^2 \\ F_0^3 &= \sum_{i=1}^r (x_{u2}^i)^2 - \sum_{i=1}^r (|x_{u2}^i| - \log(1 + x_{l2}^i))^2 \\ f_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\ f_0^2 &= q + \sum_{i=1}^q \left((x_{l1}^i)^2 - \cos 2\pi x_{l1}^i \right) \\ f_0^3 &= \sum_{i=1}^r (|x_{u2}^i| - \log(1 + x_{l2}^i))^2 \end{aligned} \quad (18)$$

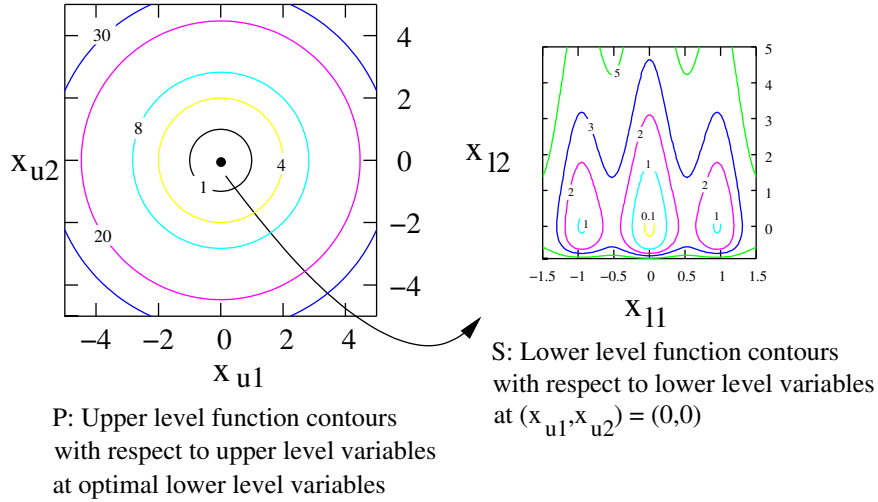


Figure 9: Upper and lower level function contours for a four variable SMD4 test problem.

The range of variables is as follows,

$$\begin{aligned}
 x_{u1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, p\} \\
 x_{u2}^i &\in [-1, 1], \quad \forall i \in \{1, 2, \dots, r\} \\
 x_{l1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, q\} \\
 x_{l2}^i &\in [0, e], \quad \forall i \in \{1, 2, \dots, r\}
 \end{aligned} \tag{19}$$

Relationship between upper level variables and lower level optimal variables is given as follows,

$$\begin{aligned}
 x_{l1}^i &= 0, \quad \forall i \in \{1, 2, \dots, q\} \\
 x_{l2}^i &= \log^{-1} |x_{u2}^i| - 1, \quad \forall i \in \{1, 2, \dots, r\}
 \end{aligned} \tag{20}$$

The values of the variables at the optima are $x_u = 0$ and x_l is obtained by the relationship given above. Both the upper and lower level functions are equal to 0 at the optima. Figure 9 represents the same information as in Figure 8 for a four variable bilevel problem.

6.5 SMD5

SMD5 is a test problem with a conflict between the two levels. The difficulty introduced is in terms of multi-modality and convergence at the lower level. The lower level problem contains the banana function such that the global optimum lies in a long, narrow, flat parabolic valley. The upper level is convex with

respect to upper level variables and optimal lower level variables.

$$\begin{aligned}
F_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
F_0^2 &= -\sum_{i=1}^q \left((x_{l1}^{i+1} - (x_{l1}^i)^2) + (x_{l1}^i - 1)^2 \right) \\
F_0^3 &= \sum_{i=1}^r (x_{u2}^i)^2 - \sum_{i=1}^r (|x_{u2}^i| - (x_{l2}^i)^2)^2 \\
f_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
f_0^2 &= \sum_{i=1}^q \left((x_{l1}^{i+1} - (x_{l1}^i)^2) + (x_{l1}^i - 1)^2 \right) \\
f_0^3 &= \sum_{i=1}^r (|x_{u2}^i| - (x_{l2}^i)^2)^2
\end{aligned} \tag{21}$$

The range of variables is as follows,

$$\begin{aligned}
x_{u1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, p\} \\
x_{u2}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, r\} \\
x_{l1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, q\} \\
x_{l2}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{22}$$

Relationship between upper level variables and lower level optimal variables is given as follows,

$$\begin{aligned}
x_{l1}^i &= 1, \quad \forall i \in \{1, 2, \dots, q\} \\
x_{l2}^i &= \sqrt{|x_{u2}^i|}, \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{23}$$

The values of the variables at the optima are $x_u = 0$ and x_l is obtained by the relationship given above. Both the upper and lower level functions are equal to 0 at the optima.

6.6 SMD6

SMD6 is a test problem with a conflict between the two levels. The problem contains infinitely many global solutions at the lower level, for any given upper level vector. Out of the entire global solution set, there is only a single lower level point which corresponds to the best upper level function value.

$$\begin{aligned}
F_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
F_0^2 &= -\sum_{i=1}^q (x_{l1}^i)^2 + \sum_{i=q+1}^{q+s} (x_{l1}^i)^2 \\
F_0^3 &= \sum_{i=1}^r (x_{u2}^i)^2 - \sum_{i=1}^r (x_{u2}^i - x_{l2}^i)^2 \\
f_0^1 &= \sum_{i=1}^p (x_{u1}^i)^2 \\
f_0^2 &= \sum_{i=1}^q (x_{l1}^i)^2 + \sum_{i=q+1, i=i+2}^{q+s-1} (x_{l1}^{i+1} - x_{l1}^i)^2 \\
f_0^3 &= \sum_{i=1}^r (x_{u2}^i - x_{l2}^i)^2
\end{aligned} \tag{24}$$

The range of variables is as follows,

$$\begin{aligned}
x_{u1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, p\} \\
x_{u2}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, r\} \\
x_{l1}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, q+s\} \\
x_{l2}^i &\in [-5, 10], \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{25}$$

Relationship between upper level variables and lower level optimal variables is given as follows,

$$\begin{aligned}
x_{l1}^i &= 0, \quad \forall i \in \{1, 2, \dots, q\} \\
x_{l2}^i &= x_{u2}^i, \quad \forall i \in \{1, 2, \dots, r\}
\end{aligned} \tag{26}$$

The values of the variables at the optima are $x_u = 0$ and x_l is obtained by the relationship given above. Both the upper and lower level functions are equal to 0 at the optima.

7 Standard test problems

Tables 2 and 3 provide a set of 8 standard test problems collected from the literature. The dimensions of the upper and lower level variables are given in the first column, and the problem formulation is defined in the second column. The third column provides the best known solution available in the literature for the chosen test problems.

8 Results

In this section, we provide the results obtained on the SMD test problems and other test problems using the BLEAQ approach. The section is divided into two parts. The first part contains the results obtained using the BLEAQ approach, which has been compared with the results obtained using a nested procedure. It was difficult to identify an approach from the existing literature, which can efficiently handle the SMD test problems with 10 variables. Therefore, we have chosen the nested approach as the benchmark for this study. The second part contains the results obtained on 8 standard constrained test problems, which have been studied by others in the past. We compare our method against the approach proposed by Wang et al. (2005), which is able to handle all the test problems successfully.

8.1 Results for SMD test problems

We report the results obtained by the nested procedure and the BLEAQ approach in this sub-section on 10-dimensional unconstrained SMD test problems. For test problems SMD1 to SMD5 we choose $p = 3$, $q = 3$ and $r = 2$, and for SMD6 we choose $p = 3$, $q = 1$, $r = 2$ and $s = 2$. Tables 4 and 5 provide the results obtained using the nested approach on these test problems. The nested approach uses an evolutionary algorithm at both the levels. For every upper level member a lower level optimization problem is solved in this approach [23]. The approach successfully handles all the test problems. However, as can be observed from Table 4, the number of function evaluation required are very high at the lower level. We use the nested approach as a benchmark to assess the savings obtained from the BLEAQ approach. Tables 6 and 7 provides the results obtained using the BLEAQ approach. Fourth and Fifth column in Table 6 provides the median function evaluations required at the upper and lower levels respectively. The numbers in the brackets provide a ratio of the function evaluations required using nested approach against the function evaluations required

Table 2: Description of the selected standard test problems (TP1-TP4).

Problem	Formulation	Best Known Sol.
TP1 $M = 2$ $m = 2$	Minimize $F_0(x_u, x_l) = (x_u^1 - 30)^2 + (x_u^2 - 20)^2 - 20x_l^1 + 20x_l^2$, s.t. $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = (x_u^1 - x_l^1)^2 + (x_u^2 - x_l^2)^2 \\ 0 \leq y_i \leq 10, \quad i = 1, 2 \end{array} \right\},$ $x_u^1 + 2x_u^2 \geq 30, x_u^1 + x_u^2 \leq 25, x_u^2 \leq 15$	$F_0 = 225.0$ $f_0 = 100.0$
TP2 $M = 2$ $m = 2$	Minimize $F_0(x_u, x_l) = 2x_u^1 + 2x_u^2 - 3x_l^1 - 3x_l^2 - 60$, s.t. $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = (x_l^1 - x_u^1 + 20)^2 + \\ (x_u^2 - x_l^2 + 20)^2 \\ x_u^1 - 2x_l^1 \geq 10, x_u^2 - 2x_l^2 \geq 10 \\ -10 \geq y_i \geq 20, \quad i = 1, 2 \end{array} \right\},$ $x_u^1 + x_u^2 + x_l^1 - 2x_l^2 \leq 40,$ $0 \leq x_i \leq 50, \quad i = 1, 2.$	$F_0 = 0.0$ $f_0 = 100.0$
TP3 $M = 2$ $m = 2$	Minimize $F_0(x_u, x_l) = -(x_u^1)^2 - 3(x_u^2)^2 - 4x_l^1 + (x_l^2)^2$, s.t. $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = 2(x_u^1)^2 + (x_l^1)^2 - 5x_l^2 \\ (x_u^1)^2 - 2x_u^1 + (x_u^2)^2 - 2x_l^1 + x_l^2 \geq -3 \\ x_u^2 + 3x_l^1 - 4x_l^2 \geq 4 \\ 0 \leq y_i, \quad i = 1, 2 \end{array} \right\},$ $(x_u^1)^2 + 2x_u^2 \leq 4,$ $0 \leq x_i, \quad i = 1, 2$	$F_0 = -18.6787$ $f_0 = -1.0156$
TP4 $M = 2$ $m = 3$	Minimize $F_0(x_u, x_l) = -8x_u^1 - 4x_u^2 + 4x_l^1 - 40x_l^2 - 4x_l^3$, s.t. $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = x_u^1 + 2x_u^2 + x_l^1 + x_l^2 + 2x_l^3 \\ x_l^2 + x_l^3 - x_l^1 \leq 1 \\ 2x_u^1 - x_l^1 + 2x_l^2 - 0.5x_l^3 \leq 1 \\ 2x_u^2 + 2x_l^1 - x_l^2 - 0.5x_l^3 \leq 1 \\ 0 \leq y_i, \quad i = 1, 2 \end{array} \right\},$ $0 \leq x_i, \quad i = 1, 2$	$F_0 = -29.2$ $f_0 = 3.2$

Table 3: Description of the selected standard test problems (TP5-TP8).

Problem	Formulation	Best Known Sol.
TP5	<p>Minimize $F_0(x_u, x_l) = rt(x_u)x_u - 3x_l^1 - 4x_l^2 + 0.5t(x_l)x_l$, (x_u, x_l) s.t.</p> $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = 0.5t(x_l)hx_l - t(b(x_u))x_l \\ -0.333x_l^1 + x_l^2 - 2 \leq 0 \\ x_l^1 - 0.333x_l^2 - 2 \leq 0 \\ 0 \leq y_i, \quad i = 1, 2 \end{array} \right\},$ <p>where $h = \begin{pmatrix} 1 & 3 \\ 3 & 10 \end{pmatrix}, b(x) = \begin{pmatrix} -1 & 2 \\ 3 & -3 \end{pmatrix} x, r = 0.1$ $t(\cdot)$ denotes transpose of a vector</p>	$F_0 = -3.6$ $f_0 = -2.0$
TP6	<p>Minimize $F_0(x_u, x_l) = (x_u^1 - 1)^2 + 2x_l^1 - 2x_u^1$, (x_u, x_l) s.t.</p> $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = (2x_l^1 - 4)^2 + \\ (2x_l^2 - 1)^2 + x_u^1 x_l^1 \\ 4x_u^1 + 5x_l^1 + 4x_l^2 \leq 12 \\ 4x_l^2 - 4x_u^1 - 5x_l^1 \leq -4 \\ 4x_u^1 - 4x_l^1 + 5x_l^2 \leq 4 \\ 4x_l^1 - 4x_u^1 + 5x_l^2 \leq 4 \\ 0 \leq y_i, \quad i = 1, 2 \end{array} \right\},$ <p>$0 \leq x_u^1$</p>	$F_0 = -1.2091$ $f_0 = 7.6145$
TP7	<p>Minimize $F_0(x_u, x_l) = -\frac{(x_u^1 + x_l^1)(x_u^2 + x_l^2)}{1 + x_u^1 x_l^1 + x_u^2 x_l^2}$, (x_u, x_l) s.t.</p> $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = \frac{(x_u^1 + x_l^1)(x_u^2 + x_l^2)}{1 + x_u^1 x_l^1 + x_u^2 x_l^2} \\ 0 \leq y_i \leq x_i, \quad i = 1, 2 \end{array} \right\},$ <p>$(x_u^1)^2 + (x_u^2)^2 \leq 100$ $0 \leq x_i, \quad i = 1, 2$</p>	$F_0 = -1.98$ $f_0 = 1.98$
TP8	<p>Minimize $F_0(x_u, x_l) = 2x_u^1 + 2x_u^2 - 3x_l^1 - 3x_l^2 - 60$, (x_u, x_l) s.t.</p> $y \in \underset{(y)}{\operatorname{argmin}} \left\{ \begin{array}{l} f_0(x_u, x_l) = (x_l^1 - x_u^1 + 20)^2 + \\ (x_l^2 - x_u^2 + 20)^2 \\ 2x_l^1 - x_u^1 + 10 \leq 0 \\ 2x_l^2 - x_u^2 + 10 \leq 0 \\ -10 \leq y_i \leq 20, \quad i = 1, 2 \end{array} \right\},$ <p>$x_u^1 + x_u^2 + x_l^1 - 2x_l^2 \leq 40$ $0 \leq x_i \leq 50, \quad i = 1, 2$</p>	$F_0 = 0.0$ $f_0 = 100.0$

using BLEAQ. The nested approach requires 2 to 5 times more function evaluations at the upper level, and more than 10 times function evaluations at the lower level as compared to BLEAQ. Both the approaches are able to successfully handle all the test problems. However, BLEAQ dominates the nested approach by a significant margin, particularly in terms of the function evaluations at the lower level.

Table 4: Function evaluations (FE) for the upper level (UL) and the lower level (LL) from 11 runs of nested approach.

Pr. No.	Best		Median		Worst	
	Total LL FE	Total UL FE	Total LL FE	Total UL FE	Total LL FE	Total UL FE
SMD1	834478	1195	1628136	2473	2037784	3258
SMD2	1001588	1495	1500725	2239	2095710	3341
SMD3	868658	1232	1412300	2231	1790398	2684
SMD4	550263	730	1106389	1634	1337435	1988
SMD5	1257659	1666	1947316	2875	2561079	3528
SMD6	1243533	1624	2326072	3076	2946779	3812

Table 5: Accuracy for the upper and lower levels, and the lower level calls from 11 runs of nested approach.

Pr. No.	Median	Median	Median	LL Evals LL Calls
	UL Accuracy	LL Accuracy	LL Calls	
SMD1	0.0051	0.0016	2473	647.02
SMD2	0.0015	0.0005	2239	653.82
SMD3	0.0087	0.0026	2231	649.59
SMD4	0.0078	0.0027	1634	694.91
SMD5	0.0012	0.0032	2875	717.13
SMD6	0.0096	0.0071	3076	767.03

8.2 Convergence Study

In this sub-section we provide the results on the convergence of the algorithm towards the bilevel optimal solution. We performed a convergence study for the first two SMD test problems with 10-dimensions, and the results are presented in Figures 10 and 11 for one particular run. The figures show the progress of the elite member at each of the generations. The upper plot shows the convergence towards the upper level optimal function value, and the lower plot shows the convergence towards the lower level optimal function value. The algorithm

Table 6: Function evaluations (FE) for the upper level (UL) and the lower level (LL) from 11 runs of the proposed BLEAQ.

Pr. No.	Best Func. Evals.		Median Func. Evals.		Worst Func. Evals.	
	LL	UL	LL (Savings)	UL (Savings)	LL	UL
SDM1	99315	610	110716 (14.71)	740 (3.34)	170808	1490
SDM2	70032	376	91023 (16.49)	614 (3.65)	125851	1182
SDM3	110701	620	125546 (11.25)	900 (2.48)	137128	1094
SDM4	61326	410	81434 (13.59)	720 (2.27)	101438	1050
SDM5	102868	330	126371 (15.41)	632 (4.55)	168401	1050
SDM6	5558	658	8393 (277.14)	946 (3.25)	10017	1322

Table 7: Accuracy for the upper and lower levels, and the lower level calls from 11 runs of the proposed BLEAQ.

Pr. No.	Median	Median	Median	$\frac{\text{LL Evals}}{\text{LL Calls}}$
	UL Accuracy	LL Accuracy	LL Calls	
SDM1	0.006828	0.003521	528	202.47
SDM2	0.003262	0.002745	522	176.09
SDM3	0.009122	0.004364	603	225.91
SDM4	0.006957	0.002716	574	146.39
SDM5	0.004103	0.003773	513	243.68
SDM6	0.000000	0.000000	167	50.24

preserves the elite member at the upper level, so we observe a continuous improvement in the upper plot. However, in a bilevel problem an improvement in the elite at the upper level does not guarantee a continuous improvement in the lower level function value. Therefore, we observe that the lower level convergence plot is not a continuously reducing plot rather contains small humps.

Next, we evaluate the algorithm’s performance in approximating the actual Ψ mapping. For this we choose the problem SMD1, which has the following Ψ mapping.

$$\begin{aligned} x_{l1}^i &= 0, \quad \forall i \in \{1, 2, \dots, p\} \\ x_{l2}^i &= \tan^{-1} x_{u2}^i, \quad \forall i \in \{1, 2, \dots, r\} \end{aligned} \quad (27)$$

We set $p = 3$, $q = 3$ and $r = 2$ to get a 10-dimensional SMD1 test problem. The Ψ mapping for SMD1 test problem is variable separable. Therefore, in order to show the convergence of the approximation on a 2-d plot, we choose the variable x_{l2}^1 , and show its approximation with respect to x_{l2}^1 . The true relationship between the variables is shown in Figure 12, along with the quadratic approximations generated at various generations. It can be observed that the

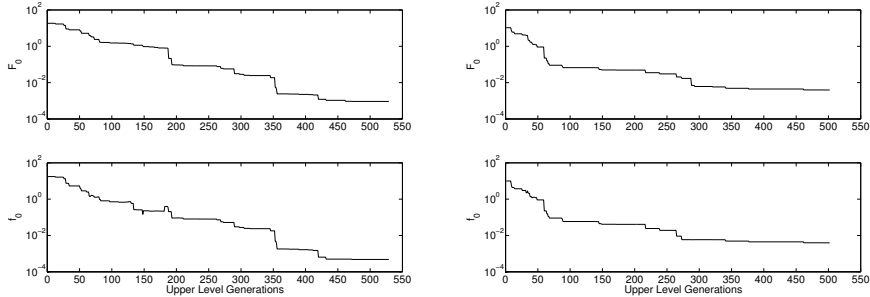


Figure 10: Convergence plot for SMD1. Figure 11: Convergence plot for SMD2.

approximations in the vicinity of the true bilevel optimum improves with increasing number of generations.

8.3 Results for constrained test problems

In this sub-section, we provide results for 8 standard constrained test problems chosen from the literature. We compare our results against the approach proposed by Wang et al. (2005). The reason for the choice of this approach as a benchmark is that the approach was successful in solving all the chosen constrained test problems. The results obtained using the BLEAQ and WJL [27] approach has been provided in Tables 8, 9 and 10. Table 8 provides the minimum, median and maximum function evaluations required to solve the chosen problems using the BLEAQ approach. Table 9 provides the accuracy obtained at both the levels, in terms of absolute difference from the best known solution to a particular test problem. The numbers in the brackets provide the best solution known from the literature for each of the test problems. The table also provides the median number of lower level calls, and the average number of lower level function evaluations required per lower level call. Table 10 compares the mean function evaluations at the upper and lower levels required by BLEAQ against that required by WJL. In their paper, Wang et al. have reported the function evaluations as sum of function evaluations for the two levels. The reported metric in their paper is the average function evaluations from multiple runs of their algorithm. We have computed a similar metric for BLEAQ, and the results are reported in the table. It can be observed that WJL requires close to an order of magnitude times more function evaluations for most of the test problems. This clearly demonstrates the efficiency gain obtained using the BLEAQ approach. It also suggests that the mathematical insights used along with the evolutionary principles in the BLEAQ approach is helpful in converging quickly towards the bilevel optimal solution.

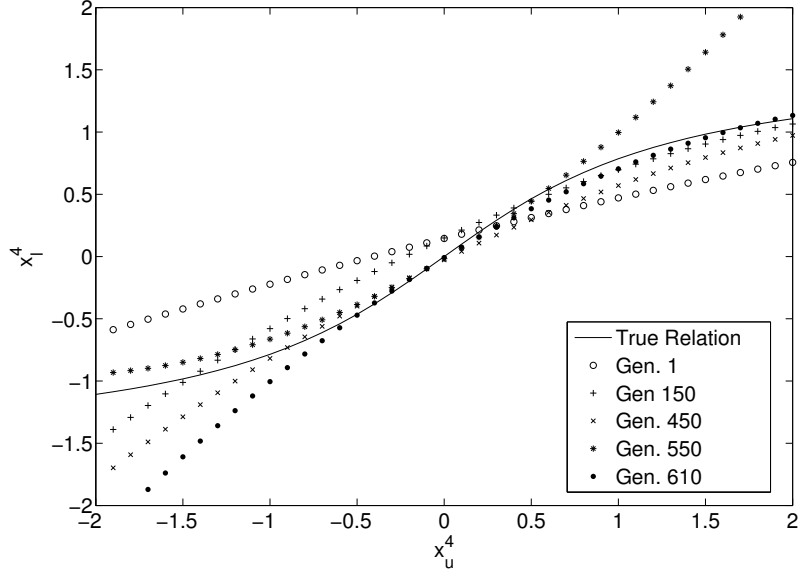


Figure 12: Quadratic relationship convergence.

Table 8: Function evaluations (FE) for the upper level (UL) and the lower level (LL) from 11 runs of the proposed BLEAQ.

Pr. No.	Best Func. Evals.		Median Func. Evals.		Worst Func. Evals.	
	LL	UL	LL	UL	LL	UL
TP1	14115	718	15041	780	24658	1348
TP2	12524	1430	14520	1434	16298	2586
TP3	4240	330	4480	362	6720	518
TP4	14580	234	15300	276	15480	344
TP5	10150	482	15700	1302	15936	1564
TP6	14667	230	17529	284	21875	356
TP7	234622	3224	267784	4040	296011	5042
TP8	10796	1288	12300	1446	18086	2080

9 Conclusions

In this paper, we have propose an efficient bilevel evolutionary algorithm (BLEAQ) which works by approximating the optimal solution mapping between the lower level optimal solutions and the upper level variables. The algorithm not only converges towards the the optimal solution of the bilevel optimization problem, but also provides the optimal solution mapping at the optima. This provides

Table 9: Accuracy for the upper and lower levels, and the lower level calls from 11 runs of the proposed BLEAQ.

Pr.	Median	Median	Median	$\frac{\text{LL Evals}}{\text{LL Calls}}$
	UL Accuracy	LL Accuracy	LL Calls	
TP1	0.000000 (225.0)	0.000000 (100.0)	206	72.76
TP2	0.012657 (0.0)	0.000126 (100.0)	235	61.79
TP3	0.000000 (-18.678711)	0.000000 (-1.015625)	112	40.00
TP4	0.040089 (-29.2)	0.007759 (3.2)	255	60.00
TP5	0.008053 (-3.6)	0.040063 (-2.0)	203	78.50
TP6	0.000099 (-1.2091)	0.000332 (7.6145)	233	75.23
TP7	0.093192 (-1.98)	0.093192 (1.98)	3862	95.42
TP8	0.001819 (0.0)	0.000064 (100.0)	200	61.50

Table 10: Comparison of BLEAQ against the results achieved by WJL approach.

Pr. No.	Mean LL Func. Evals.		
	BLEAQ	WJL	Savings
TP1	16228	85499	5.27
TP2	17210	256227	14.89
TP3	5256	92526	17.60
TP4	16690	291817	17.48
TP5	16738	77302	4.62
TP6	17717	163701	9.24
TP7	261387	1074742	4.11
TP8	14105	213522	15.14

valuable information, as to how the lower level optimal solution changes based on changes in the upper level variable vector in the vicinity of the bilevel optima. The algorithm has been tested on two sets of test problems. The first set of test problems are recently proposed SMD test problems which are scalable in terms of number of variables. The method has been tested on a 10-dimensional instance of these test problems. The second set of test problems are 8 standard test problems chosen from the literature. These problems are constrained and have relatively smaller number of variables. The results obtained using the BLEAQ approach has been compared against a nested strategy for the SMD test problems, and against the WJL approach for the standard constrained test problems. For both the sets, BLEAQ offers significant improvement in the number of function evaluations at both the levels.

10 Acknowledgements

Ankur Sinha and Pekka Malo would like to acknowledge the support provided by Liikesivistysrahasto and Helsinki School of Economics foundation. Authors of the paper would like to acknowledge the conversations with Prof. Yu-Ping Wang.

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