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A Hybrid Bayesian Approach for Pessimistic Bilevel Problems with a New Formulation

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Abstract. In many real-world problems, finding the optimal decision for a decision-maker depends on another decision-maker's response, and it is called bilevel optimization in mathematical programming. It contains two levels of optimization problems while one appears as a constraint of another one called follower and leader, respectively. In many real-world scenarios, the lower level has multiple global optima and the upper level needs to make worst-case assumptions about the decision of the lower level, called the pessimistic case of the bilevel problem. Various approaches have been implemented over the years to solve generic bilevel problems, but few of them could be extended to pessimistic cases. In this short paper, we first propose a new formulation for the pessimistic case. In this way, we take advantage of the hierarchical structure of bilevel problems to make the results more accurate for pessimistic cases. Then, we implement a black-box approach to solve the pessimistic upper level problem to decrease the necessary function evaluations. The performance of the problem is examined by solving a test benchmark problem from the literature.

1 Introduction

Many large-scale decision-making processes are *hierarchical* in terms of the obtained outcome of any decision taken by the upper-level authority to optimize their goals is affected by another decision considered as the response of lower-level entities who aim to optimize their own goals. For any given upper-level decision, there is a parametric lower-level optimization problem. The structure of these problems is asymmetric: the leader has perfect knowledge about the followers' objectives and constraints, while the follower must first observe the leader's decision before making their own decisions. Bilevel optimization problems have been used to formulate many real-world hierarchical problems over the years. It has worked successfully in the field of traffic and transportation [24, 25, 9], production and capacity planning [17, 23], management science [5, 10], energy networks [16, 34] and defence industry [1, 15].

There are two roots in terms of the research on decision-making problems with a hierarchical structure. The first one is in the domain of mathematical programming and the second one is in the domain of game theory. In the context of game theory, von Stackelberg [30] built a descriptive model of decision behaviour and provided game-theoretic equilibria. In the context of mathematical programming, an inner optimization problem appears as a constraint of an outer optimization problem which is called the bilevel optimization problem (BOP) [6]. They were introduced by J. Bracked and J. McGill, and a defence application was published by the same authors in the following year [7]. BOPs were modelled as mathematical programs at this time and are difficult to handle mathematically because of the hierarchical optimization structure. It may introduce difficulties such as non-convexity and disconnectedness between the upper-level and lower-level problems, even for simple instances. It has been shown that bilevel programming is strongly NP-hard [19], and it has been proven that just evaluating a solution is also an NP-hard task [31].

An uncertainty appears when the lower level problem is multi-modal, meaning that it has several global optima. Considering the presence of multiple lower-level optimal solutions for some x_u values, there are two approaches have been proposed in [12], called optimistic and pessimistic approaches. In the optimistic case, the upper level assumes that the lower level will select the most optimal solution also for the upper level. In the pessimistic approach, the upper level is making the worst assumption while optimizing her problem about the lower level. The assumption in the optimistic approach is a cooperation of the lower level with the upper level without any benefit, which is not realistic. On the other hand, the pessimistic approach can be considered more cautious and can be explained minimising the risk for the worst case. Hence, finding the solutions for the pessimistic case has vast importance in practice. For instance, an interdiction game has various applications such as critical infrastructure defence, nuclear weapon projects and attacker-defender problems. The leading decision-maker needs to consider the non-cooperative defender to make the optimal decision. In general, the framework for solving these problems is hierarchical sequential decision-making considering the worst-case assumptions which is the pessimistic case of bilevel problems.

There are several approaches have been developed to solve pessimistic BOPs, including classical and evolutionary algorithms. In the classical approaches, [13] focused on specific mathematical properties such as solving linear pessimistic BOPs and [22] proposed an algorithm to solve pessimistic quadratic-linear BOPs. In the hybrid and evolutionary approaches, [3] developed a particle swarm optimization-based approach. [2] proposed a differential evolution-

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based algorithm with a multi-objective lower level problem. A fully evolutionary algorithm is proposed in [4] and they optimized the upper level for both optimistic and pessimistic approaches and then presented both. A survey about solving pessimistic BOPs and the optimality condition can be found in [21, 28]. To the best of our knowledge, there is no hybrid method with a black-box approach at upper level and exact approach at lower level to solve *pessimistic* BOPs.

The proposed approaches in the literature are expensive-to-evaluate in terms of function evaluations because of the nature of the evolutionary algorithms. In this study, we propose a new formulation for the pessimistic approach to tackle this obstacle with multi-objective upper level problems and aim to solve with a hybrid approach. The upper level decision maker has full knowledge about the follower and its constraints, so following this idea, we restructure the upper level problem by adding lower level objectives in the opposite direction. Then, we aim to solve multi-objective upper level problems. The algorithm has a nested structure, so we first optimize black-box upper level objectives and select the best candidate from the Pareto front. Then for each upper level decision, the lower level optimization is conducted. The Bayesian method solves the upper-level multi-objective problem by optimizing the hypervolume improvement acquisition function. In this way, there is no need to make any assumption about the mathematical structure of the problem such as differentiability, non-convexity, etc. It also gives us the leverage of batch selection which comes with making multiple decisions at the same time to observe lower level responses. An exact algorithm solves the lower level problem to avoid the local minima and we focus on upper level decision-making with the pessimistic approach. We conducted experiments with the test benchmark problem with known global optima.

The rest of the paper is organized as follows. The optimistic and pessimistic formulations are defined in Section 2. In Section 3, we proposed the new formulation and explained the steps of the algorithm. The experimental details and empirical results are explained in Section 4. Finally, we conclude the paper in Section 6 and discuss with the future directions of the research.

2 Preliminaries

In this section, we provide a general formulation of BOPs and preliminaries for the proposed algorithm. Also, we discuss and formulate optimistic and pessimistic positions for BOPs which are being assumed by the leader.

We shall represent the leader decision by x_u and the follower response by x_l^*. A decision pair x_u, x_l^* represents the leaders' decision and an optimal feasible solution of the follower. Both optimistic and pessimistic formulations are shared in Definitions 1 and 2.

Definition 1. *For the upper-level objective function $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ and lower-level objective function $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, optimistic bilevel optimization problem is given by*

$$\begin{aligned} &\min_{x_u} \; F(x_u, x_l) \\ &\text{s.t. } x_l \in \underset{x_l}{\text{argmin}} \left\{ \begin{matrix} f(x_u, x_l) : g_j(x_u, x_l) \leq 0, \\ j = 1, 2, \ldots, J \end{matrix} \right\} \\ &G_k(x_u, x_l) \leq 0, \; k = 1, 2, \ldots, K \end{aligned} \tag{1}$$

where $x_u \in \mathcal{X}_U, x_l \in \mathcal{X}_L$ are vector-valued upper-level and lower-level decision variables, and $\mathcal{X}_U \subseteq \mathbb{R}^n$, $\mathcal{X}_L \subseteq \mathbb{R}^m$ decision spaces, G_k and g_j represent the constraints of the bilevel problem.

Definition 2. *For the upper-level objective function $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ and lower-level objective function $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, pessimistic bilevel optimization problem is given by*

$$\begin{aligned} &\min_{x_u} \max_{x_l} \; F(x_u, x_l) \\ &\text{s.t. } x_l \in \underset{x_l}{\text{argmin}} \left\{ \begin{matrix} f(x_u, x_l) : g_j(x_u, x_l) \leq 0, \\ j = 1, 2, \ldots, J \end{matrix} \right\} \\ &G_k(x_u, x_l) \leq 0, \; k = 1, 2, \ldots, K \end{aligned} \tag{2}$$

where $x_u \in \mathcal{X}_U, x_l \in \mathcal{X}_L$ are vector-valued upper-level and lower-level decision variables, and $\mathcal{X}_U \subseteq \mathbb{R}^n$, $\mathcal{X}_L \subseteq \mathbb{R}^m$ decision spaces, G_k and g_j represent the constraints of the bilevel problem.

Bayesian optimization (BO) is a method to optimize expensive-to-evaluate black-box functions. BO uses a probabilistic surrogate model, typically Gaussian process (GP) [27], $p(f|\mathcal{D})$ to model the objective function f based on previously observed data points, that can be declared as $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$. GPs are models that are specified by a mean function $\mu(\mathbf{x}; \{\mathbf{x}_n, y_n\}, \theta) : \mathbb{R}^d \to \mathbb{R}$ and predictive variance function $\sigma(\mathbf{x}; \{\mathbf{x}_n, y_n\}, \theta) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$. Surrogate model $p(f|\mathcal{D})$ is assisted by an acquisition function $\alpha : \mathcal{X} \to \mathbb{R}$. We represent acquisition functions depending on the previous observations as $\alpha(\mathbf{x}; \{\mathbf{x}_n, y_n\}, \theta)$ where θ is Gaussian parameters such as a kernel for the model. Because the objective function is expensive to evaluate and the surrogate-based acquisition function is not, it can be optimized more easily than the true function to yield $\mathbf{x}_{new}$. The acquisition function selects the point $\mathbf{x}_{new}$ that maximizes the acquisition function $\mathbf{x}_{new} = argmax_{\mathbf{x} \in \mathcal{X}} \alpha(\mathbf{x})$. Then, it evaluates the objective function $y_{new} = f(\mathbf{x}_{new})$ and updates the data set with new observations $\mathcal{D} \leftarrow \mathcal{D} \cup (\mathbf{x}_{new}, y_{new})$.

In the GP, $\mu(x)$ can be viewed as the prediction of the function value, and $\sigma(x)$ is a measure of the uncertainty of the prediction. Multi-objective BO tackles the problem of optimizing a vector-valued objective $\mathbf{f}(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}^d$ with $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_d(\mathbf{x}))$ for a vector-valued decision variable $\mathbf{x} \in \mathbb{R}^d$. Because of the nature of the multi-objective black-box problems, we assume that there is no known analytical expression. Multi-objective optimization problems generally do not have a single best solution, so we must find a solution set instead of a single solution: the set of Pareto-optimal solutions. We say that $\mathbf{f}(\mathbf{x})$ dominates another solution $\mathbf{f}(\mathbf{x}')$ if $f^{(i)}(\mathbf{x}) \succ f^{(i)}(\mathbf{x}')$ for all $i = 1, 2, \ldots, M$ and there exists $i' \in \{1, 2, \ldots, M\}$ such that $f^{i'}(\mathbf{x}) \succ f^{i'}(\mathbf{x}')$. So we can express the Pareto-optimal solution set by $P^* = \{\mathbf{f}(\mathbf{x}) \text{ s.t. } \nexists \mathbf{x}' \in X : \mathbf{f}(\mathbf{x}') \succ \mathbf{f}(\mathbf{x})\}$ and $X^* = \{\mathbf{x} \in X \text{ s.t. } \mathbf{f}(\mathbf{x}) \in P^*\}$. After obtaining the Pareto-front, the decision maker can make decisions using the trade-off between objectives, or any preferences.

Hypervolume improvement (HVI) is often used as a measure of improvement in multi-objective problems [32]. Several methods have been proposed. Expected Hypervolume Improvement (EHVI) is an updated version of Expected Improvement (EI) to HVI, and determined by $J(\mathbf{x}) = \mathbb{E}_{p(f(x)|D_n)}[HVI(f(\mathbf{x}))]$. It aims to maximize the expected hypervolume improvement at each Bayesian iteration and consider it as acquisition function. More details can be found in [32].

3 Methodology

3.1 A New Formulation for Pessimistic BOPs

Bilevel problems have asymmetric structure, meaning that upper level has complete information about lower level objectives and constraints despite the lower level having no idea about upper level ones.

Also, the pessimistic approach assumes that the upper level will make a decision with the worst case assumption about the decision of lower level. Therefore, we can reformulate the single-objective upper level problem by adding the lower level objective with opposite direction as in Equation 3.

$$\begin{aligned} &\min_{x_u} \ \big\{F(x_u, x_l), -f(x_u, x_l)\big\} \\ &\text{s.t. } G_k(x_u, x_l) \leq 0, k = 1, 2, \ldots, K \end{aligned} \tag{3}$$

where $G_k(x_u, x_l)$ is upper level constraints. Then the upper level is supposed to be optimized a multi-objective manner and the optimal decision is chosen from the Pareto front solution set that contains multiple feasible solutions. Multiple approaches are proposed for selecting the decision from the Pareto front, such as [8, 14]. As the Pareto front has multiple feasible solutions, we made a random selection at each step.

For generalization, Equation 3 can be expressed as pessimistic multi-objective BOPs as follows:

$$\begin{aligned} &\min_{x_u} \begin{Bmatrix} F_1(x_u, x_l), ..., F_{M_u}(x_u, x_l), \\ -(f_1(x_u, x_l), ..., f_{M_l}(x_u, x_l)) \end{Bmatrix} \\ &\text{s.t. } x_l \in \underset{x_l}{\text{argmin}} \begin{Bmatrix} f_1(x_u, x_l), ..., f_{M_l}(x_u, x_l) \\ g_j(x_u, x_l) \leq 0, \ j = 1, 2, \ldots, J \end{Bmatrix} \\ &\quad G_k(x_u, x_l) \leq 0, \ k = 1, 2, \ldots, K \end{aligned} \tag{4}$$

where the upper level objective functions are $F_i(x_u, x_l)$, $i = 1, 2, \ldots, M_u$ and the lower level objective functions are $f_i(x_u, x_l)$, $i = 1, 2, \ldots, M_l$ where $x_u \in \mathcal{X}_u$ and $x_l \in \mathcal{X}_l$. $G_k(x_u, x_l)$ and $g_j(x_u, x_l)$ represent upper and lower level constraints respectively. j and k values represent the number of constraints at the upper and lower level. The pessimistic upper level objective in Equation 4 is equal to Equation 3 when M_u and M_u are both equal to 1.

3.2 Proposed Method

In this section, we explain the proposed algorithm for pessimistic BOPs. First, we give brief information about the algorithm, then we explain with the details.

The proposed algorithm is a hybrid method to solve pessimistic BOPs. Briefly, it works as follows. A size of N_u initial decisions, $\mathbf{x_u}$, is randomly selected from upper-level search space. We used Sobol sampling for the initial random selection. For each upper-level decision, the lower-level problem is optimized using a sequential least squared programming (SLSQP) algorithm [20]. The solution set obtained after lower-level optimization $(\mathbf{x}_u, \mathbf{x}_l^*)$ is used to find upper-level fitnesses $F_i(\mathbf{x}_u, \mathbf{x}_l^*)$ for $i = 1, 2, \ldots, M_u$ and lower level fitnesses $f_i(\mathbf{x}_u, \mathbf{x}_l^*)$ for $i = 1, 2, \ldots, M_l$. We train the GP model with the data set $(\mathbf{x}_u, y_i)$ where $y_i = \{F_i(\mathbf{x}_u, \mathbf{x}_l^*), -f_i(\mathbf{x}_u, \mathbf{x}_l^*)\}$. We use Bayesian Optimization to choose the next candidate with qEHVI acquisition function. The lower-level optimization process is repeated for each pessimistic upper level decision $\mathbf{x}_u$. It is important to note that dealing with constraints is the most challenging aspect of BOPs. To avoid upper-level constraint violation, we made the random selection from upper level Pareto-front considering the lower level constraints. The algorithm runs for 50 iterations for the whole multi-objective bilevel optimization process.

We assume that we have the pessimistic upper level multi-objective problem with opposite direction lower level objective. We use GP to model the objective functions $\mathbf{F} = \{F_1(\mathbf{x}_u, \mathbf{x}_l), ..., F_{M_u}(\mathbf{x}_u, \mathbf{x}_l)\}$ and $\mathbf{f} = \{f_1(\mathbf{x}_u, \mathbf{x}_l), ..., f_{M_l}(\mathbf{x}_u, \mathbf{x}_l)\}$ where M_u and M_l is the number of upper-level objective, respectively. Let us assume that we have the observed upper-level and lower-level decisions and upper-level objective values, then the observation data is as follows:

$$D = \begin{Bmatrix} (\mathbf{x}_{u_1}, \mathbf{x}_{l_1}, \mathbf{F}(\mathbf{x}_{u_1}, \mathbf{x}_{l_1}), -\mathbf{f}(\mathbf{x}_{u_1}, \mathbf{x}_{l_1})), \\ \ldots, \\ (\mathbf{x}_{u_n}, \mathbf{x}_{l_n}, \mathbf{F}(\mathbf{x}_{u_n}, \mathbf{x}_{l_n}), -\mathbf{f}(\mathbf{x}_{u_n}, \mathbf{x}_{l_n})) \end{Bmatrix} \tag{5}$$

where n is the number of observations. The GP model is constructed with mean function and predictive variance function is defined by:

$$\begin{aligned} &\mu(\mathbf{x}; \{\mathbf{x}_{u_n}, \mathbf{x}_{l_n}, \mathbf{F}(\mathbf{x}_{u_n}, \mathbf{x}_{l_n}), -\mathbf{f}(\mathbf{x}_{u_n}, \mathbf{x}_{l_n})\}, \theta) \\ &\sigma(\mathbf{x}; \{\mathbf{x}_{u_n}, \mathbf{x}_{l_n}, \mathbf{F}(\mathbf{x}_{u_n}, \mathbf{x}_{l_n}), -\mathbf{f}(\mathbf{x}_{u_n}, \mathbf{x}_{l_n})\}, \theta) \end{aligned} \tag{6}$$

where θ is the model parameters. An acquisition function for multi-objective optimization is Expected Hypervolume Improvement. Maximizing hypervolume (HV) is a procedure for finding the maximum coverage with Pareto fronts [35]. We use the q-expected hypervolume improvement acquisition function (qEHVI) for a MOBO procedure at the upper-level. qEHVI computes the exact gradient of the Monte-Carlo estimator using auto-differentiation, allowing it to employ efficient and effective gradient-based optimization methods. More details about the qEHVI can be found in [11]. The acquisition function selects the next upper-level decision by $\mathbf{x}_u^* = \arg\max_{\mathbf{x} \in \mathcal{X}} \alpha(\mathbf{x})$. Then we evaluate the lower-level optimization and, after finding the optimum lower-level decision $\mathbf{x}_l^*$ regarding the upper-level decision, we update the data set with new observations $D \leftarrow D \cup (\mathbf{x}_u^*, \mathbf{x}_l^*, \mathbf{F}(\mathbf{x}_u^*, \mathbf{x}_l^*), -\mathbf{f}(\mathbf{x}_u^*, \mathbf{x}_l^*))$. We reiterate this procedure until the termination criteria are met. It is good to note that in the GP, $\mu(\cdot)$ can be viewed as the prediction of the function value and $\sigma(\cdot)$ is a measure of the uncertainty of the prediction. The details of the algorithm can be found in Algorithm 1.

Algorithm 1 PROPOSED ALGORITHM

Inputs: $\mathbf{F}_u(\mathbf{x}_u, \mathbf{x}_l) : \mathbf{x_u} \in \mathbb{X}_u, \mathbf{x_l} \in \mathbb{X}_l$,
Number of iteration *n*,
Reference point

1: Initial decision set $D = \{\mathbf{x}_{u_i}, \mathbf{F}(\mathbf{x}_{u_i}, \mathbf{x}_{l_i}^*,), -\mathbf{f}(\mathbf{x}_{u_i}, \mathbf{x}_{l_i}^*\}_{i=1}^n$ with size of n,
2: $\mathbf{x_l^*}$: Initialize Best Lower-Level Decisions as parameters from SLSQP Algorithm,
3: Initialize *Multi-objective Gaussian Model* with Observations $\{\mathbf{x}_u, \mathbf{F}(\mathbf{x}_u, \mathbf{x}_l^*), -\mathbf{f}(\mathbf{x}_{u_i}, \mathbf{x}_{l_i}^*\}$
4: **for** i = 0 : *N* **do**
5: Suggest new points by optimizing *q-EHVI* acquisition function
6: **for** j = 0 : q **do**
7: For each upper-level decision $\mathbf{x}_u$, find optimal $\mathbf{x}_l^*$ by applying SLSQP Algorithm
8: Calculate fitness scores $\mathbf{F}_u^*$ and $\mathbf{f}_u^*$
9: **end for**
10: Update the data set $D = (\mathbf{x}_{u_i}, \mathbf{F}(\mathbf{x}_{u_i}, \mathbf{x}_{l_i}^*), \mathbf{f}(\mathbf{x}_{u_i}, \mathbf{x}_{l_i}^*))_{i=1}^n$
11: **end for**
12: **Return** Optimum decisions $\mathbf{x}_u^*, \mathbf{x}_l^*$ and corresponding objective values, $F(\mathbf{x}_u^*, \mathbf{x}_l^*)$ and $f(\mathbf{x}_u^*, \mathbf{x}_l^*)$.

4 Experiments and Preliminary Results

In this section, we provide the preliminary results of the test problem to illustrate the performance of the algorithm to reach the pessimistic

Table 1. Optimal Results for the Test Problem

Solutions	x_u	x_l	$F(x_u, x_l)$
Optimistic	0.2106	1.799	-1.755
Pessimistic	0	0.2929	-0.2929

solution to the problem. The test problem is taken from [33] and called *mb_1_1_17* in the literature. We reformulate the problem and defined the pessimistic formulation as follows:

$$\begin{aligned} &\underset{x_u}{\text{Minimize}} \;\; F(x_u, x_l) = \left\{ \begin{array}{c} (x_u)^2 - x_l, \\ -\left((x_l - 1 - \frac{x_u}{10})^2 - \frac{x_u}{2} - \frac{1}{2}\right)^2 \end{array} \right\} \\ &\text{s.t.} \;\; x_l \in \underset{x_l}{\text{argmin}} \left\{ f(x_u, x_l) = \left((x_l - 1 - \frac{x_u}{10})^2 - \frac{x_u}{2} - \frac{1}{2}\right)^2 \right\}, \\ &\quad 0 \leq x_u \leq 1, \; 0 \leq x_l \leq 3. \end{aligned} \tag{7}$$

Table 1 shares the global optima for optimistic and pessimistic formulations. The problem has multiple global optima at the lower level, so solving the lower level optimization problem is crucial for both upper and lower level objective values. We applied the Algorithm 1 to the test problem that reformulated in Equation 7. The experiments run on a a single core of 1.4 GHz Quad Core i5, 8Gb 2133 Mhz LPDDR3 RAM. The algorithm is executed 30 times for the test function and the results are shown in Table 2.

Table 2. The Results Obtained by the Proposed Algorithm after 30 Run

Pessimistic Results				
Run	x_u	x_l	$F(x_u, x_l)$	Runtime (s)
1	0.0	0.295984	-0.295984	11.568
2	0.0	0.284260	-0.284260	12.394
3	0.0	0.302214	-0.302214	12.167
4	0.0	0.293317	-0.293317	8.988
5	0.0	0.291576	-0.291576	7.567
6	0.0	0.299777	-0.299777	8.752
7	0.0	0.283305	-0.283305	9.533
8	0.0	0.306050	-0.306050	4.694
9	0.0	0.290590	-0.290590	6.444
10	0.0	0.291880	-0.291880	11.532
11	0.0	0.298138	-0.298138	12.341
12	0.0	0.295053	-0.295053	7.966
13	0.0	0.287621	-0.287621	7.497
14	0.0	0.290137	-0.290137	6.396
15	0.0	0.285583	-0.285583	7.963
16	0.0	0.298160	-0.298160	10.752
17	0.0	0.291455	-0.291455	6.269
18	0.0	0.300341	-0.300341	10.180
19	0.0	0.290959	-0.290959	10.129
20	0.0	0.306742	-0.306742	10.095
21	0.0	0.290348	-0.290348	8.422
22	0.0	0.288043	-0.288043	8.974
23	0.0	0.280132	-0.280132	14.473
24	0.0	0.300028	-0.300028	8.651
25	0.0	0.287369	-0.287369	11.703
26	0.0	0.290636	-0.290636	8.040
27	0.0	0.298473	-0.298473	6.208
28	0.0	0.288104	-0.288104	10.138
29	0.0	0.291824	-0.291824	10.549
30	0.0	0.295658	-0.295658	5.953
Min	0.0	0.280132	-0.306742	4.694
Median	0.0	0.293125	-0.293125	9.211
Max	0.0	0.306742	-0.280132	14.473

We can see the pessimistic upper level decision and lower level response for each run in Table 2. Also, we report the min, max and median results for each run including runtimes. We can see that the solutions found by the proposed algorithm after pessimistic reformulation reached the optimal solution with an accuracy of 0.0002. The runtime is approximately 9 seconds per run. Recently, [4] proposed an evolutionary approach and compared its performance with state-of-the-art algorithms, and they present the approach is successful. We compared our results with them and discussed the brief results. Compared with the fully evolutionary approach in [4], the proposed algorithm runs almost 4.4 times faster with 100 times better accuracy for the pessimistic reformulation. It is shown that the proposed algorithm with the pessimistic reformulation approximates well the global optima while managing well to overcome the multiple local optima of the lower level problem.

5 Limitations

The proposed hybrid approach uses the Bayesian optimization at the upper level to approximate Pareto-optima. The Bayesian optimization and Gaussian surrogate model is not very successful when the problem is high-dimensional, and it appears as a limitation of the proposed approach. There are few studies that focus on high-dimensional Bayesian optimization recently [18]. Also, the new formulation of the proposed approach is reshaping the single-objective problems to multi-objective, which is harder to optimize compared with single-objective problems. Many algorithms do not guarantee the optima at the Pareto-optimal solution set. That comes with a challenge in candidate selection for upper-level decisions on pessimistic problems.

6 Conclusions and Future Work

In this short paper, we propose a new formulation for pessimistic bilevel optimization problems and a hybrid algorithm containing a black-box approach at the upper level. Then we gave both general optimistic and pessimistic formulations. After that, we explained the motivation behind the proposed formulation and the algorithm. The proposed algorithm contains a Bayesian optimization approach to the pessimistic upper level problem. The Gaussian process-based surrogate model uses both upper and lower level objectives, and then we solved the lower level problem with an exact algorithm. The experiments show that the proposed algorithm with the reformulation approximates well to the known global optima for the test benchmark problem.

It is well known that bilevel optimization with both single- and multi-objective problems is widely used for decision-making systems [26]. The approaches developed and presented in this paper can be applied to several practical problems with pessimistic formulation, such as negotiations [36] in diplomacy or optimizing the tax policy of authority while optimizing the specific objectives of a mining company. Another interesting application to work on is the defence industry in terms of attacker-defender Stackelberg games. For instance, the positioning of the missile interceptors to counter an attack threat or interdicting nuclear weapons are some of them. The black-box approach at the upper level as presented in this paper is not dependent on the specifications of the problems. In this way, the simulation-optimization approach [29] can be applied to multiple problems.

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