Adaptive discretization algorithms for unbounded semi-infinite programs

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Abstract: The proof of convergence of adaptive discretization-based algorithms for semi-infinite programs (SIPs) usually relies on compact host sets for the upper- and lower-level variables. This assumption is violated in some applications, and we show that indeed convergence problems can arise when discretization-based algorithms are applied to SIPs with unbounded host sets. To mitigate these convergence problems, we first examine the assumptions underlying the algorithm proposed in [*Mitsos. Optimization, 2011*], which uses the algorithm proposed by [*Blankenship and Falk. JOTA, 1976*] as the lower-bounding procedure. We give sharper, slightly relaxed, assumptions with which we achieve the same convergence guarantees. We show that the convergence guarantees also hold for certain SIPs with unbounded host sets based on these sharpened assumptions. However, convergence guarantees cannot be given for SIPs with unbounded host sets in the general case. For these cases, we propose additional assumptions which restore the convergence guarantee. Using these additional assumptions, we present numerical case studies with unbounded host sets. Finally, we review which applications are tractable with the proposed additional assumptions.

Keywords— semi-infinite programming, unbounded, adaptive discretization

1 Introduction

Adaptive discretization-based algorithms are widely used for the solution of semi-infinite programs (SIPs), generalized semi-infinite programs, and bilevel programs, e.g., [14, 17, 18, 20, 33]. For a recent review of applications and adaptive discretization-based algorithms for SIPs, the reader may refer to [9]. In this paper, we focus on the lower-bounding procedure and assumptions proposed in [19] and consider SIPs in the form of

$$\begin{aligned} f^* = &\min_{\boldsymbol{x}\in\mathcal{X}} f(\boldsymbol{x}) \\ &\text{s.t.}\ \forall \boldsymbol{y}\in\mathcal{Y}\,[g(\boldsymbol{x},\boldsymbol{y})\leqslant 0] \\ &|\mathcal{Y}| = \infty. \end{aligned} \tag{SIP}$$

[19] applies a convergent lower-bounding procedure as well as proposes a convergent upper-bounding procedure to compute in finite time a feasible point of (SIP) with a certificate of ε^f-optimality. The upper-bounding procedure of Mitsos is a slight adaption of the lower-bounding procedure, which in turn is the algorithm by [3]. Moreover, many adaptive discretization-based algorithms for (generalized) semi-infinte programs and bilevel programs have identical predecessors, i.e., [3, 26], and are conceptually closely related, e.g., [5, 7, 8, 12, 21, 22, 25, 27–32]. Therefore, we expect that the results within this paper, i.e., convergence guarantees with the sharper, slightly relaxed, assumptions and recovered convergence guarantees in case of unbounded host sets, directly carry over from one algorithm to the other.

The proof of convergence of algorithms for the global solution of SIPs relies, among other assumptions, on compact host sets. This is true both for discretization-based and other methods as well as local methods allowing nonconvex lower-level problem [1, 2, 10, 23]. Typically, the upper- and lower-level variables $\boldsymbol{x}$ and $\boldsymbol{y}$ have a technical

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or physical meaning and thus, in most cases, inherit finite bounds from their physical or technical origin. Furthermore, these finite bounds are usually attainable yielding closed and therefore compact upper- and lower-level host sets $\mathcal{X}$ and $\mathcal{Y}$.

However, one might not know the finite bounds of the variables. Furthermore, SIPs stemming from specific applications or reformulations may exhibit unbounded upper- and/or lower-level host sets. In the following, we give examples of problem classes where SIPs with unbounded host sets can arise. Note that in some of the applications, finite bounds of the variables may be computed or generated by additional assumptions. In most of the following examples, (arbitrary) bounds are usually used in practice. An unbounded lower-level set $\mathcal{Y}$ may occur, e.g., in approximation theory where one wants to approximation a function with a minimal estimation error, not only over a compact set, but over all $\mathbb{R}^n$ (Chebyshev approximation). Another interesting example of obtaining unbounded variables is replacing an embedded optimization problem with its optimality conditions. Consider, for instance

$$\begin{aligned} f^k = \min_{x \in [0,2]} \quad & x \\ \text{s.t.}\, & px = p \end{aligned} \tag{1}$$

with the parameter $p \in [-1, 1]$. Since it is a linear problem, it can be replaced by primal and dual feasibility along with strong duality. However, the dual variable for the optimal solution is equal to $1/p$ and is thus unbounded for $p \neq 0$; it is arbitrary for $p = 0$. An unbounded upper-level variable host set $\mathcal{X}$ occurs, e.g., in design centering, in epigraph reformulations of min-max programs or in approximation theory, e.g., classical Chebyshev problem, where the parameter values are unbounded, or reverse Chebyshev approximation, where the approximation error is fixed and the region where the approximation is not worse than the fixed approximation error is computed [12, 30].

In order to address such applications, we will investigate whether adaptive discretization-based algorithms are directly applicable to SIPs with unbounded host sets, i.e., whether the assumption of compact host sets can be relaxed. By relaxing the assumption of compact host sets, we will also consider SIPs with bounded but noncompact host sets, e.g., host sets consisting of half-open intervals or open intervals. For cases where this is not directly possible, we will derive additional assumptions to enable the application.

In Section 2, we first introduce the basic notation used throughout this paper and review the assumptions in [19]. Second, we prove convergence of the lower-bounding procedure. In the proof, we use sharper and slightly relaxed assumptions compared to [19]. We show that our relaxed assumptions are implied by the original assumptions of [19]. Section 3 shows that the lower-bounding procedure may exhibit convergence problems if the host sets are not compact. In Section 4, we give additional assumptions to apply the lower-bounding procedure to SIPs with noncompact and unbounded host sets. In Section 5, we present two case studies as a proof-of-concept for our findings. Finally, we give a conclusion and outlook in Section 6.

2 Preliminaries

In this section, we briefly review the notation, formulation, definitions, and assumptions of the lower-bounding procedure in [19].

2.1 Notations, formulation and definitions of the lower-bounding procedure of [19]

[19] considers (SIP), with the following lower-bounding and lower-level problem.

Definition 1 (*Discrete lower-bounding problem*) The discrete lower-bounding problem (LBP) with $\mathcal{Y}^k \subsetneq \mathcal{Y}$ is

$$\begin{aligned} f^k = &\min_{\boldsymbol{x}\in\mathcal{X}} f(\boldsymbol{x}) \\ &\text{s.t.}\ \forall \boldsymbol{y} \in \mathcal{Y}^k \left[g(\boldsymbol{x},\boldsymbol{y}) \leqslant 0\right]. \end{aligned} \tag{LBP}$$

In literature, (LBP) is also often called discrete upper-level problem.

Definition 2 (*Lower-level problem*) The lower-level problem (LLP) for fixed upper-level variables $\bar{\boldsymbol{x}}$ is

$$g^*(\bar{\boldsymbol{x}}) = \max_{\boldsymbol{y}\in\mathcal{Y}} g(\bar{\boldsymbol{x}},\boldsymbol{y}). \tag{LLP}$$

The iterative lower-bounding procedure in [19] solves (LBP) and then (LLP) in each iteration k. The solution of (LBP) is a lower bound on the solution of (SIP). If the optimal value of the (LLP) is nonpositive, the lower-bounding procedure has furnished the optimal solution to (SIP). Otherwise, the optimal solution is used to populate the discretization set $\mathcal{Y}^k$ for subsequent iterations.

The following summarizes the notation used and the definition of compact sets used throughout this paper.

Notation 1 (*Optimal solution of* (LBP)) We denote the optimal solution point of (LBP) by $\boldsymbol{x}^k$ and the sequence of optimal solutions by $\left\{\boldsymbol{x}^k\right\}_{k=0}^m = \left\{\boldsymbol{x}^0, \boldsymbol{x}^1, \boldsymbol{x}^2, \ ..., \boldsymbol{x}^m\right\}$. To simplify the notation, we omit indexing numbers wherever possible, i.e., $\left\{\boldsymbol{x}^k\right\}$.

Notation 2 (*Optimal solution of* (LLP)) We denote the optimal solution point of (LLP) by $\boldsymbol{y}^k$ and the sequence of optimal solutions by $\left\{\boldsymbol{y}^k\right\}_{k=0}^m = \left\{\boldsymbol{y}^0, \boldsymbol{y}^1, \ \boldsymbol{y}^2, ..., \boldsymbol{y}^m\right\}$. To simplify the notation, we omit indexing numbers wherever possible, i.e., $\left\{\boldsymbol{y}^k\right\}$.

Notation 3 (*Feasible set*) We use for the set of all feasible points in the host set of (SIP) the notation

$$\mathcal{X}^{\text{feas}} := \left\{\boldsymbol{x} \in \mathcal{X} : \forall \boldsymbol{y} \in \mathcal{Y}\left[g(\boldsymbol{x},\boldsymbol{y}) \leqslant 0\right]\right\}. \tag{2}$$

Notation 4 (*Infeasible set*) We use for the set of all infeasible points in the host set of (SIP) the notation

$$\mathcal{X}^{\text{infeas}} := \left\{\boldsymbol{x} \in \mathcal{X} : \exists \boldsymbol{y} \in \mathcal{Y} : g(\boldsymbol{x},\boldsymbol{y}) > 0\right\}. \tag{3}$$

Definition 3 (*Compact set*) $\mathcal{K} \subsetneq \mathbb{R}^n$ is compact if any open cover of $\mathcal{K}$ has a finite subcover. More explicitly, $\mathcal{K}$ is compact if whenever $\mathcal{K} \subseteq \bigcup_{\alpha\in\mathcal{I}} \mathcal{A}_\alpha$, where each $\mathcal{A}_\alpha$ is open, there exists a finite number of indices $\alpha_1, \alpha_2, ..., \alpha_m \in \mathcal{I}$ such that $\mathcal{K} \subseteq \bigcup_{j=1}^{j=m} \mathcal{A}_{\alpha_j}$ (c.f., [15]).

Notation 5 (*Compact infeasible subset of* $\mathcal{X}^{infeas}$) We use the symbol $\mathcal{K}^{\text{infeas}}$ for compact subsets of $\mathcal{X}^{\text{infeas}}$.

2.2 Assumptions

The existing global discretization-based algorithms use a global solver to compute the subproblems which are (mixed-integer) (non)linear problems ((MI)(N)LP). By considering SIPs with unbounded host sets, we obviously inherit the need for global solvers that can handle optimization problems with unbounded host sets. In the case of linear programs, this does not pose a problem as, e.g., the simplex method can handle unbounded host sets [24]. In the more general case of (MI)NLPs, e.g., BARON is able to treat some problems with unbounded variables systematically by trying to compute appropriate bounds from problem constraints [16] but substantial theoretical and practical challenges remain. In what follows, we focus on the SIP algorithm's convergence properties for unbounded host sets and do not discuss these challenges.

The presented lower-bounding procedure in [19] relies on the following assumptions (c.f., Lemma 2.2 in [19], revised in Lemma 2 in [13]):

Assumption 1 (*Compactness of Sets*) The sets $\mathcal{X} \subseteq \mathbb{R}^{n_x}$ and $\mathcal{Y} \subseteq \mathbb{R}^{n_y}$ are compact.

Assumption 2 (*Continuous Functions*) The functions f and g are continuous on $\mathcal{X}$ and $\mathcal{X} \times \mathcal{Y}$, respectively.

Assumption 3 (*Appr. Solution of* (LLP)) At each iteration k, (LLP) is solved approximately for the solution of the lower-bounding problem $\boldsymbol{x}^k$ either establishing $\max_{\boldsymbol{y} \in \mathcal{Y}} g\left(\boldsymbol{x}^k, \boldsymbol{y}\right) \leqslant 0$, or furnishing a point $\boldsymbol{y}^k$ such that $g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) \geqslant \alpha g^*\left(\boldsymbol{x}^k\right) > 0$. With α being constant over all iterations and $\alpha \in (0,1)$.

Assumption 3 is relaxed compared to the assumption in [3], where exact solution of (LLP) is assumed. However, as will be shown below, the problems associated with unbounded host sets persist even if the (LLP) is solved exactly.

2.3 Proof of convergence of the lower-bounding procedure

The proof presented in this paper relies on slightly relaxed assumptions compared to those made by [19]. Basically, we split the assumptions made by [19] and some properties, which result from them, into multiple sharpened assumptions. These sharpened assumptions are often challenging to prove a priori. In these cases, we later present alternative, stricter, assumptions, which are easier to prove and that imply the sharpened assumptions. The sharpened assumptions motivate the additional assumptions for SIPs with unbounded host sets in Section 4.

Assumption 1 is relaxed to

Assumption 4 It holds (a) $\mathrm{cl}\left(\mathcal{X}^{\text{infeas}}\right) \subseteq \mathcal{X}$ and (b) $\mathcal{X}^{\text{infeas}}$ is bounded.

Assumption 4 allows for unbounded host sets and also for bounded but not closed sets. Assumption 4(a) can be verified, at least in principle, a priori by checking if there exist points that belong to $\mathrm{cl}\left(\mathcal{X}^{\text{infeas}}\right)$ but not to $\mathcal{X}$: if $\forall \boldsymbol{x} \in \mathrm{cl}\left(\mathcal{X}\right) \setminus \mathcal{X} \left[\max_{\boldsymbol{y} \in \mathcal{Y}} g\left(\boldsymbol{x}, \boldsymbol{y}\right) < 0\right]$, Assumption 4(a) holds. As $\mathrm{cl}\left(\mathcal{X}\right) \setminus \mathcal{X}$ is potentially an open set, Assumption 4(a) can be checked more conservatively by verifying that the optimal value of $\max_{\boldsymbol{x} \in \mathrm{cl}(\mathrm{cl}(\mathcal{X}) \setminus \mathcal{X}), \boldsymbol{y} \in \mathcal{Y}} g\left(\boldsymbol{x}, \boldsymbol{y}\right)$ is greater than zero. As this optimization problem is an adaption of (LLP), the computational burden is in most cases tractable. Assumption 4(b) can be checked by computing

$$x^{\text{infeas,UBD}} = \sup_{\boldsymbol{x} \in \mathcal{X}, \boldsymbol{y} \in \mathcal{Y}} \|\boldsymbol{x}\| \quad \text{s.t. } g\left(\boldsymbol{x}, \boldsymbol{y}\right) \geqslant 0. \tag{4}$$

If $x^{\text{infeas,UBD}}$ is bounded, Assumption 4(b) is satisfied. Assumption 2 and the property of uniform continuity of g on $\mathcal{X} \times \mathcal{Y}$ follow from Assumptions 1 and 2. In the following we relax these two assumptions.

Assumption 5 The function f is lower semi-continuous at all $\boldsymbol{x} \in \partial\mathcal{X}^{\text{infeas}}$.

Assumption 6 It holds

$$\forall \varepsilon > 0 \; \exists \delta_1 > 0 : \; \forall \boldsymbol{x}^k \in \left\{\boldsymbol{x}^k\right\} \cap \mathcal{X}^{\text{infeas}}, \boldsymbol{x} \in \mathcal{X}^{\text{infeas}} \left[\left\|\boldsymbol{x}^k - \boldsymbol{x}\right\| < \delta_1\right] \\ \Rightarrow \left|g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\right| < \varepsilon. \tag{5}$$

We first prove that the proposed assumptions are indeed relaxed compared to the original assumptions, i.e., the latter imply the former.

Lemma 1 *Assumptions 4 to 6 hold if Assumptions 1 and 2 are satisfied.*

Proof First, we show that Assumption 1 implies Assumption 4. $\mathcal{X}$ is compact according to Assumption 1. Since $\mathcal{X}^{\text{infeas}} \subseteq \mathcal{X}$, we directly get $\text{cl}\left(\mathcal{X}^{\text{infeas}}\right) \subseteq \mathcal{X}$. $\mathcal{X}$ is bounded by compactness and, therefore, $\mathcal{X}^{\text{infeas}}$ is also bounded.
Second, according to Assumption 2, f is continuous on $\mathcal{X}$ and hence lower semi continuous on $\partial\mathcal{X}^{\text{infeas}} \subseteq \mathcal{X}$, or Assumption 5 holds.
Third, from Assumptions 1 and 2 follows uniform continuity of g on $\mathcal{X} \times \mathcal{Y}$ and we have

$$\forall \varepsilon > 0 \; \exists \delta_1 > 0 : \; \forall \boldsymbol{x}^k, \boldsymbol{x} \in \mathcal{X} \left[\left\|\boldsymbol{x}^k - \boldsymbol{x}\right\| < \delta_1\right] \Rightarrow \left|g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\right| < \varepsilon. \tag{6}$$

Then, it also holds

$$\forall \varepsilon > 0 \; \exists \delta_1 > 0 : \; \forall \boldsymbol{x}^k \in \left\{\boldsymbol{x}^k\right\} \cap \mathcal{X}^{\text{infeas}}, \boldsymbol{x} \in \mathcal{X}^{\text{infeas}} \left[\left\|\boldsymbol{x}^k - \boldsymbol{x}\right\| < \delta_1\right] \\ \Rightarrow \left|g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\right| < \varepsilon \tag{7}$$

because $\left\{\boldsymbol{x}^k\right\} \cap \mathcal{X}^{\text{infeas}} \subseteq \mathcal{X}$ and $\mathcal{X}^{\text{infeas}} \subseteq \mathcal{X}$. □

Next, we prove convergence of the lower-bounding procedure using Assumption 3 and the relaxed Assumptions 4 to 6.

Theorem 1 *If Assumptions 3 to 6 are satisfied, the adaptive discretization-based lower-bounding procedure in [19] converges to the optimal objective value, i.e., $f^k \to f^*$ for $k \to \infty$. If the SIP is infeasible, the lower-bounding procedure terminates finitely with proof of infeasibility.*

Note that [19] excludes infeasible SIPs by assumption, c.f., Assumption 13 in Appendix B.

Proof We first show that we move away from any *compact set of infeasible points* within finitely many iterations. Second, we consider the case of an *infeasible SIP*. We show that the algorithm terminates finitely with proof of infeasibility. Third, we consider the case of a *feasible SIP* and show that the algorithm terminates finitely with a globally optimal solution, or the algorithm produces the optimal solution in the limit.

1. Consider a *compact set of infeasible points* $\mathcal{K}^{\text{infeas}} \subseteq \mathcal{X}^{\text{infeas}}$. In the following, we restrict the iterations to be in this set, i.e., $\boldsymbol{x}^k \in \{\boldsymbol{x}^k\} \cap \mathcal{K}^{\text{infeas}}$. Due to compactness of $\mathcal{K}^{\text{infeas}}$ and Assumption 3, it follows that $\boldsymbol{x}^k$ is infeasible and hence the infimum of g^* is positive. Recall that $g(\boldsymbol{x}^k, \boldsymbol{y}^k) \leqslant 0$ would imply that $\boldsymbol{x}^k$ is feasible, $\boldsymbol{x}^k$ is not a member of $\mathcal{K}^{\text{infeas}}$, and we have left $\mathcal{K}^{\text{infeas}}$. From compactness of $\mathcal{K}^{\text{infeas}}$ follows that the infimum is attained. We have
$$\exists \mu > 0 : \ \forall \boldsymbol{x}^k \in \left\{\boldsymbol{x}^k\right\} \cap \mathcal{K}^{\text{infeas}} \left[g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) \geqslant \alpha g^*\left(\boldsymbol{x}^k\right) \geqslant \mu > 0\right]. \tag{8}$$
Since Assumption 6 holds for all $\varepsilon > 0$, it also holds
$$\begin{aligned}\exists \delta_1 > 0 : \ \forall \boldsymbol{x}^k \in \left\{\boldsymbol{x}^k\right\} \cap \mathcal{X}^{\text{infeas}}, \boldsymbol{x} \in \mathcal{X}^{\text{infeas}} \left[\left\|\boldsymbol{x}^k - \boldsymbol{x}\right\| < \delta_1\right] \\ \Rightarrow \left|g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\right| < \mu.\end{aligned} \tag{9}$$
We obtain for the deduction in (9) the two cases
$$\begin{aligned}\text{Case 1: } g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right) \geqslant 0: \\ \Rightarrow \quad & g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right) < \mu \\ \overset{(8)}{\Longrightarrow} \mu - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right) \leqslant\, & g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right) < \mu \\ \Rightarrow 0 < g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\end{aligned} \tag{10}$$
$$\begin{aligned}\text{Case 2: } g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right) < 0: \\ \Rightarrow \quad & g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) < g\left(\boldsymbol{x}, \boldsymbol{y}^k\right) \\ \overset{(8)}{\Longrightarrow} 0 < \mu \leqslant\, & g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) < g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\end{aligned} \tag{11}$$
Therefore, it holds
$$\begin{aligned}\exists \delta_1 > 0 : \ \forall \boldsymbol{x}^k \in \left\{\boldsymbol{x}^k\right\} \cap \mathcal{X}^{\text{infeas}}, \boldsymbol{x} \in \mathcal{X}^{\text{infeas}} \left[\left\|\boldsymbol{x}^k - \boldsymbol{x}\right\| < \delta_1\right] \\ \Rightarrow 0 < g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\end{aligned} \tag{12}$$
Thus, with each iteration, the open neighborhood $\mathcal{N}_{\delta_1}(\boldsymbol{x}^k) \cap \mathcal{K}^{\text{infeas}}$ is infeasible for the following iterations (and therefore we do not (re)visit points in this neighborhood). Since the excluded neighborhoods cannot be revisited and $\mathcal{K}^{\text{infeas}}$ is compact, after at most finitely many iterations, these neighborhoods form a finite cover of $\mathcal{K}^{\text{infeas}}$. Therefore, we only need a finite number of iterations until we have covered $\mathcal{K}^{\text{infeas}}$ (c.f., Definition 3), i.e., we prove infeasibility of all points in $\mathcal{K}^{\text{infeas}}$ after a finite number of iterations.

2. Consider now an *infeasible SIP*. $\mathcal{X}^{\text{infeas}}$ is compact by Assumption 4. The proof of finite termination with proof of infeasibility directly follows from the proof for case 1 above with $\mathcal{K}^{\text{infeas}} = \mathcal{X}^{\text{infeas}}$. It follows that (LBP) is infeasible after a finite number of iterations.

3. Finally, consider a *feasible SIP*.

   (a) If (SIP) is unbounded, the problem will be determined to be unbounded in the first iteration. (LBP) is a valid relaxation of (SIP), i.e., $f^k \leqslant f^*$. As (SIP) is by assumption unbounded, the first iteration must yield an unbounded result.

   (b) If the optimal solution is finite, i.e., $\|\boldsymbol{x}^*\| < \infty$, we will show by contradiction that a feasible and optimal point is generated in the limit.
   By Assumption 4, there exists a compact set $\tilde{\mathcal{X}} \supsetneq \mathcal{X}^{\text{infeas}}$ containing the

optimal point. By compactness of $\tilde{\mathcal{X}}$, we can choose an infinite subsequence $\{\boldsymbol{x}^k\}$ that converges to $\hat{\boldsymbol{x}} \in \tilde{\mathcal{X}}$.
Now, assume the *limit point is infeasible* $\hat{\boldsymbol{x}} \in \mathcal{X}^{\text{infeas}}$. There exists a compact set $\mathcal{K}^{\text{infeas}} \ni \hat{\boldsymbol{x}}$. By proof from case 1 above, we move away from any infeasible set $\mathcal{K}^{\text{infeas}}$ within finite time. Therefore, the infeasible point $\hat{\boldsymbol{x}}$ is not a limit point that gives us the desired contradiction.
It remains to show that the *feasible limit point* is optimal. (LBP) is a valid relaxation of (SIP). Hence, we have $f^k \leqslant f^*$. The limit point $\hat{\boldsymbol{x}}$ is feasible, i.e., $f(\hat{\boldsymbol{x}}) \geqslant f^*$. With lower semi-continuous of f at all $\forall \boldsymbol{x} \in \partial\mathcal{X}^{\text{infeas}}$ and with $f^k \leqslant f^*$ follows $f(\hat{\boldsymbol{x}}) = f^*$.

□

Following the proof of Lemma 1 and Theorem 1, we can also prove that the lower-bounding procedure in [19] converges in the infeasible case under the original Assumptions 1 to 3.

The upper-bounding procedure in [19] is conceptually similar to the lower-bounding procedure. For the sake of completeness, the proof of convergence and the slightly changed assumptions for the case of unbounded host sets of the upper-bounding procedure are shown in Appendix B.3.

3 Illustrative examples of SIPs with unbounded host sets

We first show examples where assumptions Assumptions 3 to 6 do not hold and discuss how the lower-bounding procedure in [19] may fail. All examples follow the same pattern. They contain an upper- or lower-level variable that i) has an unbounded host set and ii) can be chosen arbitrarily in the sense that the variable does not affect the (UBP) or (LLP) objective, respectively. Using this property, we can choose a sequence of points that generates arbitrarily weak discretization cuts, thus violating Assumption 6. This leads to a convergence to an infeasible point in the limit with no proof of infeasibility

3.1 Illustrative example for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded

Consider the SIP

$$\begin{aligned} f^* = &\min_{x \in \mathcal{X}} -x \\ &\text{s.t. } \forall \boldsymbol{y} \in \mathcal{Y}\left[-y_1^2 (y_2 - x)^2 + 1 \leqslant 0\right] \\ &\quad \mathcal{X} = [0, 2] \\ &\quad \mathcal{Y} = \mathbb{R}^2. \end{aligned} \tag{E1}$$

Note that the corresponding LLP has infinitely many solutions. The optimal solutions of the (LLP) are $\boldsymbol{y}^*(\bar{x}) = (\tilde{y}, \bar{x})^T$ or $\boldsymbol{y}^*(\bar{x}) = (0, \tilde{y})^T$ with arbitrary $\tilde{y} \in \mathbb{R}$. We have $\forall x \in \mathcal{X}\left[g^*(x) = 1 > 0\right]$. Therefore, (E1) is infeasible.

We show that the lower-bounding procedure in [19] may converge to an infeasible point. We start with an empty discretization $\mathcal{Y}^0 = \varnothing$. The optimal solution of the (UBP) is $x^0 = 2$ with an optimal objective value of $f^{*,0} = -2$. Then, $\boldsymbol{y}^0 = (2, 2)^T$ is a globally optimal solution of (LLP). Using $\boldsymbol{y}^k = \left(2^{k+1}, x^k\right)^T$ for all subsequent iterations and considering the (UBP) objective, the last introduced discretization point determines the optimal solution in the next iteration. See also Figure 1 for graphical illustration. x^{k+1} can be computed by

$$\begin{aligned} g\left(x^{k+1}, \boldsymbol{y}^{k}\right) &\leqslant 0 \\ -\left(y_1^{k}\right)^2\left(y_2^{k} - x^{k+1}\right)^2 + 1 &\leqslant 0 \\ -\left(2^{k+1}\right)^2\left(x^{k} - x^{k+1}\right)^2 + 1 &\leqslant 0 \\ \Rightarrow x^{k+1} = x^{k} - \frac{1}{2^{k+1}}. \end{aligned}$$

Therefore, we have for any iteration $k \geqslant 1$

$$x^{k} = x^{0} - \sum_{i=1}^{k} \frac{1}{2^{i}}.$$

With $\sum_{i=1}^{k} \frac{1}{2^i}$ being the geometrical series, we obtain $\lim_{k\to\infty} x^0 - \sum_{i=1}^{k} \frac{1}{2^i} = 1$ with

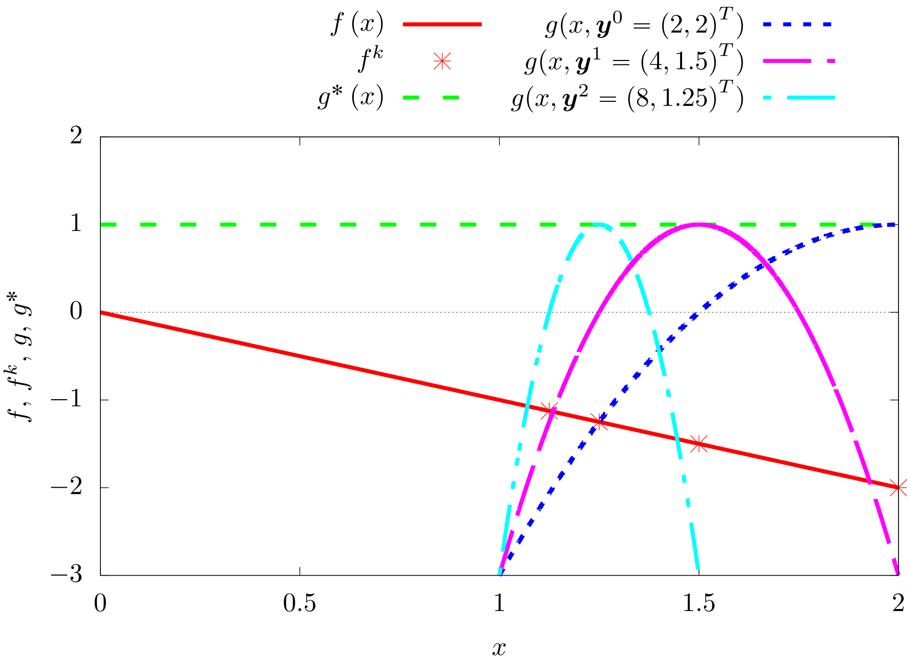

Fig. 1: Illustrative example (E1) for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded with parametric solutions of (LLP). (E1) is infeasible.

an objective value of $f^{k=\infty} = -1$. Therefore, the lower-bounding procedure converges to an infeasible point in the limit, and no proof of infeasibility is given within finite time.

The same convergence issues arise when we consider an SIP with $\mathcal{X}$ compact and $\mathcal{Y}$ bounded but not closed, c.f., Appendix A.1. For the sake of simplicity, we considered the infeasible SIP (E1). Recall that [19] excludes infeasible SIPs. Therefore, (E1) would not be considered (assuming the extension to unbounded host sets). The reader may refer to the Appendix A.2 for a feasible but conceptually equivalent SIP that exhibits the same convergence issues.

We show in (E1) that in certain cases the lower-bounding procedure can converge to an infeasible point. Similarly, also, the upper-bounding procedure in [19] may never produce a SIP-feasible point. For a detailed example, the reader may refer to Appendix B.2.

3.2 Illustrative example for $\mathcal{X}$ unbounded and $\mathcal{Y}$ compact

Consider the SIP

$$\begin{aligned} f^* = &\min_{\boldsymbol{x}\in\mathcal{X}} \begin{cases} -1\ , & x_2 \geqslant 1 \\ -x_2, & x_2 < 1 \end{cases} \\ &\text{s.t. } \forall y \in \mathcal{Y}\left[-x_1\left(x_2-y\right)^2+1 \leqslant 0\right] \\ &\mathcal{X} = [0,+\infty)\times[0,2] \\ &\mathcal{Y} = [0,2]. \end{aligned} \tag{E3}$$

The optimal value function of the corresponding (LLP) is $g^*(\bar{\boldsymbol{x}}) = 1 > 0,\ \forall \bar{\boldsymbol{x}} \in \mathcal{X}$ with the optimal solution $y^*(\bar{\boldsymbol{x}}) = \bar{x}_2$. Therefore, (E3) is infeasible. Note that the objective function only depends on x_2 and is constant in the interval $x_2 \in [1,2]$. Again, we show below that the lower-bounding procedure can converge to an infeasible point in the limit. First, start with an empty discretization set $\mathcal{Y}^0 = \varnothing$. For iteration $k = 0$, choose $\boldsymbol{x}^0 = (4,2)^T$ as the optimal solution, with an objective value of $f^0 = -1$. For the corresponding (LLP), we have $y^0 = 2$. Using for iteration $k \geqslant 1$ and all following iterations $x_1^k = 2^{k+2}$ and considering the (UBP) objective, we can choose $x_2^k = 2 - \sum_{i=1}^{k} \frac{1}{2^i}$, see Figure 2 for graphical illustration. With $\sum_{i=1}^{k} \frac{1}{2^i}$ being the

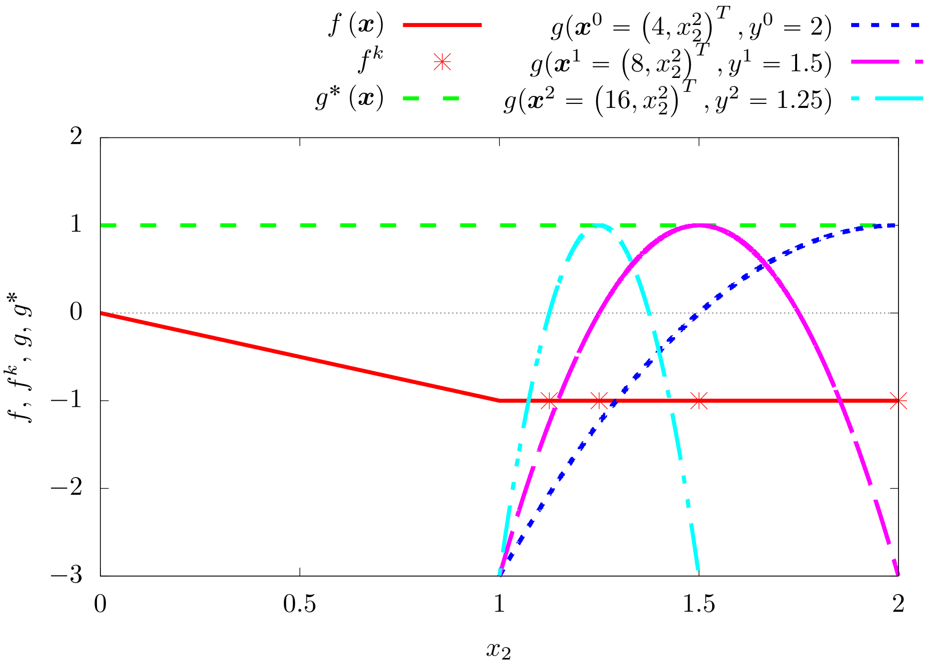

Fig. 2: Illustrative example (E3) for $\mathcal{X}$ unbounded and $\mathcal{Y}$ compact with parametric solutions of LLP. (E3) is infeasible.

geometrical series, we obtain $\lim_{k\to\infty} x_2 = \lim_{k\to\infty} x_2^0 - \sum_{i=1}^{k} \frac{1}{2^i} = 1$ with an objective value of $f^* = -1$. Therefore, the lower-bounding procedure does not prove infeasibility of (E3) within finite time.

Again, for the sake of simplicity, an infeasible SIP with a non-differentiable function f has been considered. Similar adaptations as in Appendix A.2 can be made to obtain a feasible SIP with n-times differentiable functions, which exhibit the same convergence issues. Furthermore, similar adaptions as in Appendix A.1 can be made to obtain an SIP with compact $\mathcal{Y}$ and bounded but non-compact $\mathcal{X}$, which exhibits the same convergence issues.

4 Additional assumptions

This section discusses assumptions, which are often easy to check and which imply Assumptions 4 to 6 for SIPs with unbounded host sets. With these assumptions we are able to alleviate some of the convergence issues shown in Section 3.

4.1 Additional assumptions for $\mathcal{X}$ unbounded $\mathcal{Y}$ compact

First, note that if the lower-bounding procedure produces a feasible point, it terminates with a global solution. Thus, it suffices to consider that the algorithm generates points in $\mathcal{X}^{\text{infeas}}$. Therefore, we restrict our discussion to the following cases:

1. $\mathcal{X}^{\text{infeas}}$ is bounded
2. $\mathcal{X}^{\text{infeas}}$ is unbounded and
   (a) no additional assumptions
   (b) $\mathcal{X}^{\text{feas}} \neq \varnothing$ and f is continuous and coercive on $\mathcal{X}$
   (c) the (SIP) stems from the min-max program

$$\begin{aligned} f^* = &\min_{\boldsymbol{x}\in\mathcal{X}} \max_{\boldsymbol{y}\in\mathcal{Y}} q\left(\boldsymbol{x},\boldsymbol{y}\right) \\ &\mathcal{Y} \subsetneq \mathcal{R} \\ &\mathcal{X} \subseteq \mathcal{R}, \end{aligned} \tag{13}$$

with $q(\boldsymbol{x},\boldsymbol{y})$ being coercive in $\boldsymbol{x}$ for all $\boldsymbol{y}$. We consider in the following the epigraph reformulation of this min-max program, which reads

$$\begin{aligned} f^* = \min_{\boldsymbol{x}\in\mathcal{X},\mu\in\mathcal{E}} \quad & \mu \\ \text{s.t.}\ & \forall \boldsymbol{y} \in \mathcal{Y}\left[q\left(\boldsymbol{x},\boldsymbol{y}\right) \leqslant \mu\right] \\ & \mathcal{Y} \subsetneq \mathcal{R} \\ & \mathcal{E},\mathcal{X} \subseteq \mathcal{R}. \end{aligned} \tag{14}$$

Feasible SIPs can belong to cases 1 or 2. Infeasible SIPs always belong to case 2 since it follows directly from $\mathcal{X}$ unbounded and $\mathcal{X}^{\text{feas}} = \varnothing$ that $\mathcal{X}^{\text{infeas}}$ is unbounded.

4.1.1 Case 1: $\mathcal{X}^{\text{infeas}}$ bounded

In the case of bounded $\mathcal{X}^{\text{infeas}}$, we can prove convergence of the algorithm.

Assumption 7 The set $\mathcal{Y} \subsetneq \mathbb{R}^{n_y}$ is compact, $\text{cl}\left(\mathcal{X}^{\text{infeas}}\right) \subseteq \mathcal{X} \subseteq \mathbb{R}^{n_x}$, and $\mathcal{X}^{\text{infeas}}$ is bounded.

Proposition 1 *Under Assumptions 2, 3 and 7, the lower-bounding procedure converges.*

Proof First, from Assumption 7 follows Assumption 4. Second, from Assumption 2 follows Assumption 5. Third, from Assumptions 2 and 7 follows Assumption 6. By Theorem 1, the lower-bounding procedure converges. □

In some instances, one can show (analytically) that Assumption 7 is satisfied by proving $\lim_{\|\boldsymbol{x}\|\to+\infty} \max_{\boldsymbol{y}} g\left(\boldsymbol{x},\boldsymbol{y}\right) < 0$ holds for any sequence $\left\{\boldsymbol{x}^k\right\}$ with $\left\|\boldsymbol{x}^k\right\| \to \infty$ for $k \to \infty$.

4.1.2 Case 2(a): $\mathcal{X}^{\text{infeas}}$ unbounded and no additional assumptions

In this general case, the existence of a finite cover of the set $\mathcal{X}^{\text{infeas}}$ cannot be guaranteed. Even if we exclude an open neighborhood of points whose size tends to infinity in each iteration, we cannot guarantee convergence.
As a counterexample, revisit (E3) and replace g with the piecewise-defined function

$$g(x, \boldsymbol{y}) = \begin{cases} -x_2 (x_1 - y)^2 + 1, & x_1 \leqslant y \\ 1, & x_1 > y \end{cases} \tag{15}$$

In this case, the open ball we exclude in each iteration is infinite. However, the same convergence issues arise when using the same sequence of (LLP) solutions given in (E3).

The function g in Equation (15) is continuous but not differentiable on $\mathcal{X} \times \mathcal{Y}$. Similar to Remark 1, we can obtain a function belonging to differentiability class C^n that produces the same convergence issues.

4.1.3 Case 2(b): $\mathcal{X}^{\text{infeas}}$ unbounded and f is continuous and coercive on $\mathcal{X}$ and $\mathcal{X}^{\text{feas}} \neq \varnothing$

If f is continuous and coercive on $\mathcal{X}$ and $\mathcal{X}^{\text{feas}} \neq \varnothing$, we can prove convergence of the lower-bounding procedure.

Assumption 8 The set $\mathcal{Y} \subsetneq \mathbb{R}^{n_y}$ is compact and $\text{cl}\left(\mathcal{X}^{\text{infeas}}\right) \subseteq \mathcal{X} \subseteq \mathbb{R}^{n_x}$. f is continuous and coercive on $\mathcal{X}$ and $\mathcal{X}^{\text{feas}} \neq \varnothing$

Proposition 2 *Under Assumptions 2, 3 and 8, the lower-bounding procedure converges.*

Proof Because f is coercive on $\mathcal{X}$, $\mathcal{X}^{\text{feas}} \neq \varnothing$, and $f^k \leqslant f^*$, we have $\exists M \in \mathbb{R}$ such that $\|\boldsymbol{x}\|_\infty \geqslant M \Rightarrow f(\boldsymbol{x}) > f^* \geqslant f^k$. Thus there exists a compact interval $\mathcal{K} = \left[\boldsymbol{x}^L, \boldsymbol{x}^U\right]$ with $\left\|\boldsymbol{x}^i\right\|_\infty \geqslant M$, $i = L, U$ which includes all iterates $\boldsymbol{x}^k$. In the following, we replace $\mathcal{X}$ by $\mathcal{K}$ and show that all necessary assumptions for Theorem 1 hold. First, from Assumption 8 follows Assumption 4. Second, from Assumption 8 follows Assumption 5. Third, from continuity of g (Assumption 2) and compactness of $\mathcal{K}$ and $\mathcal{Y}$ follow uniform continuity of g and Assumption 6 is satisfied. By Theorem 1, the lower-bounding procedure converges. □

4.1.4 Case 2(c): $\mathcal{X}^{\text{infeas}}$ unbounded and SIP has the form of a epigraph reformulation

In the special case that (SIP) is the epigraph reformulation of a min-max problem with a coercive objective function, no convergence problems arise.

Assumption 9 (SIP) has the form of (14), q is continuous and coercive in $\boldsymbol{x}$ for all $\boldsymbol{y}$, and $\mathcal{Y}$ is compact.

Proposition 3 *Under Assumptions 2, 3 and 9, the lower-bounding procedure converges.*

Proof From continuity and coerciveness of q in $\boldsymbol{x}$ $\forall \boldsymbol{y}$ follows the optimal point exists, is finite, and attainable. It also follows, $\exists M$ such that $\forall \boldsymbol{y}, \boldsymbol{x} : \|\boldsymbol{x}\| > M\Big[q(\boldsymbol{x}, \boldsymbol{y}) \geqslant \max_{\boldsymbol{y} \in \mathcal{Y}} q(\boldsymbol{x}^*, \boldsymbol{y}) = \mu^*\Big]$. Because of the epigraph form of (14), the construction of (LBP), and the global solution of the subproblems, we also have $\forall k, l : k > l\left[\mu^* \geqslant q\left(\boldsymbol{x}^k, \boldsymbol{y}^l\right)\right]$. Combining these results above, there exists a compact $\mathcal{K}$ such that $\left\{\boldsymbol{x}^k\right\} \subseteq \mathcal{K} \subsetneq \mathcal{X}$ and $\boldsymbol{x}^* \in \mathcal{K}$. Using $\mathcal{K}$ instead of $\mathcal{X}$ in (14), we obtain a new SIP, called $\widetilde{\text{SIP}}$. From compactness of $\mathcal{K}$ follows Assumption 4 is satisfied. From Assumption 9 follows Assumption 5. From continuity of g and compactness of $\mathcal{K}$ and $\mathcal{Y}$ follows Assumption 6. By Theorem 1, the lower-bounding procedure converges. It remains to show that the solution of $\widetilde{\text{SIP}}$ and of the original SIP are equivalent. $\widetilde{\text{SIP}}$ is a restriction of (14) because $\mathcal{K} \subsetneq \mathcal{X}$. Since the optimal point of (14) is also feasible in $\widetilde{\text{SIP}}$, the optimal solutions are equivalent. □

4.2 Additional assumptions for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded

If one of the following assumptions holds instead of Assumption 1, no convergence issues occur.

Assumption 10 The set $\mathcal{X} \subsetneq \mathbb{R}^{n_x}$ is compact and $\mathcal{Y} \subseteq \mathbb{R}^{n_y}$. The function g is uniformly continuous on $\mathcal{X} \times \mathcal{Y}$.

Assumption 11 The set $\mathcal{X} \subsetneq \mathbb{R}^{n_x}$ is compact and $\forall \varepsilon > 0\ \exists \delta_2 > 0 : \forall \boldsymbol{x}^k \in \left\{\boldsymbol{x}^k\right\}, \boldsymbol{x} \in \mathcal{X}\left[\left\|\boldsymbol{x}^k - \boldsymbol{x}\right\| < \delta_2\right]$ holds $\left|g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\right| < \varepsilon$.

Assumption 12 The optimal solution $\boldsymbol{y}^k$ of (LLP) exists for all iterates $\boldsymbol{x}^k$, and the sequence $\left\{\boldsymbol{y}^k\right\}$ does not diverge, i.e., $\lim_{k\to\infty} \left\|\boldsymbol{y}^k\right\| < \infty$.

Proposition 4 *Under Assumptions 2, 3 and 10, the lower-bounding procedure converges.*

Proof First, from Assumption 10 follows Assumption 4. Second, from Assumption 2 follows Assumption 5. Third, from Assumption 10 follows Assumption 6. By Theorem 1, the lower-bounding procedure converges. □

Proposition 5 *Under Assumptions 2, 3 and 11, the lower-bounding procedure converges.*

The proof is conceptually equivalent to the proof of Proposition 4 and is thus omitted.

Proposition 6 *Under Assumptions 2, 3 and 12, the lower-bounding procedure converges.*

Proof Consider

$$\begin{aligned} &\min_{\tilde{\boldsymbol{x}} \in \widetilde{\mathcal{X}}} f(\tilde{\boldsymbol{x}}) \\ &\quad \text{s.t.} \quad \forall \tilde{\boldsymbol{y}} \in \widetilde{\mathcal{Y}}\left[g(\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}) \leqslant 0\right] \end{aligned} \qquad (\widetilde{\text{SIP}})$$

with $\widetilde{\mathcal{X}} = \mathcal{X}$ and the compact interval $\widetilde{\mathcal{Y}} \subseteq \mathcal{Y}$ such that $\left\{\boldsymbol{y}^k\right\} \in \widetilde{\mathcal{Y}}$. With Assumption 2 follows uniform continuity of g on $\widetilde{\mathcal{Y}} \times \widetilde{\mathcal{X}}$. ($\widetilde{\text{SIP}}$) fulfills Assumptions 1 to 3. Therefore, Theorem 1 and its proof are applicable.
We will show by contradiction that the optimal objective value of the limit point

of ($\widetilde{\text{SIP}}$) and the original SIP are equivalent, i.e., $f(\tilde{\boldsymbol{x}}^*) = f(\boldsymbol{x}^*)$. First, assume $f(\tilde{\boldsymbol{x}}^*) < f(\boldsymbol{x}^*)$. Since the functions g and f are the same for ($\widetilde{\text{SIP}}$) and the original SIP, we have $\exists \boldsymbol{y} \in \mathcal{Y} : g(\tilde{\boldsymbol{x}}^*, \boldsymbol{y}) > 0$, i.e., $\tilde{\boldsymbol{x}}^*$ is infeasible in the original SIP. Assumption 12 and $k \to \infty$ $g(\tilde{\boldsymbol{x}}^*, \tilde{\boldsymbol{y}}^k) > 0$ proves $\tilde{\boldsymbol{x}}^*$ infeasible and gives us the desired contradiction. Second, assume $f(\tilde{\boldsymbol{x}}^*) > f(\boldsymbol{x}^*)$ which gives us (due to the same functions g and f) $\tilde{\mathcal{X}}^{\text{feas}} \subsetneq \mathcal{X}^{\text{feas}}$. But from $\tilde{\mathcal{Y}} \subseteq \mathcal{Y}$, follows $\tilde{\mathcal{X}}^{\text{feas}} \supseteq \mathcal{X}^{\text{feas}}$ which gives us the desired contradiction. From $f(\tilde{\boldsymbol{x}}^*) \nless f(\boldsymbol{x}^*)$ and $f(\tilde{\boldsymbol{x}}^*) \ngtr f(\boldsymbol{x}^*)$ follows $f(\tilde{\boldsymbol{x}}^*) = f(\boldsymbol{x}^*)$. □

4.2.1 Discussion of the Assumptions 10 to 12

Assumption 10 can be checked a priori. The following proposition covers Assumption 11.

Proposition 7 *Assumption 11 is implied by Assumption 10 but the reverse does not hold.*

Proof Consider $\tilde{\mathcal{X}} \times \tilde{\mathcal{Y}}$ with $\tilde{\mathcal{X}} \supseteq \bigcup_k \{\boldsymbol{x} \in \mathcal{X} | \, \|\boldsymbol{x}^k - \boldsymbol{x}\| < \delta_2\}$ and $\tilde{\mathcal{Y}} \supseteq \{\boldsymbol{y}^k\}$. If g is uniform continuous on $\mathcal{X} \times \mathcal{Y}$, g is also uniform continuous on $\tilde{\mathcal{X}} \times \tilde{\mathcal{Y}} \supseteq \mathcal{X} \times \mathcal{Y}$. Assumption 11 is therefore implied by Assumption 10. Revisit E1 with the non-uniform continuous function g on $\mathcal{X} \times \mathcal{Y}$, i.e., Assumption 10 is not satisfied. Choose for the LLP solution $\boldsymbol{y}^k = (1, x^k)^T$. $\mathcal{X}$ being a compact set, we can choose the compact set $\hat{\mathcal{Y}} \supseteq \{\boldsymbol{y}^k\}$. It follows, g is uniform continuous on $\mathcal{X} \times \hat{\mathcal{Y}}$ but not on $\mathcal{X} \times \mathcal{Y}$ □

Assumptions 11 and 12 generally cannot be proven a priori. Therefore, they are not directly applicable. However, stronger conditions than required for Assumption 12 can be checked a priori. For example, one may choose some large number M a priori and check during runtime whether $\|\boldsymbol{y}^k\| < M$ holds. One way to achieve this may be to require the solver to minimize the magnitude of the variable values among all global solutions of (LLP). The auxiliary problem

$$\begin{aligned} \min_{\boldsymbol{y} \in \mathcal{Y}} \; & \|\boldsymbol{y}\| \\ \text{s.t.}\; & g(\bar{\boldsymbol{x}}, \bar{\boldsymbol{y}}) = g(\bar{\boldsymbol{x}}, \boldsymbol{y}). \end{aligned} \tag{AUX}$$

is solved with $\bar{y}$ being the optimal solution of the (LLP). Note that only an approximate solution of the (LLP) is required, c.f., Assumption 3. Therefore, a relaxation of the equality constraint is possible. The optimal solution of (AUX) is then used to populate the set $\mathcal{Y}^k$.

One could also prove that Assumption 12 holds, by computing upper and lower bounds for each lower-level variable y_i a priori. The following optimization-based bound tightening based approach computes upper and lower bounds for all y_i, i.e., y_i^{UBD} and y_i^{LBD}, respectively. However, there is no guarantee of success.

$$\begin{aligned} y_i^{\text{LBD}} = \min_{\boldsymbol{x} \in \mathcal{X}, \boldsymbol{y} \in \mathcal{Y}} \; & y_i \\ \text{s.t.}\; & g(\boldsymbol{x}, \boldsymbol{y}) \geqslant 0 \end{aligned} \tag{16}$$

$$\begin{aligned} y_i^{\text{UBD}} = \max_{\boldsymbol{x} \in \mathcal{X}, \boldsymbol{y} \in \mathcal{Y}} \; & y_i \\ \text{s.t.}\; & g(\boldsymbol{x}, \boldsymbol{y}) \geqslant 0 \end{aligned} \tag{17}$$

Note the direction of the inequality in (16) and (17) as we want to compute the maximum and minimum value of y_i on $\text{cl}(\mathcal{X}^{\text{infeas}}) \times \mathcal{Y}$.

4.3 Additional assumptions for $\mathcal{X}$ unbounded and $\mathcal{Y}$ unbounded

For SIPs with unconstrained upper- and lower-level hosts, convergence guarantees can be recovered if a suitable combination of the assumptions presented in Section 4.2 and Section 4.1 are adopted. Note that this is possible, as none of the corresponding pairs are mutually exclusive.

5 Numerical case studies

We present two illustrative case studies from Chebyshev approximation. These are a proof-of-concept for our findings rather than a complete numerical study which is beyond the scope of this paper. The corresponding (LBP) and (LLP) of the considered cases studies are written in the domain specific language provided by libALE [6]. The implementation of the lower-bounding procedure of [19] is provided by the library for discretization-based semi-infinite programming solvers (libDIPS) [4]. The numerical case studies are carried out on a Windows Server 2016 Standard with an Intel(R) Xeon(R) CPU E5-2640 v3 @2.60GHz processor and 128GB of RAM. All subproblems are solved using Baron version 19.12.7., accessed through GAMS version 30.2.0 [11, 16]. Note that Baron cannot handle trigonometric functions, which limits the applicability, and does not give certificate of global optimality for complex subproblems.

5.1 Case study for $\mathcal{X}$ unbounded and $\mathcal{Y}$ compact

Consider the min-max problem inspired by Chebyshev-approximation

$$
\begin{aligned}
f^* = \min_{\boldsymbol{x}\in\mathcal{X}} \max_{\boldsymbol{y}\in\mathcal{Y}} & \Big\| \left(-\exp\left(-(y-3)^2\right) + 0.2\exp(y-3) + 1\right) \\
& \quad - \left(x_1 + x_2 y + x_3 y^2 + x_4 y^3 + x_5 y^4\right) \Big\|_2 \\
& \mathcal{X} \subseteq \mathcal{R}^5 \\
& \mathcal{Y} = [1,5]\,.
\end{aligned} \tag{18}
$$

We reformulate (18) to

$$
\begin{aligned}
f^* = \min_{\boldsymbol{x}\in\mathcal{X},\mu\in\mathcal{E}} \quad & \mu \\
\text{s.t.} \quad & \forall \boldsymbol{y}\in\mathcal{Y}\Big[\Big(\left(-\exp\left(-(y-3)^2\right) + 0.2\exp(y-3) + 1\right) \\
& \qquad - \left(x_1 + x_2 y + x_3 y^2 + x_4 y^3 + x_5 y^4\right)\Big)^2 \leqslant \mu\Big] \\
& \mathcal{X} \subsetneq \mathcal{R}^5 \\
& \mathcal{Y} = [1,5] \\
& \mathcal{E} = [0,+\infty)\,.
\end{aligned} \tag{19}
$$

Note that we have in this example the case 2(c), i.e., $\mathcal{X}^{\text{infeas}}$ is unbounded and the SIP has the form of an epigraph reformulation (Section 4.1.4). The lower-bounding terminates after 11 iterations (total CPU time 19.510 s, relative and absolute termination tolerance $\varepsilon^r = \varepsilon^a = 0.001$) with an optimal solution of $\boldsymbol{x}^* = (-2.111,\ 6.471,\ -4.377,\ 1.091,\ -0.088)^T$ and with a maximal error of the fit of 0.028 (Figure 3).

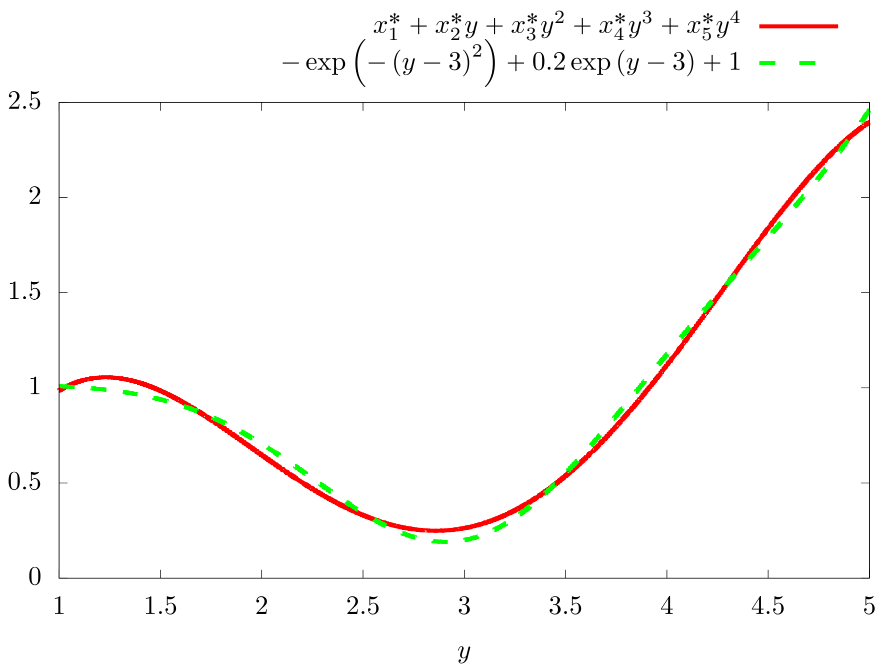

Fig. 3: Case study for $\mathcal{X}$ unbounded and $\mathcal{Y}$ compact.The original function is plotted as a green dashed line and the approximation function as a red solid line.

5.2 Case study for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded

Consider

$$\begin{aligned} f^* = \min_{(\mu,\boldsymbol{x})^T \in \mathcal{X}} \quad & \mu \\ \text{s.t. } \forall \boldsymbol{y} \in \mathcal{Y} & \left[\left(\left(\frac{3}{y^2} - \frac{2}{y^3} \right) - \left(\exp\left(x_1 \left(x_2 y + x_3 \right)^2 \right) \right) \right)^2 \leqslant e \right] \\ & \mathcal{X} = [0, 100] \times [-10, 10]^3 \\ & \mathcal{Y} = [1, +\infty) \,. \end{aligned} \tag{20}$$

(20) corresponds to a reformulated min-max Chebyshev-approximation problem, where $\left(\frac{3}{y^2} - \frac{2}{y^3}\right)$ is approximated by $\exp\left(x_1 \left(x_2 y + x_3\right)^2\right)$ over $[1, +\infty)$ with $\boldsymbol{x}$ being the parameters to be estimated. For (20), we assume that Assumption 12 holds. The lower-bounding procedure terminates after 8 iterations (total CPU time 23.300 s, relative and absolute termination tolerance $\varepsilon^r = \varepsilon^a = 0.001$) with the optimal parameters $\boldsymbol{x}^* = (-0.010, -4.285, 1.248)^T$ (Figure 4).

6 Conclusion and outlook

Unconstrained upper and/or lower variable host sets in SIPs may arise, e.g., in (inverse) Chebyshev approximation, epigraphic reformulations, design centering, or in problems where an embedded optimization problem is replaced by its dual problem. In this paper, we showed in this paper that adaptive discretization-based algorithms are not

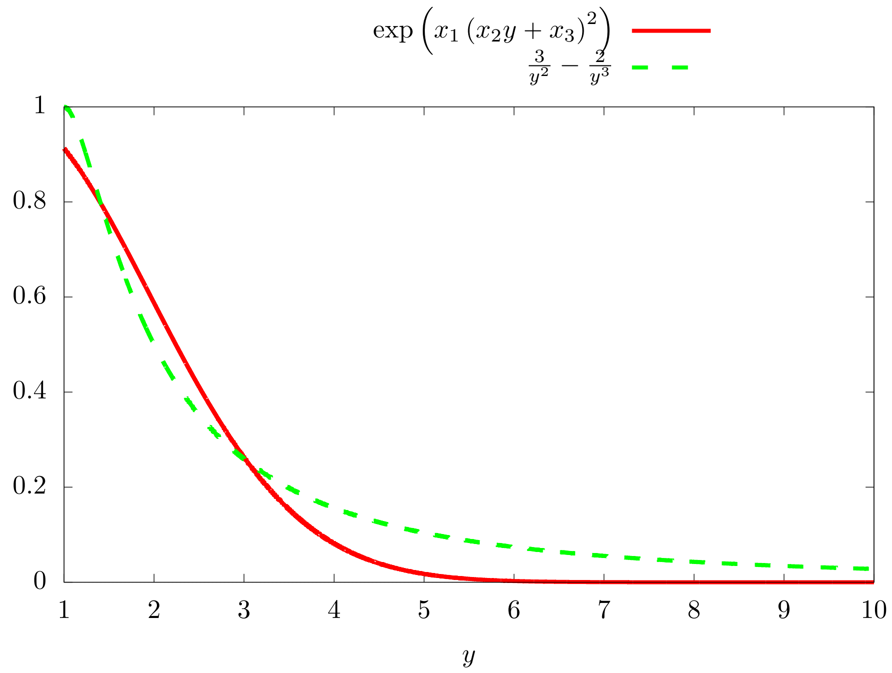

Fig. 4: Case study for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded. The original function is plotted as a green dashed line and the approximation function as a red solid line.

suitable for all SIPs with unconstrained host sets since convergence problems may arise.

Therefore, we investigated whether adaptive discretization-based algorithms, such as the lower bounding procedure of [19], are applicable to SIPs with unbounded host sets. First, we briefly reviewed the assumptions of the lower-bounding procedure of [19]. Instead of the original assumptions in [19], we used sharper, (slightly) relaxed, assumptions for our proof of the convergence of the lower bound procedure. In essence, the sharpened, slightly relaxed, assumptions establish a weaker form of uniform continuity of the constraint function on the set of all infeasible points in the host set of the SIP. In addition, the objective function must be at least semi-continuous on the boundary of the set of infeasible points. Using the sharpened assumptions, we provide additional assumptions that recover convergence guarantees for SIPs with unbounded host sets. Although the additional assumptions may be difficult to verify a priori in some cases, we give examples of stronger criteria that can be verified a priori or during run-time of the algorithm, implying the sharpened assumptions. The criteria are expected to be, at most, of the same computational burden as the subproblems of the SIPs. In addition, the criteria are expected to apply to many applications. We give two numerical case studies of SIPs with unbounded host sets, as a proof of concept.

The results discussed in this paper can be directly applied to the upper bound procedure of [19]. Moreover, we assume that our results are transferable to conceptually related adaptive discretization procedures for generalized semi-infinite programs and bilevel programs with unbounded host sets. For future work, we plan to investigate the latter and the impact of non-continuous functions. A close examination of our sharpened and slightly relaxed assumptions suggests that lower semi-continuous constraint functions do not pose a problem for adaptive discretization methods.

A Lower-bounding procedure of [19]

A.1 Illustrative example for $\mathcal{X}$ compact and $\mathcal{Y}$ bounded and not closed

The same convergence issues as in (E1) (Section 3.1) arise when we consider (E1.1) with $\mathcal{X}$ compact and $\mathcal{Y}$ bounded but not closed.

$$\begin{aligned} f^* =& \min_{x \in \mathcal{X}} -x \\ & \text{s.t. } \forall \boldsymbol{y} \in \mathcal{Y} \left[-\frac{1}{y_1} (y_2 - x)^2 + 1 \leqslant 0 \right] \\ & \mathcal{X} = [0, 2] \\ & \mathcal{Y} = (0, 0.5] \times [0, 2] . \end{aligned} \tag{E1.1}$$

The optimal solutions of (LLP) are $\boldsymbol{y}^* (\bar{x}) = (\tilde{y}, \bar{x})^T$ with $\tilde{y} \in (0, 0.5]$ or $\boldsymbol{y}^* (\bar{x}) = (0, \tilde{y})^T$ with $\tilde{y} \in [0, 2]$. Starting with an empty discretization $\mathcal{Y}^0 = \varnothing$ and using $\boldsymbol{y}^k = \left(2^{-(k+1)}, x^k\right)^T$ for all iterations, the same issues arises.

In general, one could use the closure of the non-compact host sets. However, this is not possible here.

A.2 Illustrative examples for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded: Feasible SIP

Consider the feasible SIP with unbounded host sets.

$$\begin{aligned} f^* =& \min_{x \in \mathcal{X}} -x \\ & \text{s.t. } \forall \boldsymbol{y} \in \mathcal{Y} \left[\begin{cases} -y_1^2 (y_2 - x)^2 + 1 & \leqslant 0, \quad x \geqslant 1 \\ -y_1^2 (y_2 - x)^2 + 3x - 2 & \leqslant 0, \quad x < 1 \end{cases} \right] \\ & \mathcal{X} = [0, 2] \\ & \mathcal{Y} = \mathbb{R}^2 \end{aligned} \tag{E2}$$

Remark 1 The function g is continuous but not differentiable on $\mathcal{X} \times \mathcal{Y}$. This is not required according to Assumptions 1 to 3. The non-differentiability of g is of no relevance in this example, as we receive the same convergence properties when using the function

$$g(x, \boldsymbol{y}) = \begin{cases} -y_1^2 (y_2 - x)^2 + 1 & \leqslant 0, \quad x \geqslant 1 \\ -y_1^2 (y_2 - x)^2 + 3x^{2n} - 2 & \leqslant 0, \quad x < 1 \end{cases} \tag{21}$$
$$\text{with } n \in \mathbb{N}_{>0}$$

belonging to the differentiability class C^n instead.

The optimal value function of (LLP) of (E2) is

$$g^* (\bar{x}) = \begin{cases} 1, & x \geqslant 1 \\ 3\bar{x} - 2, & x < 1 \end{cases} \tag{22}$$

with the optimal value $\boldsymbol{y}^* (\bar{x}) = (\tilde{y}, \bar{x})^T$ or $\boldsymbol{y}^* (\bar{x}) = (0, \tilde{y})^T$ with $\tilde{y} \in \mathbb{R}$. The feasible set is $\mathcal{X}^{\text{feas}} = \left[0, \frac{2}{3}\right]$. The optimal solution of (E2) is $x^* = \frac{2}{3}$ with $f^* = -\frac{2}{3}$. Using the same sequence of points as in (E1), we converge to the same infeasible point $x = 1$ in the limit, c.f., Figure 5. We do not converge to the globally optimal solution, again failing our expectations.

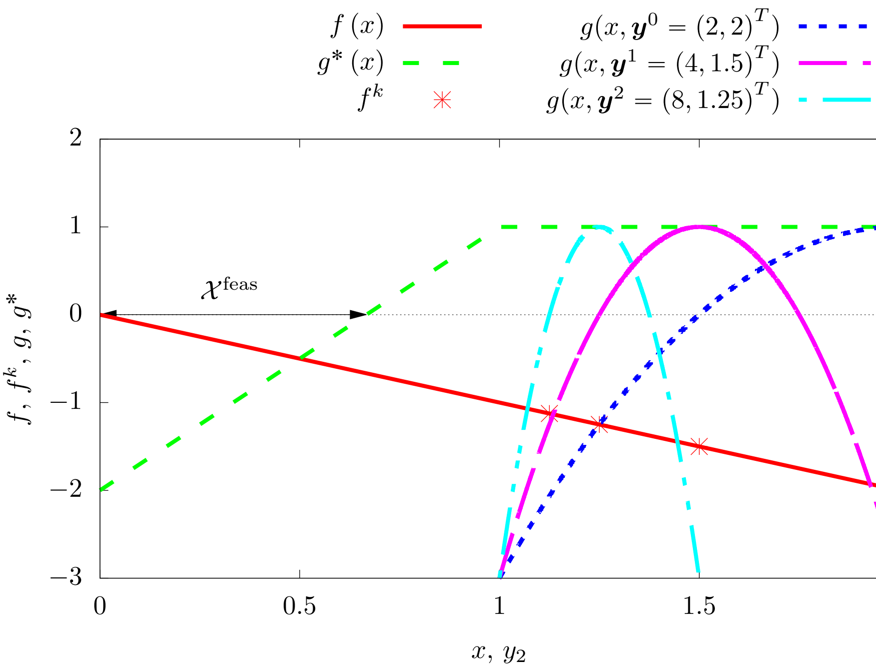

Fig. 5: Illustrative example (E2) for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded with parametric solutions of (LLP). (E2) is feasible.

B Upper-bounding procedure of [19]

B.1 Definitions and assumptions of the upper-Bounding procedure of [19]

We first review the discrete upper-bounding problem in [19].

Definition 4 (*Discrete upper-bounding problem*) The discrete upper-bounding problem (UBP) with $\mathcal{Y}^{\text{UBD},k} \subsetneq \mathcal{Y}$ is

$$f^{\text{UBD},k} = \min_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x}) \quad \text{s.t. } \forall \boldsymbol{y} \in \mathcal{Y}^{\text{UBD},k} \left[g(\boldsymbol{x}, \boldsymbol{y}) \leqslant -\varepsilon^g \right] \tag{UBP}$$

with some $\varepsilon^g > 0$. For convencience we define $g^{\text{UBD}}(\boldsymbol{x}, \boldsymbol{y}) = g(\boldsymbol{x}, \boldsymbol{y}) - \varepsilon^g$.

In the following, we use the same notations as for the lower-bounding procedure. The proof of convergence of the upper-bounding procedure in [19] relies on the existence of an ε^f-optimal SIP-Slater point.

Definition 5 (*SIP-Slater Point*) A point $\boldsymbol{x}^s$ is called a SIP-Slater point if $\forall \boldsymbol{y} \in \mathcal{Y} \left[g(\boldsymbol{x}^s, \boldsymbol{y}) < 0 \right]$.

Assumption 13 (*Existence of ε^f-optimal SIP-Slater Point*) An ε^f-optimal SIP-Slater point $\boldsymbol{x}^s$ exists such that $f(\boldsymbol{x}^s) \leqslant f^* + \varepsilon^f$ and $\forall \boldsymbol{y} \in \mathcal{Y} \left[g(\boldsymbol{x}^s, \boldsymbol{y}) \leqslant -\varepsilon^s \right]$.

B.2 Illustrative example for $\mathcal{X}$ compact and $\mathcal{Y}$ unbounded

[19] states

> at each iteration of the upper-bounding procedure, there are three potential outcomes, namely (i) (UBP) is infeasible, (ii) (UBP) is feasible and furnishes a SIP-feasible point and (iii) (UBP) is feasible but furnishes a SIP-infeasible point. In the former two cases the restriction parameter ε^g is reduced and in the latter case $\mathcal{Y}^{\mathrm{UBD},k}$ is populated.

and shows that after a finite number of updates of ε^g, the upper-bounding procedure produces a SIP-feasible point. We show that in the case of unbounded sets, the upper-bounding procedure may never produce a SIP-feasible point. Consider

$$
\begin{aligned}
f^* = & \min_{x \in \mathcal{X}} \; -x \\
& \text{s.t. } \forall \boldsymbol{y} \in \mathcal{Y} \left[\begin{cases} -y_1^2 (y_2 - x)^2 + 0.5 & \leqslant 0, \quad x \geqslant 1 \\ -y_1^2 (y_2 - x)^2 + 3x - 2.5 \leqslant 0, & x < 1 \end{cases} \right] \\
& \mathcal{X} = [0, 2] \\
& \mathcal{Y} = \mathbb{R}^2
\end{aligned}
\tag{E2}
$$

and choose $\varepsilon^g = 0.5$ in (UBP). With the chosen ε^g, (UBP) of (E2) is equivalent to the (LBP) of (E2). Figure 6 depicts the objective function f, $f^{\mathrm{UBD},k}$, $g^{*,\mathrm{UBD}}$, g^* and the feasible set of (UBP) and (E2), i.e., and $\mathcal{X}^{\mathrm{UBD,feas}}$ $\mathcal{X}^{\mathrm{feas}}$, respectively.

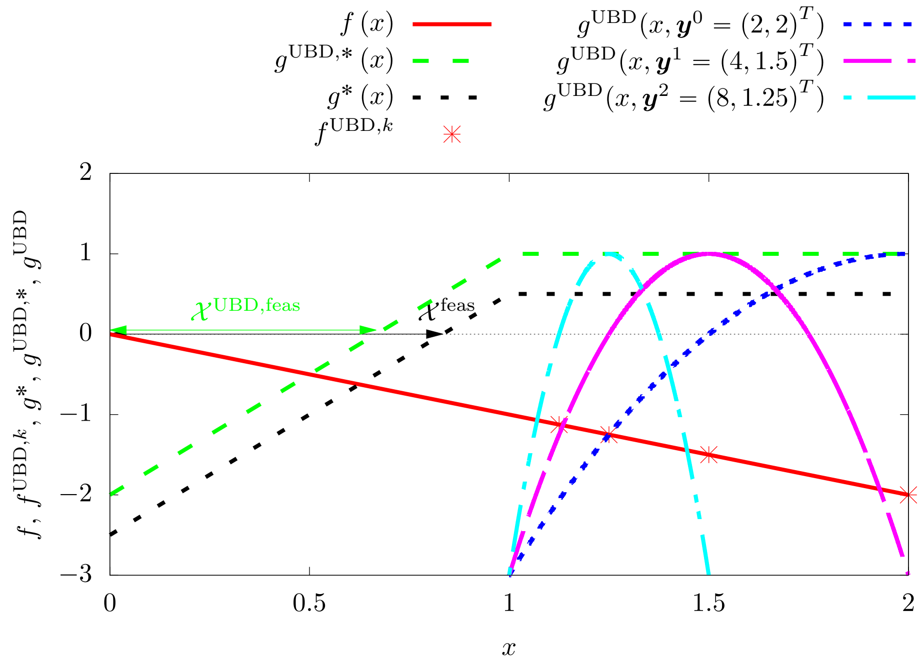

Fig. 6: Illustrative example (E2) for the upper-bounding procedure with $\mathcal{X}$ compact and $\mathcal{Y}$ unbounde. $\varepsilon^g = 0.5$.

Note that the (LLP) solution point of (E2) is independent of to ε^g. Using the same sequence of points as in (E2), the outcome is always (iii), i.e., no SIP-feasible point is furnished. Therefore, ε^g is never reduced, and the upper-bounding procedure converges to the infeasible point $x = 1$ in the limit.

B.3 Proof of convergence of the upper-bounding procedure in [19]

In [19] follows with the existence of a SIP-Slater point $\boldsymbol{x}^s$, compactness of $\mathcal{Y}$, and continuity of g (c.f, Assumptions 1 and 2), there exists a $\varepsilon^s > 0$ such that

$$\forall \boldsymbol{y} \in \mathcal{Y}\left[g\left(\boldsymbol{x}^s, \boldsymbol{y}\right) \leqslant -\varepsilon^s\right], \tag{23}$$

c.f. , [19]. This also holds for the case of unbounded $\mathcal{X}$ and compact $\mathcal{Y}$ but does not hold for the case of unbounded $\mathcal{Y}$. For example, for $y \in \mathcal{Y} = [1, +\infty)$, $g(x, y) = -\frac{1}{y}$ there exists an SIP-Slater point but $\nexists \varepsilon^s : \forall \boldsymbol{y} \in \mathcal{Y}\left[g\left(\boldsymbol{x}^s, \boldsymbol{y}\right) \leqslant -\varepsilon^s\right]$). Therefore, for the case of unbounded $\mathcal{Y}$, we slightly adapt Assumption 13 to

Assumption 14 (*Existence of ε^f-optimal and strictly feasible Point*) An ε^f-optimal and strictly feasible point $\boldsymbol{x}^s$ exists such that there exists an $\varepsilon^s > 0$ and $f\left(\boldsymbol{x}^s\right) \leqslant f^* + \varepsilon^f$ and $\forall \boldsymbol{y} \in \mathcal{Y}\left[g\left(\boldsymbol{x}^s, \boldsymbol{y}\right) \leqslant -\varepsilon^s\right]$.

Note that for $\mathcal{X}$ and compact $\mathcal{Y}$, Assumption 14 directly follows from Assumption 13. To extend the applicability to unbounded SIPs, we adapt the original Lemma to

Theorem 2 *Take any $\mathcal{Y}^{UBD,0} \subsetneq \mathcal{Y}$, any ε^f and any $r > 1$. Assume that Assumptions 3 to 6 and 14 hold. Then the upper-bounding procedure in [19] furnishes a SIP-feasible point $\boldsymbol{x}^*$ finitely, such that $f\left(\boldsymbol{x}^*\right) \leqslant f^* + \varepsilon^f$.*

The proof of Theorem 2 is, apart from slight changes, equivalent to the original proof in [19].

Proof In each iteration one of the following cases hold

i) (UBP) is infeasible

ii) (UBP) is feasible and a SIP feasible point is furnished

iii) (UBP) is feasible and a SIP infeasible point is furnished

In case i) and ii) ε^g is reduced. In case iii) $\mathcal{Y}^{\mathrm{UBD},k}$ is populated with the solution point of the corresponding (LLP).

We first show that a infinite sequence of infeasible (UBP) is not possible. By Assumption 14 there exists a point $\boldsymbol{x}^s$ such that $f\left(\boldsymbol{x}^s\right) \leqslant f^* + \varepsilon^f$ and $\forall \boldsymbol{y} \in \mathcal{Y}\left[g\left(\boldsymbol{x}^s, \boldsymbol{y}\right) \leqslant -\varepsilon^s\right]$. This point is feasible in (UBP) if $\varepsilon^g \leqslant \varepsilon^s$, regardless of $\mathcal{Y}^{\mathrm{UBD},k}$. Therefore, (UBP) is feasible if $\varepsilon^g \leqslant \varepsilon^s$. Because of $\varepsilon^g = \frac{\varepsilon^{g,0}}{r^a}$ with a being the number of reductions, after $a = \lceil \log_r \frac{\varepsilon^{g,0}}{\varepsilon^s} \rceil$ reductions, the (UBP) becomes feasible.

For (UBP) with $\varepsilon^g < \varepsilon^s$ follows $f\left(\boldsymbol{x}^k\right) \leqslant f\left(\boldsymbol{x}^s\right) \leqslant f^* + \varepsilon^f$. Hence, the solution point of (UBP) $\boldsymbol{x}^k$ is a candidate point with ε^f-optimality. If $\boldsymbol{x}^k$ is SIP-feasible, the desired result holds.

It remains to show that an infinite sequence of iii) is not possible, which also means that ε^g is no longer updated. It therefore holds for all iterations $\varepsilon^g \geqslant \varepsilon^{g,\min} \equiv \frac{\varepsilon^s}{r}$. By construction of (UBP) we have

$$\forall l, k : \ l > k\left[g\left(\boldsymbol{x}^l, \boldsymbol{y}^k\right) \leqslant -\varepsilon^g \leqslant -\varepsilon^{g,\min}\right] \tag{24}$$

Due to Assumption 6, it also holds

$$\begin{aligned} \exists \delta_1 > 0 : \ \forall \boldsymbol{x}^l \in \left\{\boldsymbol{x}^k\right\} \cap \mathcal{X}^{\mathrm{infeas}}, \boldsymbol{x} \in \mathcal{X}^{\mathrm{infeas}}\left[\left\|\boldsymbol{x}^l - \boldsymbol{x}\right\| < \delta_1\right] \\ \Rightarrow \left|g\left(\boldsymbol{x}^l, \boldsymbol{y}^k\right) - g\left(\boldsymbol{x}, \boldsymbol{y}^k\right)\right| < \frac{\varepsilon^{g,\min}}{2}. \end{aligned} \tag{25}$$

Combining (24) and (25), we have

$$\forall l, k : l > k\left[g\left(\boldsymbol{x}, \boldsymbol{y}^k\right) < -\frac{\varepsilon^{g,\min}}{2} < 0\right] \tag{26}$$

Due to Assumption 4, the limit point $\boldsymbol{x}^* \in \mathrm{cl}\,(\mathcal{X})^{\mathrm{infeas}}$ exists. From $\boldsymbol{x}^k \to \boldsymbol{x}^*$, we have

$$\forall \delta_1 \exists K : \forall l, k\, [l > k \geqslant K] \left[\left\| \boldsymbol{x}^l - \boldsymbol{x}^k \right\| < \delta_1 \right]. \tag{27}$$

Substituting $\boldsymbol{x} = \boldsymbol{x}^k$ in (26), we obtain

$$\exists K : g\left(\boldsymbol{x}^k, \boldsymbol{y}^k\right) < -\frac{\varepsilon^{g,\min}}{2} < 0. \tag{28}$$

Therefore, after a finite number of iterations K the point $\boldsymbol{x}^k$ is SIP-feasible which gives us the desired result. Combining the results above, the upper-bounding procedure furnishes a point $\boldsymbol{x}^*$ that satisfies $f\left(\boldsymbol{x}^*\right) \leqslant f^* + \varepsilon^f$ after a finite number of iterations. □

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