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Recent advances in nonconvex semi-infinite programming: Applications and algorithms

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ABSTRACT

The goal of this literature review is to give an update on the recent developments for semi-infinite programs (SIPs), approximately over the last 20 years. An overview of the different solution approaches and the existing algorithms is given. We focus on deterministic algorithms for SIPs which do not make any convexity assumptions. In particular, we consider the case that the constraint function is non-concave with respect to parameters. Advantages and disadvantages of the different algorithms are discussed. We also highlight recent SIP applications. The article closes with a discussion on remaining challenges and future research directions.

1. Introduction

This article reviews recent developments in theory, applications and algorithms for nonconvex semi-infinite programs. In such problems, finitely many variables are subject to infinitely many inequality constraints. They can be stated as

$$SIP: \quad \min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{s.t.} \quad \boldsymbol{x} \in M$$

with the set of feasible points

$$M = \{\boldsymbol{x} \in \mathbb{R}^n |\ g(\boldsymbol{x}, \boldsymbol{y}) \leq 0 \text{ for all } \boldsymbol{y} \in Y\} \tag{1}$$

and a nonempty compact index set $Y \subsetneq \mathbb{R}^m$ of the inequality constraints. The defining functions f and g are assumed to be real-valued and at least continuous on their respective domains, but we neither impose upper-level nor lower-level convexity assumptions on SIP for the most part of this paper.

1.1. Upper-level and lower-level convexity

In the case of convex $g(\cdot, \boldsymbol{y})$ for all $\boldsymbol{y} \in Y$, the feasible set M is convex, so that together with a convex objective function f, the optimization problem SIP is then convex and, in particular, each locally minimal point is also globally minimal. As these assumptions involve the upper-level variable $\boldsymbol{x}$, one speaks of upper-level convexity. An important special case is linear semi-infinite optimization, where the functions f and $g(\cdot, \boldsymbol{y})$, $\boldsymbol{y} \in Y$, are (affine) linear.

In the absence of upper-level convexity, one may either keep aiming at the computational approximation of globally minimal points for SIP by resorting to global optimization techniques, or one is content with the computation of locally optimal points.

The lower-level problem of SIP is concerned with checking feasibility of a point $\boldsymbol{x}$. This constitutes the main algorithmic challenge in semi-infinite optimization because feasibility of $\boldsymbol{x}$ is defined in terms of the infinitely many constraints $g(\boldsymbol{x}, \boldsymbol{y}) \leq 0$, $\boldsymbol{y} \in Y$. In an optimization reformulation, they may be written as $\overline{g}(\boldsymbol{x}) := \max_{\boldsymbol{y} \in Y} g(\boldsymbol{x}, \boldsymbol{y}) \leq 0$, so that feasibility of $\boldsymbol{x}$ may be checked by testing the optimal value $\overline{g}(\boldsymbol{x})$ of the lower-level problem

$$LLP(\boldsymbol{x}): \quad \max_{\boldsymbol{y}} g(\boldsymbol{x}, \boldsymbol{y}) \quad \text{s.t.} \quad \boldsymbol{y} \in Y$$

for nonpositivity. This also motivates to call $\boldsymbol{y}$ the lower-level variable.

For given $\boldsymbol{x}$, the problem $LLP(\boldsymbol{x})$ is convex if Y is a convex set and if $g(\boldsymbol{x}, \cdot)$ is concave on Y. We refer to these assumptions as lower-level convexity. Under lower-level convexity, each locally maximal value of $LLP(\boldsymbol{x})$ coincides with the globally maximal value $\overline{g}(\boldsymbol{x})$ and may, thus, be used to check feasibility of $\boldsymbol{x}$. We emphasize that in the absence of lower-level convexity, it is not an option to check only locally maximal values of $LLP(\boldsymbol{x})$ for nonpositivity because infeasible points $\boldsymbol{x}$ may then erroneously be identified as feasible. Consequently, as opposed to the situation without upper-level convexity, a lack of lower-level convexity entails a need for some sort of global optimization technique to solve $LLP(\boldsymbol{x})$.

The present survey mainly covers standard semi-infinite programs (SIPs), while also theory, methods, and applications of generalized semi-infinite optimization (GSIP) received considerable attention over the last two decades. In these problems, the index set Y is allowed to depend on the upper-level variable $\boldsymbol{x}$, that is, the feasible set has the form

$$M_{GSIP} = \{\boldsymbol{x} \in \mathbb{R}^n |\ g(\boldsymbol{x}, \boldsymbol{y}) \leq 0 \text{ for all } \boldsymbol{y} \in Y(\boldsymbol{x})\} \tag{2}$$

with a set-valued mapping $Y: \mathbb{R}^n \rightrightarrows \mathbb{R}^m$.

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1.2. Standard references

As basic references, we mention (Hettich and Kortanek, 1993) for an introduction to semi-infinite optimization, (Hettich and Zencke, 1982; Polak, 1997; Reemtsen and Görner, 1998) for algorithmic approaches to SIPs as well as Goberna and López (1998) and Goberna and López (2018) for linear semi-infinite optimization. The foundations of GSIPs are treated in the monograph (Stein, 2003).

More recent reviews on theory, applications and algorithms for SIP are López and Still (2007), Guerra Vázquez et al. (2008), Shapiro (2009) and Stein (2012). Internet resources include the SIP bibliography (López and Still, 2012) with several hundreds of references and the NEOS SIP directory (Goberna, 2013). Note that these recent reviews mainly cover optimality conditions and stability results for SIPs, while the present survey focuses on applications and algorithmic aspects.

1.3. Motivating example

In anticipation of the presentation of current SIP application areas in Section 3, let us briefly sketch Chebyshev approximation as a classical example.

Example 1. *(Chebyshev approximation)* Historically, the systematic study of semi-infinite optimization is motivated by Chebyshev approximation problems (cf. López and Still, 2007). In fact, consider the approximation of a continuous function F on a nonempty compact set $Y \subsetneq \mathbb{R}^m$ by an element from the family of continuous functions $a(\boldsymbol{p},\cdot)$, $\boldsymbol{p} \in P$, with parameter set $P \subseteq \mathbb{R}^n$. Measuring the deviation of F from $a(p,\cdot)$ on Y by the Chebyshev norm $\|F(\cdot)-a(\boldsymbol{p},\cdot)\|_{\infty,Y} := \max_{\boldsymbol{y}\in Y} |F(\boldsymbol{y})-a(\boldsymbol{p},\boldsymbol{y})|$ leads to the Chebyshev approximation problem

$$CA: \quad \min_{\boldsymbol{p}} \|F(\cdot)-a(\boldsymbol{p},\cdot)\|_{\infty,Y} \quad \text{s.t.} \quad \boldsymbol{p} \in P.$$

Its epigraphical reformulation yields the semi-infinite program

$$\begin{aligned} SIP_{CA}: \quad \min_{\boldsymbol{p},q} q \quad \text{s.t.} \quad & F(\boldsymbol{y})-a(\boldsymbol{p},\boldsymbol{y}) \le q, \ \boldsymbol{y} \in Y, \\ & -F(\boldsymbol{y})+a(\boldsymbol{p},\boldsymbol{y}) \le q, \ \boldsymbol{y} \in Y, \\ & \boldsymbol{p} \in P, \end{aligned}$$

with two semi-infinite constraints.

In case that the family $a(\boldsymbol{p},\cdot)$, $\boldsymbol{p} \in P$, depends linearly on $\boldsymbol{p}$ and P is polyhedral, SIP_{CA} enjoys upper-level convexity and is even a linear SIP. This is the case, e.g., for polynomial functions $a(\boldsymbol{p},\cdot)$ of fixed maximal degree and with unconstrained coefficient vector $\boldsymbol{p}$. The usually missing lower-level convexity in SIP_{CA} can be treated algorithmically for example by the Remez algorithm, if the index variable $\boldsymbol{y}$ is scalar (Hettich and Kortanek, 1993; Hettich and Zencke, 1982).

1.4. Relations to other problem classes

While this survey does not focus on them, we point out some fruitful relations of SIP to several other problem classes in optimization, in particular to robust optimization, to mathematical programs with complementarity constraints, to disjunctive programs, and to game theory.

Example 2. *(Robust optimization)* Optimization under uncertainty is a long-standing goal, cf. (Halemane and Grossmann, 1983; Sahinidis, 2004). The two main approaches to deal with uncertainty are (two-stage) stochastic programming, e.g., (Birge and Louveaux, 1997) and worst-case or robust optimization (Ben-Tal and Nemirovski, 1999).

In the optimization problem

$$P(\boldsymbol{t}): \quad \min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{t},\boldsymbol{x}) \quad \text{s.t.} \quad g_i(\boldsymbol{t},\boldsymbol{x}) \le 0, \ i \in I,$$

with finite index set I, let the continuous functions f, g_i, $i \in I$, depend on some uncertain parameter $\boldsymbol{t}$. Then, the robust optimization approach prescribes that the worst case for $\boldsymbol{t}$ is considered to construct a robust counterpart. Indeed, letting $T \subsetneq \mathbb{R}^r$ denote a nonempty and compact uncertainty set and with the upper envelopes

$$\overline{f}(\boldsymbol{x}) = \max_{\boldsymbol{t}\in T} f(\boldsymbol{t},\boldsymbol{x}) \quad \text{and} \quad \overline{g}_i(\boldsymbol{x}) = \max_{\boldsymbol{t}\in T} g_i(\boldsymbol{t},\boldsymbol{x}), \ \ i \in I,$$

one may consider the robust counterpart

$$RO: \quad \min_{\boldsymbol{x}\in\mathbb{R}^n} \overline{f}(\boldsymbol{x}) \quad \text{s.t.} \quad \overline{g}_i(\boldsymbol{x}) \le 0, \ i \in I,$$

of the family $P(\boldsymbol{t})$, $\boldsymbol{t} \in T$. Its epigraphical reformulation leads to

$$\begin{aligned} SIP_{RO}: \quad \min_{(\boldsymbol{x},z)\in\mathbb{R}^n\times\mathbb{R}} z \quad \text{s.t.} \quad & f(\boldsymbol{t},\boldsymbol{x}) \le z \text{ for all } \boldsymbol{t} \in T, \\ & g_i(\boldsymbol{t},\boldsymbol{x}) \le 0 \text{ for all } \boldsymbol{t} \in T, \ i \in I, \end{aligned}$$

with finitely many semi-infinite constraints.

While considerable attention has been paid to robust optimization in its own right, this survey considers it to be an application of semi-infinite programming. As such, the solution of robust optimization problems and variants of the formulation RO are discussed along with other applications of semi-infinite programming in Section 3.

Example 3. *(Mathematical programs with complementarity constraints)* Mathematical programs with complementarity constraints (MPCCs) consider the minimization of some objective function over a feasible set whose description contains complementarity constraints. Under the assumption of lower-level convexity and some mild regularity assumption, SIPs may be recast as MPCCs as follows.

Let $Y = \{\boldsymbol{y} \in \mathbb{R}^m | \, \boldsymbol{v}(\boldsymbol{y}) \le \boldsymbol{0}\}$ be described by a function $\boldsymbol{v}: \mathbb{R}^m \to \mathbb{R}^s$ with convex and continuously differentiable component functions, let Y satisfy the Slater condition $\boldsymbol{v}(\bar{\boldsymbol{y}}) < \boldsymbol{0}$ for some $\bar{\boldsymbol{y}}$ (where the inequalities $\le$ and $<$ are meant componentwise), and let $g(\boldsymbol{x},\cdot)$ be concave and continuously differentiable for each $\boldsymbol{x}$. Then, the bilevel reformulation (Stein and Still, 2002)

$$BL_{SIP}: \quad \min_{\boldsymbol{x},\boldsymbol{y}} f(\boldsymbol{x}) \quad \text{s.t.} \quad g(\boldsymbol{x},\boldsymbol{y}) \le 0, \ \boldsymbol{y} \text{ is an optimal point of } LLP(\boldsymbol{x})$$

of SIP can be reformulated by means of the lower-level Karush-Kuhn-Tucker conditions as

$$\begin{aligned} MPCC_{SIP}: \quad \min_{\boldsymbol{x},\boldsymbol{y},\boldsymbol{\gamma}} f(\boldsymbol{x}) \quad \text{s.t.} \quad & g(\boldsymbol{x},\boldsymbol{y}) \le 0, \\ & \nabla_{\boldsymbol{y}} g(\boldsymbol{x},\boldsymbol{y}) - \nabla \boldsymbol{v}(\boldsymbol{y})\boldsymbol{\gamma} = \boldsymbol{0}, \\ & \boldsymbol{0} \le \boldsymbol{\gamma} \perp -\boldsymbol{v}(\boldsymbol{y}) \ge \boldsymbol{0}, \end{aligned}$$

where the last is a complementarity constraint. This approach can easily be transferred to GSIPs and makes solutions methods for MPCCs (Luo et al., 1996) available for SIPs and GSIPs (Stein, 2003).

Example 4. *(Disjunctive optimization)* In disjunctive optimization, problem constraints may be coupled not only by conjunctions, but by general logical expressions containing conjunctions and disjunctions. For example, a logical expression consisting only of disjunctions between the constraints $G_j(\boldsymbol{x}) \le 0$, $j = 1, \dots, s$, leads to the disjunctive feasible set

$$M_{DP} = \bigcup_{j=1}^{s} \{\boldsymbol{x} \in \mathbb{R}^n | \, G_j(\boldsymbol{x}) \le 0\}.$$

On the other hand, for a one-dimensional lower-level variable y let $g(\boldsymbol{x},y) := y$ and $v_j(\boldsymbol{x},y) := y - G_j(\boldsymbol{x})$, $j = 1, \dots, s$. This yields the index set

$$Y(\boldsymbol{x}) = \{y \in \mathbb{R} | \ y \le G_j(\boldsymbol{x}), \ j = 1, \dots, s\} = (-\infty, \min_{j=1,\dots,s} G_j(\boldsymbol{x})],$$

the function

$$\overline{g}(\boldsymbol{x}) = \max_{y\in Y(\boldsymbol{x})} y = \min_{j=1,\dots,s} G_j(\boldsymbol{x})$$

and the feasible set

$$M_{GSIP} = \{\boldsymbol{x} \in \mathbb{R}^n | \ \overline{g}(\boldsymbol{x}) \le 0\} = \{\boldsymbol{x} \in \mathbb{R}^n | \min_{j=1,\dots,s} G_j(\boldsymbol{x}) \le 0\} = M_{DP}.$$

As the lower-level problem is a one-dimensional linear program, it particularly enjoys lower-level convexity.

In Kirst and Stein (2016), it is shown how also disjunctive programs with general logical expressions may be reformulated as GSIPs with convex lower-level problems, and how this connection helps to solve disjunctive programs with GSIP methods. We remark that it is also possible to incorporate disjunctive optimization ideas into GSIP solution techniques (Kirst and Stein, 2019).

Example 5. *(Equilibrium selection)* Consider an N-player Nash equilibrium problem where each player $\nu \in \{1,\dots,N\}$ seeks a globally minimal point of the problem

$$Q^{\nu}(\boldsymbol{x}^{-\nu}): \qquad \min_{\boldsymbol{x}^{\nu}} \theta_{\nu}(\boldsymbol{x}^{\nu},\boldsymbol{x}^{-\nu}) \quad \text{s.t.} \quad \boldsymbol{x}^{\nu} \in X^{\nu},$$

which depends on the vector $\boldsymbol{x}^{-\nu}$ of all other players' decision vectors via its objective function θ_{ν}. As opposed to this dependence, in a standard Nash equilibrium problem, the strategy sets X^{ν}, $\nu = 1,\dots,N$, are assumed to be independent of $\boldsymbol{x}^{-\nu}$. No cooperation between the players is assumed. Rather, a vector $\boldsymbol{x}^{\star} \in \mathbb{R}^n$ can be considered an equilibrium if for each ν its subvector $\boldsymbol{x}^{\star,\nu}$ is a globally minimal point of $Q(\boldsymbol{x}^{\star,-\nu})$. In this situation none of the players possesses a rational incentive to deviate from their respective optimal point $\boldsymbol{x}^{\star,\nu}$. We denote the (possibly empty) set of all such so-called Nash equilibria by E.

When E contains more than one element, equilibrium selection problems aim to explain why players prefer some equilibria over others. This can be modelled by a selection function $f : \mathbb{R}^n \to \mathbb{R}$ and the equilibrium selection problem

$$ESP: \qquad \min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{s.t.} \quad \boldsymbol{x} \in E.$$

Note that a Nash equilibrium problem differs from ESP in that it merely aims at finding a feasible point of ESP. The Nash equilibrium problem is called player-convex if each strategy set X^{ν} is convex and each function $\theta_{\nu}(\cdot,\boldsymbol{x}^{-\nu})$ is convex for given $\boldsymbol{x}^{-\nu}$. If the latter function is also continuously differentiable, then by the variational reformulation $\boldsymbol{x}^{\star,\nu} \in X^{\nu}$ is an optimal point of $Q(\boldsymbol{x}^{\star,-\nu})$ if and only if the variational inequality

$$\langle \nabla_{\boldsymbol{x}^{\nu}} \theta_{\nu}(\boldsymbol{x}^{\nu},\boldsymbol{x}^{-\nu}), \boldsymbol{z}^{\nu} - \boldsymbol{x}^{\nu} \rangle \geq 0 \text{ for all } \boldsymbol{z}^{\nu} \in X^{\nu}$$

holds. It is not hard to see that thus $\boldsymbol{x}^{\star} \in X := X^1 \times \dots \times X^N$ is a Nash equilibrium if and only if the aggregated variational inequality

$$\langle F(\boldsymbol{x}), \boldsymbol{z} - \boldsymbol{x} \rangle \geq 0 \text{ for all } \boldsymbol{z} \in X$$

with $F := (\nabla_{\boldsymbol{x}^1}\theta_1,\dots,\nabla_{\boldsymbol{x}^N}\theta_N)$ is satisfied. The set of Nash equilibria may hence be written as

$$E = \{x \in \mathbb{R}^n \mid \langle F(\boldsymbol{x}), \boldsymbol{z} - \boldsymbol{x} \rangle \geq 0 \text{ for all } \boldsymbol{z} \in X\},$$

and the equilibrium selection problem becomes the semi-infinite program

$$SIP_{ESP}: \qquad \min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{s.t.} \quad \langle F(\boldsymbol{x}), \boldsymbol{z} - \boldsymbol{x} \rangle \geq 0 \text{ for all } \boldsymbol{z} \in X$$

enjoying lower-level convexity. Note that in the situation of a generalized Nash equilibrium problem, where also the strategy sets $X^{\nu}(\boldsymbol{x}^{-\nu})$ are allowed to depend on the other players' decisions, the above reformulation of equlibrium selection yields a GSIP. For more details on such formulations we refer to Lampariello et al. (2020).

1.5. Article structure

This article is structured as follows. In Section 2 we survey recent algorithmic approaches to nonconvex semi-infinite optimization. Section 3 illustrates the suitability of these methods for a list of modern applications of semi-infinite optimization. We close the article with some final remarks in Section 4.

2. Methods

As mentioned previously, SIPs can be reformulated to MPCCs only under the assumption of lower-level convexity, in which case the KKT conditions are sufficient to enforce lower-level optimality. By the same token, it has been proposed to solve SIPs by solving a joint set of upper and lower-level KKT conditions via homotopy methods (Fan et al., 2018; Liu, 2007). In the general case of a nonconvex lower-level problem however, these approaches are not applicable. In the following, we survey solution approaches for SIPs with nonconvex lower-level problems. These approaches have in common that they establish feasibility of a point in a SIP by globally solving the lower-level problem, either explicitly or implicitly.

2.1. Discretization methods

The basic principle of discretization methods is the derivation of approximations of SIP by replacing the index set Y by a finite subset $Y_k \subsetneq Y$. Using this *discretization* instead of the original index set, gives rise to a relaxation of the feasible set M:

$$M_{LBP}(Y_k) = \{\boldsymbol{x} \in \mathbb{R}^n \mid g(\boldsymbol{x},\boldsymbol{y}) \leq 0 \text{ for all } \boldsymbol{y} \in Y_k\} \supseteq M.$$

The set $M_{LBP}(Y_k)$ is given in terms of finitely many constraints and gives rise to a finite relaxation of SIP, which we term a lower bounding problem,

$$LBP(Y_k): \qquad \min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{s.t.} \quad \boldsymbol{x} \in M_{LBP}(Y_k).$$

Based on this lower bounding problem, one can construct a conceptual discretization method by considering a predetermined sequence $\{Y_k\}$ of successively finer discretizations

$$Y_k \subsetneq Y_{k+1} \subsetneq Y \text{ for all } k.$$

Then, the conceptual discretization method consists of solving $LBP(Y_k)$ for the predefined sequence of discretizations in order to obtain a sequence of approximate solutions of SIP. López and Still (2007) show that under the assumptions of continuous functions and compactness of Y, this sequence of approximate solutions approaches a solution of SIP, if the Hausdorff distance between Y_k and Y vanishes for $k \to \infty$.

While the conceptual discretization method is theoretically sound, it has the drawback that it generally requires many iterations and large $|Y_k|$ in order to yield a level of accuracy that is sufficient in practice. This in turn may render the solution of $LBP(Y_k)$ intractable for large k. Accordingly, recent advances in discretization methods build on an adaptive discretization method that usually requires smaller discretizations. Initially proposed by Blankenship and Falk (1976), based on Remez (1962) the adaptive discretization method prescribes the following steps.

1. Choose an initial discretization $Y_0 \subsetneq Y$ and let $k = 0$.
2. Solve $LBP(Y_k)$ and obtain a solution $\boldsymbol{x}_k$.
3. Solve $LLP(\boldsymbol{x}_k)$ and obtain a solution $\boldsymbol{y}_k$.
4. If $g(\boldsymbol{x}_k,\boldsymbol{y}_k) \leq 0$, return $\boldsymbol{x}_k$ (feasible optimal solution).
5. Let $Y_{k+1} = Y_k \cup \{\boldsymbol{y}_k\}$ and go to step 2 with $k \leftarrow k+1$.

From one iteration to the next, the discretization is refined with the points $\boldsymbol{y}_k$ that cause the largest violation of the semi-infinite constraint for a given iterate $\boldsymbol{x}_k$. By this approach, the lower bounding problem is tightened successively to more accurately approximate SIP. Notably, for adaptive discretization to be successful, it must be ensured that the points $\boldsymbol{y}_k$ are global solutions of the lower-level problem.

Blankenship and Falk (1976) show that for continuous functions and compact host sets, the sequence $\{\boldsymbol{x}_k\}$ of iterates approaches a solution of SIP in the limit. Furthermore, in the case of an infeasible SIP, the lower bounding problem becomes infeasible in finitely many iterations, proving the infeasibility of SIP, see e.g., (Mitsos and Tsoukalas, 2015). The major drawback of the adaptive discretization method is the fact that the generation of points feasible in SIP can only be guaranteed in the limit. Accordingly, a practical implementation of the method must allow for a positive feasibility tolerance with respect to the semi-infinite constraints. Recent advances building on this method have focused on remedying this point in particular while also weakening the underlying assumptions and extending the method to more general problems such as GSIPs (Still, 1999; 2001).

We mention that Step 5 of the above adaptive discretization scheme may be modified by additionally allowing to drop points from Y_k when the new set Y_{k+1} is formed. Such exchange methods were suggested in, e.g., Hettich and Kortanek (1993) and Goberna and López (1998) for linear SIPs, and they also received some attention for the solution of convex SIPs (Zhang et al., 2010). However, since we are not aware of successful dropping rules in the nonconvex case, the present review does not further comment on this topic.

2.1.1. Feasible point adaptations

Mitsos (2011) proposes to address the problem of finding feasible points by introducing an upper bounding problem

$$UBP(Y_k,\varepsilon^g): \qquad \min_{x} f(x) \quad \text{s.t.} \quad x \in M_{UBP}(Y_k,\varepsilon^g),$$

wherein $M_{UBP}(Y_k,\varepsilon^g)$ is obtained by restricting the right-hand side of a set of discretized constraints by $\varepsilon^g > 0$.

$$M_{UBP}(Y_k,\varepsilon^g) \ = \ \{x \in \mathbb{R}^n |\ g(x,y) \le -\varepsilon^g \text{ for all } y \in Y_k\}$$

Notably, for arbitrary $Y_k \subsetneq Y$ and $\varepsilon^g > 0$, $M_{UBP}(Y_k,\varepsilon^g)$ is generally neither a superset nor a subset of Y. Accordingly, $UBP(Y_k,\varepsilon^g)$ is generally neither a relaxation nor a restriction of SIP. However, through population of Y_k and reduction of ε^g, $UBP(Y_k,\varepsilon^g)$ can be restricted and relaxed, respectively. Under the assumption that there exists a point that satisfies a Slater condition with respect to the semi-infinite constraint, $UBP(Y_k,\varepsilon^g)$ can be used to construct an upper bounding procedure that yields a feasible point in finitely many steps. Furthermore, if such a Slater point is also ε-optimal in SIP, the upper bounding procedure produces an ε-optimal solution in finitely many steps. Together with the convergent lower bounds produced by the basic adaptive discretization method, Mitsos (2011) proposes an algorithm that is guaranteed to terminate finitely with an ε-optimal solution.

Tsoukalas and Rustem (2011) build on the adaptive discretization method by proposing an algorithm centered around the oracle problem

$$ORA(Y_k,f_{ORA}): \qquad \min_{x\in\mathbb{R}} \max\{f(x) - f_{ORA}, \max\{g(x,y) \mid y \in Y_k\}\},$$

where f_{ORA} is a target objective value. Given a discretization $Y_k \subsetneq Y$ and some $f_{ORA} \in \mathbb{R}$, the optimal objective value of $ORA(Y_k,f_{ORA})$ indicates whether f_{ORA} is attainable by SIP. Indeed, if the optimal objective value is positive, f_{ORA} is unattainable for SIP and therefore a lower bound. If on the other hand, the optimal objective value is nonpositive, the obtained solution point x_k can be checked for feasibility by solving $LLP(x_k)$. As in the original adaptive discretization method, this either yields a proof of feasibility (and an upper bound) or a point that is added to the discretization. Tsoukalas and Rustem (2011) propose an algorithm that chooses f_{ORA} according to bisection on the objective space and successively solves the oracle problem and the lower-level problem to solve SIP. Given initial guesses for the lower and upper bounds and under appropriate assumptions, the algorithm is guaranteed to terminate finitely with an ε-optimal solution. As pointed out by Mitsos and Tsoukalas (2015), the assumptions made are slightly stronger than the ones made in Mitsos (2011).

Djelassi and Mitsos (2017) compare the two aforementioned algorithms and identify a strong relation between $UBP(Y_k,\varepsilon^g)$ and $ORA(Y_k,f_{ORA})$. Indeed, while $UBP(Y_k,\varepsilon^g)$ is subject to a set of restricted constraints, the objective of $ORA(Y_k,f_{ORA})$ is to maximize such a restriction balanced with the minimization of $f(x)$. Djelassi and Mitsos (2017) thus propose an algorithm that exploits this relation by using a slight adaptation of $ORA(Y_k,f_{ORA})$ in order to generate updates for the restriction parameter ε^g. The algorithm inherits the guarantees for convergence and finite termination from Mitsos (2011) while improving upon both of its predecessors in terms of performance on a standard SIP test set (Watson, 1983).

In addition to guaranteeing feasible points finitely, Mitsos (2011) and Djelassi and Mitsos (2017) slightly weaken the requirements for the solution of subproblems, particularly the LLP. Indeed, while Blankenship and Falk (1976) assume the exact global solution of the LLP, (Mitsos, 2011) only assumes that the solution accuracy is sufficient to conclusively determine feasibility of a given iterate. Similarly Djelassi and Mitsos (2017) assume that subproblems can be solved to an arbitrary absolute optimality tolerance, which is set as needed according to a refinement scheme. However, Harwood et al. (2019) point out that in both cases, the proofs of convergence fail to consider a case where these assumptions are insufficient. In order to remedy this issue, they propose a relative optimality tolerance for the solution of the lower-level problem. Djelassi (2020) points out that a similar result can be achieved by using absolute tolerance and using a more aggressive version of the tolerance refinement scheme from Djelassi and Mitsos (2017).

Beyond guarantees for the generation of feasible solutions, the methods discussed previously may also provide superior performance to the original adaptive discretization method in practice. Indeed, due to the provision of convergent upper bounds, the feasible point adaptations may terminate earlier based on ε-optimality than the original method terminates based on ε-feasibility. However, this is not due to an improvement of the underlying discretization-based approximation of SIP. In the following section, we discuss an approach of such an improvement based on the ideas from reduction methods.

2.1.2. Reduction-based adaptation

Pure reduction methods rest on assumptions under which for a given $x \in X$, the set of global solutions to $LLP(x)$ is finite. Given this property and additional smoothness assumptions, the feasible set of SIP can be approximated in a neighborhood of x by only considering these finitely many solutions to $LLP(x)$ and their sensitivity with respect to x. Then, one can devise a conceptual reduction method that successively performs local optimization steps of the approximation and updates the approximation by solutions of $LLP(x)$ (López and Still, 2007). Note however, that this method calls for finding all global optimizers in $LLP(x)$ repeatedly, which renders it intractable for the general case of SIPs with nonconvex lower-level problems.

Nevertheless, from the perspective of discretization methods, the reduction-based approximation has the advantage that it considers the sensitivity of the global optimizers of $LLP(x)$. Indeed, the discretization points added according to the adaptive discretization method can be understood as zeroth-order approximations of lower-level optimizers. Seidel and Küfer (2020) highlight this relation and propose to include sensitivity information about the discretization points in the discretization-based approximation. They show that their newly proposed discretization scheme provides a quadratic rate of convergence to a stationary point of SIP where the original adaptive discretization scheme only converges linearly. Djelassi (2020) points out that this inclusion of sensitivities in the lower bounding problem $LBP(Y_k)$ generally entails a loss of its bounding properties. As a consequence, the inclusion of sensitivities cannot be applied directly to the bounding algorithms discussed in the previous section. In order to remedy this problem, Djelassi (2020) proposes an alternative formulation of the discretization-based subproblems that preserves their bounding properties. However, due to the involvement of nonsmooth functions in this formulation, it is doubtful whether the same quadratic rate of convergence as in Seidel and Küfer (2020) can be obtained here.

2.1.3. Generalizations & specializations

Beyond the solution of SIPs, the adaptive discretization method has been applied to other problem classes that are closely related to SIPs. Indeed, only shortly after the original publication of the method by Blankenship and Falk (1976), Falk and Hoffman (1977) proposed a specialization to min-max programs of the following form.

$$MMP: \qquad \min_{x\in X} \max_{y\in Y} f(x,y)$$

As shown previously for the Chebyshev approximation problem in Example 1, this min-max program can be recast in its epigraphical formulation as the SIP

$$SIP_{MMP}: \qquad \min_{x\in X,\eta\in\mathbb{R}} \eta \quad \text{s.t.} \quad \eta \geq f(\boldsymbol{x},\boldsymbol{y}) \text{ for all } \boldsymbol{y}\in Y.$$

Falk and Hoffman (1977) proposed to solve this SIP using the adaptive discretization method. Notably and unlike the general SIP case, the problem of generating feasible points finitely does not arise here. Indeed, any feasibility gap due to the semi-infinite constraint in SIP_{MMP} translates to an optimality gap in MMP. By the same token, given any $\boldsymbol{x}\in X$, the solution of the lower-level problem of MMP provides a value for η such that $(\boldsymbol{x},\eta)$ is feasible in SIP_{MMP}.

More recent advances in this area focus on the solution of generalizations of SIPs rather than specializations. As such, the oracle approach proposed by Tsoukalas and Rustem (2011) for the solution of SIPs was initially proposed by Tsoukalas et al. (2009) for the solution of GSIPs, bilevel programs and min-max programs with coupling constraints. In contrast to the SIP variant, the original publication prescribes the solution of subproblems by stochastic methods and does not provide a proof of convergence. The method proposed by Mitsos (2011) is extended to GSIPs in Mitsos and Tsoukalas (2015). Furthermore, the methods in Mitsos (2011) and Djelassi and Mitsos (2017) are extended to existence-constrained SIPs, which possess three rather than two levels in Djelassi and Mitsos (2021).

Both Tsoukalas et al. (2009) and Mitsos and Tsoukalas (2015) pay particular attention to a concern that generally arises when discretization methods are applied to GSIPs. In the SIP case, it is trivial to obtain a subproblem that only considers a subset of the index set since the index set is independent of the upper-level variables. In the GSIP case however, the index set depends on the upper-level variables and the construction of discretization-based subproblems must take account of this fact. Then, the derivation of valid subproblems usually involves logical constraints that are only imposed when the underlying discretization point is lower-level feasible. Tsoukalas et al. (2009) and Mitsos and Tsoukalas (2015) employ such constraints and recast them as nonsmooth constraints. Furthermore, in order to ensure convergence of the discretization-based approximations, both approaches ensure that each new discretization point satisfies a Slater condition with respect to the coupling lower-level constraints. Since such a Slater condition can only be satisfied by inequality constraints, these approaches do not permit the presence of coupling lower-level equality constraints. However, under a uniqueness assumption for the solution of such coupling equality constraints, convergence of discretization methods can be recovered (Djelassi et al., 2019; Stuber and Barton, 2015).

2.2. Overestimation methods

In this section we discuss methods that overestimate the optimal objective value of the LLP. Underlying all these methods is the observation that this overestimation entails a restriction of the SIP. Indeed, letting $\hat{g}:\mathbb{R}^n\to\mathbb{R}$ overestimate $\bar{g}$ on $\mathbb{R}^n$, it holds that

$$g(\boldsymbol{x},\boldsymbol{y}) \leq \bar{g}(\boldsymbol{x}) \leq \hat{g}(\boldsymbol{x}) \text{ for all } \boldsymbol{y}\in Y,\ \boldsymbol{x}\in\mathbb{R}^n.$$

Accordingly, the overestimation problem

$$OE: \qquad \min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{s.t.} \quad \hat{g}(\boldsymbol{x}) \leq 0$$

is a restriction of SIP and any solution of OE is also feasible in SIP. Furthermore, there are several overestimation approaches for which OE is either finite or can be reformulated as a finite problem.

Overestimation methods for the solution of SIPs employ such finite problems in order to generate feasible points in SIP. Furthermore, the methods usually prescribe a refinement of the overestimation such that it can be shown that a sequence of iterates converges to a solution of SIP. The refinement usually involves some kind of tessellation or branching of the lower-level variable space. In the following, we separate overestimation methods into two groups according to the kind of overestimation they employ (interval or relaxation-based).

2.2.1. Interval methods

Bhattacharjee et al. (2005a,b) proposed the first deterministic algorithm for the global optimization of SIPs. As is typical in deterministic global optimization, they perform a branch-and-bound in the upper-level variables. In each node, they construct both lower and upper bounds. For the lower bound, they use a discretization method. The key novelty is that they propose to overestimate the lower-level objective function using natural interval extensions, which yields a restriction of the SIP. The restriction is a finite smooth nonconvex NLP. Any feasible point of this NLP is also a feasible point of the SIP and thus provides an upper bound to the optimal objective value. Following standard practice in deterministic global optimization, Bhattacharjee et al. (2005b) solve this nonconvex restriction using local NLP solvers. They prove finite convergence of their algorithm to an approximate optimal solution of the SIP. The key assumption is the existence of SIP Slater points. Note that also (Bianco and Piazzi, 2001) use interval extensions for the LLP in a genetic algorithm for the solution of SIPs.

Marendet et al. (2020) propose a branch-and-bound algorithm for the solution of SIPs with box-constrained LLPs. They build on an existing interval-based global optimization solver and extend its capabilities for the treatment of semi-infinite constraints. In particular, they perform branching on the upper-level variables while maintaining for each node of the branch-and-bound tree a tessellation that provides a superset of the lower-level optimal solutions for the given node. Then, upper and lower bounds on the optimal lower-level objective are obtained via natural interval extensions applied over the tessellation. Convergence of these bounds and in turn convergence of the branch-and-bound scheme are achieved by successively refining the tessellations. Beyond this extension of the branch-and-bound scheme, Marendet et al. (2020) also propose the use of constraint programming techniques in order to tighten the bounds on the lower-level optimal objective.

2.2.2. Relaxation methods

Unlike the interval methods from Bhattacharjee et al. (2005a,b), the adaptive convexification method from Floudas and Stein (2007) and Stein and Steuermann (2012) is a local method for the upper-level problem which guarantees semi-infinite feasibility by global optimization ideas for the lower-level problem. As an upper-level local method it generally needs lower numerical effort than methods which aim both at lower-level and upper-level global optimality. The main idea of adaptive convexification is to tessellate the index set Y into finitely many smaller sets and to convexify the resulting subproblems. Ideas of spatial branching are used to refine the tessellation.

In the special case of a scalar index set Y the tessellation is formed by closed subintervals. For any such subinterval Y' a seperate lower-level problem $LLP'(\boldsymbol{x})$ is considered, in which $g(\boldsymbol{x},\cdot)$ is maximized over Y'. Since Y' is convex, a possible nonconvexity of $LLP'(\boldsymbol{x})$ can only be due to the nonconcavity of $g(\boldsymbol{x},\cdot)$ on Y'. Floudas and Stein (2007) then suggest to overestimate $g(\boldsymbol{x},\cdot)$ on Y' by a concave function $\hat{g}(\boldsymbol{x},\cdot)$ which is constructed by techniques of the αBB method from Adjiman et al. (1998a,b). If no additional information is available, the αBB method generates a concave overestimator by adding an appropriately scaled quadratic relaxation function to the original function $g(\boldsymbol{x},\cdot)$, where the size of the scaling factor is determined by interval arithmetic.

The concavity of the overestimators entails that all lower-level problems of the approximating SIP are convex, so that it may be solved via the MPCC reformulation from Example 3. In fact, the implementation from Floudas and Stein (2007) computes a stationary point $\bar{x}$ of the MPCC and terminates if it is also stationary for the original SIP within given tolerances. Otherwise the algorithm refines the tessellation in the spirit of a discretization method by splitting the current subintervals at the active indices of $\bar{x}$.

While Floudas and Stein (2007) focus on the discussed case of a scalar index set, Stein and Steuermann (2012) generalize this approach to higher dimensional index sets which, in addition, are not necessarily box-shaped. The resulting algorithm is shown to be well-defined, convergent and finitely terminating.

Another approach to improve on the interval-based methods from Bhattacharjee et al. (2005a,b) is the approach of Mitsos et al. (2008b). The aim therein is the global solution of SIPs in the absence of any convexity assumptions. Recall that a restriction of the LLP leads to a relaxation of the SIP, and a relaxation of the LLP to a restriction of the SIP. Mitsos et al. (2008b) used these properties to respectively construct lower and upper bounds to the optimal objective value of the SIP. The relaxation of the LLP is performed via convex relaxations of the lower-level objective function. This results in general to nonconvex optimization problems. As the relaxations of the LLP are tighter than the interval-based method in Bhattacharjee et al. (2005a,b), the upper bound to the SIP is potentially also tighter. Mitsos et al. (2008b) discuss alternative methods to construct the relaxations, along with advantages and disadvantages. For the lower bounding problem, a combination of discretization and lower-level necessary optimality conditions are proposed.

2.3. Other methods

Some recently proposed methods cannot be neatly categorized as dicretization or overestimation methods.

Indeed, Okuno and Fukushima (2020) propose a sequential quadratic programming approach for SIPs that uses an exchange method to solve its semi-infinite quadratic suproblems. Therein, an exchange method is essentially a discretization method that selectively drops discretization points. In general, it is difficult to obtain sensible dropping rules for SIPs with nonconvex lower-level problems. Okuno and Fukushima (2020) circumvent this issue by applying the exchange method to subproblems with linearized semi-infinite constraints.

Lv et al. (2019) consider SIP in terms of the lower-level optimal value function, which generally yields a nonconvex nonsmooth problem. They propose an infeasible bundle method in order to solve this nonsmooth problem (and the underlying SIP) to local optimality. Similar to discretization methods, the bundle method maintains and successively refines an approximation of the lower-level optimal value function. However since the bundle method directly approximates the lower-level optimal value function, it requires evaluations of its subgradient in addition to the global solution of the lower-level problem.

2.4. Related methods in bilevel programming

Due to the close relation of SIPs and bilevel programs, we also mention that the basic concepts of the methods discussed here are also applicable in bilevel programming absent convexity assumptions. As such, the adaptive discretization method is used to solve bilevel programs in Mitsos et al. (2008a), Mitsos (2010), Tsoukalas et al. (2009), Wiesemann et al. (2013) and Djelassi et al. (2019). Similarly, a relaxation-based branch-and-bound method for the solution of bilevel programs is proposed in Kleniati and Adjiman (2014a, 2014b, 2015).

3. Applications

Over the last decades, several interesting applications of SIP have been proposed and solved. Some applications however still remain intractable.

3.1. Chebyshev approximation

While the Chebyshev approximation problem from Example 1 can be solved for scalar index sets by the Remez algorithm (Remez, 1962), Floudas and Stein (2007) illustrate the benefits of the adaptive convexification method from Section 2.2.2 for this problem class. Although their method can generally be only expected to solve the upper-level problem locally, the special structure of polynomial Chebyshev approximation allows to provide not only upper bounds for the minimal value of SIP_{CA} via the generated feasible points, but the splitting points of the generated index set tessellations can also be used to form upper-level LP relaxations. In the numerical example from Floudas and Stein (2007) the resulting lower bounds on the minimal value provide a certificate that the terminal feasible point of the adaptive convexification method is 10^{-3}-optimal. We also remark that the applicability of the Remez algorithm is restricted to scalar index sets, while the modern SIP solution methods from Section 2 allow the treatment of higher dimensional index sets.

3.2. Design centering

Design centering problems consist in maximizing some measure $f(\boldsymbol{x})$, for example the volume, of a parametrized body $Y(\boldsymbol{x})$ while it is inscribed into a container set $G(\boldsymbol{x})$,

$$\max_{\boldsymbol{x}} \ f(\boldsymbol{x}) \quad \text{s.t.} \quad Y(\boldsymbol{x}) \subseteq G(\boldsymbol{x}).$$

They have been studied extensively, see for example (Gritzmann and Klee, 1994; Horst and Tuy, 1996; Nguyen and Strodiot, 1992; Polak, 1982; Stein, 2006), and they are also related to the so-called set containment problem from Mangasarian (2002).

In applications, the set $G(\boldsymbol{x})$ often is independent of $\boldsymbol{x}$ and has a complicated structure, while $Y(\boldsymbol{x})$ possesses a simpler geometry. For example, in the robot maneuverability problem, Graettinger and Krogh (1988) determine lower bounds for the volume of a complicated container set G by inscribing an ellipsoid $Y(\boldsymbol{x})$ into G.

The design centering problem of cutting a gem of maximal volume with prescribed shape features from a raw gem is treated in Nguyen and Strodiot (1992) and, with the bilevel algorithm for semi-infinite optimization from Stein and Still (2003) in Winterfeld (2008).

The connection with semi-infinite optimization becomes apparent when the container set is described by a functional constraint as $G(\boldsymbol{x}) = \{\boldsymbol{y} \in \mathbb{R}^m |\ g(\boldsymbol{x}, \boldsymbol{y}) \le 0\}$. Then, the inclusion constraint $Y(\boldsymbol{x}) \subseteq G(\boldsymbol{x})$ is equivalent to the GSIP constraint

$$g(\boldsymbol{x}, \boldsymbol{y}) \le 0 \text{ for all } \boldsymbol{y} \in Y(\boldsymbol{x}),$$

so that the design centering problem becomes a GSIP. A standard SIP appears if the body Y is independent of $\boldsymbol{x}$, while the container $G(\boldsymbol{x})$ is allowed to vary with $\boldsymbol{x}$. Many design centering problems can actually be reformulated as standard SIPs, if the $\boldsymbol{x}$-dependent transformations of $Y(\boldsymbol{x})$ consist of, for example, translation, rotation, and scaling, whose inverse transformations can as well be imposed on the container set.

Examples for the solution of nonconvex design centering problems by the adaptive convexification method from Section 2.2.2 are provided by Floudas and Stein (2007) and Stein and Steuermann (2012).

3.3. Kinetic model reduction

Model reduction is in general very important for engineering when the full model results in intractable problems, in particular for online applications. A plethora of methods exist for model reduction. Among them we want to concentrate on optimization-based error-control methods.

In particular, consider reactive flows, involving thousands of species and reactions. A prime application for such models is the fundamental understanding and optimization of internal-combustion engines for the simultaneous increase of efficiency and mitigation of exhaust pollutants. Such applications require spatially-distributed dynamic models. This results in systems of partial differential equations in four independent variables, namely time and the three spatial coordinates. In addition to mass balance (continuity equation), and energy/momentum balance, for each species a species mass balance needs to be resolved. The number of partial differential equations is approximately equal to the number of species. Species balances contain production terms due to the chemical reactions. As a result, the number of reactions determines the coupling of the differential equations and the stiffness. Computational fluid dynamics with fully resolved chemistry is typically intractable. One approach is to introduce so-called adaptive chemistry, Schwer et al. (2003) and Green et al. (2001), wherein for different parts of the spatial domain different kinetic mechanisms are used.

One way to generate the reduced kinetic mechanisms, is to formulate an optimization problem (Bhattacharjee et al., 2003) with the objective function of minimizing the number of reactions or alternatively minimizing the weighted reactions and species (Mitsos et al., 2008c). A key idea is that the methods impose the validity of the kinetic mechanism for a finite number of points in the space of thermodynamic states (temperature, pressure and concentration of each species). The validity is given by comparing the production rates of the full model to that of the reduced model and allowing for a maximum difference. Under suitable formulation, this results in mixed-integer linear programs which are tractable with state-of-the-art solvers. However, the finite number of points in thermodynamic space does not guarantee validity of the developed models for a range of thermodynamic states. Imposing the validity for the range results in a design centering problem which can be formulated as $GSIP$ or SIP along the lines sketched in Section 3.2. For details, the reader is referred to Bhattacharjee (2003) and Oluwole et al. (2007, 2006).

Recall that semi-infinite programming is historically motivated by Chebyshev approximation, cf. López and Still (2007). As such, the occurrence of a semi-infinite program in this model reduction should not be surprising. In an abstract sense, the full model can be seen as the function to be approximated and the reduced model as the approximating function.

3.4. Robust optimization and flexibility analysis

Starting with Ben-Tal and Nemirovski (1999), a large part of the literature on robust optimization (Example 2) studies assumptions on the problems at hand, under which the robust counterpart RO is algorithmically "tractable". These assumptions usually involve upper-level as well as lower-level convexity, or are even stronger. For more recent developments in robust optimization we refer to the monograph (Ben-Tal et al., 2009).

Recently, one can observe a trend towards convex nonlinear robust problems (Mutapcic and Boyd, 2009) and even nonconvex robust optimization (Bertsimas et al., 2009). In the general case and as shown in Example 2, robust optimization formulations correspond to SIP. Accordingly, existing results from semi-infinite optimization literature can be used and in fact should be considered.

As an extension of the robust optimization framework, Ben-Tal et al. (2004) propose adjustable robust optimization. Therein and similar to two-stage stochastic programming, the decision variables are separated into "here and now" decisions and "wait and see" decisions. While the former have to be taken in anticipation of the worst case regarding uncertainty, the latter may be taken in response to the realization of uncertainty. When considering the semi-infinite formulation of such problems, the addition of the "wait and see" decisions results in an existence-constrained SIP.

Recent applications of adjustable robust optimization include investment problems (Takeda et al., 2007) and network expansion problems (Ordóñez and Zhao, 2007). Solution approaches to these problems often rely on convexity assumptions that enable the reformulation of the problem as a single-level problem. However, as pointed out previously, the general nonconvex case of existence-constrained SIPs is approachable, at least in theory, via discretization methods.

While robust optimization is a recognized field in the operations research community, similar concepts have been developed independently in the process systems engineering community under the name of flexibility analysis (Zhang et al., 2016). Indeed, the flexible design problem proposed in Grossmann and Sargent (1978) and Halemane and Grossmann (1983) amounts to an adjustable robust optimization problem for the design of chemical plants. Further contributions extend the framework of flexibility analysis by proposing auxiliary problems to measure the degree of flexibility of a given design (Grossmann et al., 1983; Swaney and Grossmann, 1985a; 1985b). As in robust optimization, flexibility analysis problems can be cast as SIPs or existence-constrained SIPs. Furthermore, flexibility analysis problems are commonly solved under monotonicity or convexity assumptions, which permit the reformulation of the problems as single-level problems.

The present review and most literature contributions consider models without dynamics. Dealing with uncertainty has also been a long-lasting goal in the (process) control community. Therein, dynamics are essential, and thus models are differential equation systems, or even differential-algebraic equation systems. For such applications, the reader is referred to Puschke et al. (2017), Puschke et al. (2018) and Puschke and Mitsos (2018) and the references therein. Note also that SIP methods have been applied to rigorously handle path constraints in dynamic systems (Chen and Vassiliadis, 2005; Fu et al., 2015); however this does not pertain to uncertainty. Solving the subproblems in these dynamic systems is extremely challenging and currently globally only tractable for small systems.

3.5. Thermodynamics

Another application of SIP and bilevel optimization is the parameter estimation in mixture thermodynamics, which are prevalent in chemical engineering. We will here focus on so-called excess Gibbs free energy models, which describe the deviation of a mixture from ideal behavior. For details the reader is referred to Bollas et al. (2009), Mitsos et al. (2009) and Glass et al. (2018a). Mathematically, the excess Gibbs free energy G_e is given as a function of temperature T, pressure P, composition $\boldsymbol{z}$ and some adjustable parameters $\boldsymbol{q}$. Typically, the composition vector $\boldsymbol{z}$ consists of molefractions; by the closure condition one species is not included. The latter are typically determined from equilibrium measurements, i.e., cases where there are more than one phases indexed by k, each with composition $\boldsymbol{z}^k$. As such, the corresponding model in the parameter estimation must predict stable equilibria.

Stable equilibrium at constant temperature T and pressure P corresponds to the global minimization of Gibbs free energy over the possible compositions $\boldsymbol{z}^k$. A necessary but not sufficient criterion for stability are the so-called isopotential equations: the chemical potential of each species is the same across each phase. Mathematically, these correspond to first-order optimality conditions of the minimization of Gibbs free energy. Specialized necessary and sufficient criteria for stability exist based on tangent-plane (Baker et al., 1982) and duality (Mitsos and Barton, 2007). Simply said, these reformulate the optimality definition to a semi-infinite constraint with the advantage of reducing the dimensionality. For instance in the case of a binary mixture with three phases, six variables and three constraints would be used in the minimization, while a single variable is used for the specialized criteria.

Most parameter estimation tools use the necessary-only criteria resulting in nonlinear programs of the form

$$\min_{\boldsymbol{q},\boldsymbol{z}^k} LS\left(\boldsymbol{z}^k\right) \quad \text{s.t.} \quad \boldsymbol{v}\left(\boldsymbol{z}^k, \boldsymbol{q}\right) = \boldsymbol{0},$$

where LS is the objective function, typically least-square errors. These nonconvex problems are typically solved with local methods resulting in suboptimal fits. More gravely, by imposing the necessary-only stability criteria, the compositions $\boldsymbol{z}^k$ are not guaranteed to be stable equilibria. This essentially means that the excess Gibbs free energy models are applied in a wrong way inside the parameter estimation. If they are then applied correctly in process simulation, very different predictions will be found.

Another approach is to solve the parameter estimation problem in a nested approach

$$\min_{\boldsymbol{q}} LS\left(\hat{z^k}(\boldsymbol{q})\right)$$

where $\widehat{z^k}$ is calculated by a thermodynamic package for a given value of $\boldsymbol{q}$. Ideally, the same thermodynamic package is used that will then be used also in process simulation. If the thermodynamic package is rigorous, stability of the predictions is guaranteed. This corresponds to a nonsmooth solution method of the bilevel formulation (Dempe, 2017). This approach is in essence used in the standard tool DPP (Westhaus and Sass, 2004). As the problem is nonsmooth, either a derivative-free method or a nonsmooth method needs to be used. In practice, one can also heuristically apply a derivative-based method.

The third approach, proposed by Bollas et al. (2009), Mitsos et al. (2009) and Glass et al. (2018a) and implemented in Glass et al. (2018b) is to consider the specialized stability criterion and solve the resulting SIP. For the case of binary mixture and two phases described by the corresponding compositions z^1, z^2 the optimization problem is roughly given by

$$\min_{\boldsymbol{q},z^1,z^2} LS(z^1, z^2) \quad \text{s.t.} \quad \boldsymbol{v}(z^1, z^2, \boldsymbol{q}) = \boldsymbol{0} \wedge g(\boldsymbol{q}, y) \leq 0, \text{ for all } y \in [0, 1]$$

It should be noted that the problems have no SIP Slater points. They can be solved approximately with the aforementioned discretization-based algorithms. With a suitable a-priori discretization in the order of 5–10 points, a quite small number of iterations is needed, typically less than 5. Thus, the main challenge is to solve the subproblems. For a moderate number of measurement points they are tractable with standard solvers. For large numbers of parameters, they are quite expensive and still an open challenge.

4. Conclusions and future challenges

The present paper gives a review of current methods and applications for SIPs with nonconvex lower-level problems. While we identify multiple directions of research in this area, we note that all discussed methods solve the lower-level problem to global optimality, either explicitly or implicitly. Accordingly, we emphasize that the discussed methods are expected to run in acceptable time only if the lower-level dimension is moderate, say up to between four and ten, depending on the problem structure. The design of methods which are able to handle larger lower-level dimensions is a basic algorithmic challenge in semi-infinite optimization. Similarly a large number of upper-level variables can be challenging.

For the development of such methods, a few benchmark problems exist as well as some comparison of algorithms. It may be helpful to organize this in a more systematic framework. Similarly, some open-source and commercial SIP solvers are available, but a larger variety is desirable.

While this paper focuses on smooth and continuous nonconvex lower-level problems, in practice semi-infinite constraints also appear in more general settings, like with nonsmooth defining functions and/or with mixed-integer variables. Some of the aforementioned methods do not make assumptions on differentiability of the functions involved and are also applicable to the mixed-integer case. However, these methods rely on the global solution of subproblems which is challenging in the nonsmooth/mixed-integer case. So overall it is fair to say that the development of theory and methods for SIPs with nonsmoothness/integer variables is still in its infancy.

As a final remark, semi-infinite constraints can as well appear in the formulation of instances of other problem classes such as multi-objective programming, bilevel programming and Nash equilibrium problems. The combination of the methods from the present survey with approaches for these problem classes is a challenging subject of future research. Similarly, an opportunity exists for the robust optimization community to use classic and recent theory, algorithms and solvers from SIP.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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