Discrete Monotonic Global Optimization

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1 Introduction

Throughout this paper, for any two vectors $x, y \in \mathbb{R}^n$ we write $x \leq y$ (x < y, resp.) to mean $x_i \leq y_i$ ($x_i < y_i$, resp.) for every i = 1, ..., n. If $a \leq b$ then the box [a, b] ((a, b], resp.) is the set of all $x \in \mathbb{R}^n$ satisfying $a \leq x \leq b$ ($a < x \leq b$, resp.). A function $f : [a, b] \to \mathbb{R}$ is said to be *increasing* if

$$a \le x \le y \le b \quad \Rightarrow \quad f(x) \le f(y).$$

Recently a general mathematical framework has been developed [3] for studying mathematical programming problems described by means of increasing functions, or more generally, differences of increasing functions. It has been shown in [3] that any mathematical programming problem of this class can be reduced to an equivalent problem of the following form, called *canonical monotonic optimization problem*:

$$\max\{f(x)| \ g(x) \le 0 \le h(x)\} \tag{CM/A}$$

where f(x), g(x), h(x) are given increasing functions on \mathbb{R}^n_+ . An easily implementable algorithm called the *Polyblock Algorithm* has been proposed for solving (CM/A). Applications of this approach to certain classes of difficult nonconvex global optimization problems have proved its efficiency ([1], [5], [6], [7]), especially when these problems, originally of large scale, can be converted into problems (CM/A) in lowdimensional space by a suitable change of variables.

If a problem involves discrete constraints, e.g. boolean constraints like $x_i \in \{0,1\}, i = 1, ..., m$, then these constraints can be written as $\sum_{i=1}^{m} x_i(1-x_i) \leq 0, 0 \leq x_i \leq 1 \ (i = 1, ..., m)$, i.e. $\sum_{i=1}^{m} x_i - \sum_{i=1}^{m} x_i^2 \leq 0, 0 \leq x_i \leq 1 \ (i = 1, ..., m)$ where the functions $\sum_{i=1}^{m} x_i, \sum_{i=1}^{m} x_i^2$ are increasing on \mathbb{R}^n_+ . Therefore, a mathematical programming problem with discrete constraints can in principle be reformulated as a monotonic optimization problem and studied by methods of monotonic optimization. However, this approach is generally not practical; moreover, its drawback is that, since the basic algorithms for continuous monotonic optimization are iterative procedures, by this approach only an approximate optimal solution can be computed in finitely many steps.

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The aim of the present paper is to suggest an alternative, more efficient approach to monotonic optimization problems with additional discrete constraints. Specifically, given a finite set S of points in the box $[a,b] = \{x \in \mathbb{R}^n_+ | a \leq x \leq b\}$ with a < b, and given increasing functions f(x), g(x), h(x) on [a,b], we will be concerned with the following general optimization problem.

$$\max\{f(x) | g(x) \le 0 \le h(x), \ x \in S\}$$

which will be referred to as the Canonical Discrete Monotonic Optimization Problem (DM/A). Setting $G = \{x \in [a,b] | g(x) \leq 0\}, H = \{x \in [a,b] | h(x) \geq 0\}$, we can rewrite it as

$$\max\{f(x) \mid x \in G \cap H \cap S\}$$
(DM/A)

In the sequel we propose to extend the basic algorithm for (continuous) monotonic optimization in [3] to obtain a *finite* algorithm for solving (DM/A). Thus, by suitable modifications of the basic algorithm for the continuous case, it will be possible to obtain an exact optimal solution of(DM/A) in finitely many steps. Furthermore, it is worth noticing that for many continuous monotonic optimization problems, although the optimum is known à priori to be achieved on a certain finite set S, an exact optimal solution cannot be obtained in finitely many steps by the basic iterative algorithms of the continuous approach. The discrete version to be proposed will help in many cases to turn this infinite procedure into a finite one, thus allowing the exact optimum in these continuous problems to be found, too, in finitely many steps.

In Sections 2 and 3, we discuss some pertinent geometric concepts, and also some basic properties of the problem. For the sake of completeness and for the convenience of the reader, all the proofs will be provided, although most of them are simple and can be found in [2] or [3], and also in [4]. In Sections 4 and 5 we present the extended polyblock algorithm for solving(DM/A) and discuss some implementation issues. Finally in Section 6, as illustration we apply the proposed approach to a discrete maximin location problem.

2 Some Geometric Concepts

A set $G \subset [a, b]$ is said to be normal if $a \leq x' \leq x$, $x \in G \Rightarrow x' \in G$. A set $H \subset [a, b]$ is conormal (reverse normal) if $a \leq x' \leq x$, $x \notin H \Rightarrow x' \notin H$. Thus the set $G = \{x \in [a, b] | g(x) \leq 0\}$ defined above (with an increasing function g(x)) is normal, whereas the set $H = \{x \in [a, b] | h(x) \geq 0\}$ (with an increasing function h(x)) is conormal.

Given a set $A \subset [a, b]$ the normal hull of A, written A^{\downarrow} , is the smallest normal set containing A. The conormal hull of A, written $\lfloor A$, is the smallest conormal set containing A.

Proposition 1 (i) The normal hull of a set $A \subset [a,b] \subset \mathbb{R}^n_+$ is the set $A^{\uparrow} = \bigcup_{z \in A} [a,z]$. If A is compact then so is A^{\uparrow} .

(ii) The conormal hull of a set $A \subset [a, b] \subset \mathbb{R}^n_+$ is the set $\lfloor A = \bigcup_{z \in A} [z, b]$. If A is compact then so is $\lfloor A$.

Proof It suffices to prove (i), because the proof of (ii) is similar. Let $P = \bigcup_{z \in A} [a, z]$. Clearly P is normal and $P \supset A$, hence $P \supset A^{\uparrow}$. Conversely, if $x \in P$ then $x \in [a, z]$ for some $z \in A \subset A^{\uparrow}$, hence $x \in A^{\uparrow}$ by normality of A^{\uparrow} , so that $P \subset A^{\uparrow}$ and therefore, $P = A^{\uparrow}$. If A is compact then A is contained in a ball B centered at 0, and if $x^k \in A^{\uparrow}, k = 1, 2, \ldots$, then since $x^k \in [a, z^k] \subset B$, there exists a subsequence $\{k_{\nu}\} \subset \{1, 2, \ldots\}$ such that $z^{k_{\nu}} \to z^0 \in A, \ x^{k_{\nu}} \to x^0 \in [a, z^0]$, hence $x^0 \in A^{\uparrow}$, proving the compactness of A^{\uparrow} . \Box

A polyblock P is the normal hull of a finite set $T \subset [a, b]$ called its vertex set. By Proposition 1, $P = \bigcup_{z \in T} [a, z]$. A vertex z of a polyblock is called proper if there is no vertex $z' \neq z$ "dominating" z, i.e. such that $z' \geq z$. An improper vertex or improper element of T is an element of T which is not a proper vertex. Oviously, a polyblock is fully determined by its proper vertex set; more precisely, a polyblock is the normal hull of its proper vertices.

Similarly, a copolyblock (reverse polyblock) Q is the conormal hull of a finite set $T \subset [a, b]$ called its vertex set. By Proposition 1, $Q = \bigcup_{z \in T} [z, b]$. A vertex z of a copolyblock is called *proper* if there is no vertex $z' \neq z$ "dominated" by z, i.e. such that $z' \leq z$. An *improper* vertex or improper element of T is an element of T which is not a proper vertex. Oviously, a copolyblock is fully determined by its proper vertex set; more precisely, a copolyblock is the conormal hull of its proper vertices.

Proposition 2 (i) The intersection of finitely many polyblocks is a polyblock.

(ii) The intersection of finitely many copolyblocks is a copolyblock.

Proof If T_1, T_2 are the vertex sets of two polybocks P_1, P_2 , respectively, then $P_1 \cap P_2 = (\bigcup_{z \in T_1} [a, z]) \cap (\bigcup_{y \in T_2} [a, y] = \bigcup_{z \in T_1, y \in T_2} [a, z] \cap [a, y] = \bigcup_{z \in T_1, y \in T_2} z \land y$ where $u = z \land y$ means $u_i = \min\{z_i, y_i\} \forall i = 1, \ldots, n$. Similarly, if T_1, T_2 are the vertex sets of two copolyblocks Q_1, Q_2 , respectively, then $Q_1 \cap Q_2 = \bigcup_{z \in T_1, y \in T_2} [z, b] \cap [y, b] = \bigcup_{z \in T_1, y \in T_2} z \lor y$ where $v = z \lor y$ means $v_i = \max\{z_i, y_i\} \forall i = 1, \ldots, n$. \Box

Proposition 3 (i) The maximum of an increasing function f(x) over a polyblock is achieved at a proper vertex of this polyblock.

(ii) The minimum of an increasing function f(x) over a copolyblock is achieved at a proper vertex of this copolyblock.

Proof We prove (i). Let \bar{x} be a maximizer of f(x) over a polyblock P. Since a polyblock is the normal hull of its proper vertices, there exists a proper vertex z of P such that $\bar{x} \in [a, z]$. Then $f(z) \geq f(\bar{x})$ because $z \geq \bar{x}$, so z must be also an optimal solution. \Box

Lemma 1 (i) If a < x < b, then the set $[a, b] \setminus (x, b]$ is a polyblock with vertices

$$u^{i} = b + (x - b)e^{i}, \quad i = 1, \dots, n.$$
 (1)

(ii) If a < x < b, then the set $[a, b] \setminus [a, x)$ is a copolyblock with vertices

$$v^{i} = a + (x_{i} - a_{i})e^{i}, \quad i = 1, \dots, n_{i}$$

Proof We prove (i). Let $K_i = \{z \in [a, b] | x_i < z_i\}$. Since $(x, b] = \bigcap_{i=1,\dots,n} K_i$, we have $[a, b] \setminus (x, b] = \bigcup_{i=1,\dots,m} ([a, b] \setminus K_i)$, proving the Lemma because $[a, b] \setminus K_i = \{z \mid a_i \leq z_i \leq x_i, a_j \leq z_j \leq b_j \ \forall j \neq i\} = [a, u^i]$. \Box

Note that u^1, \ldots, u^n are the *n* vertices of the hyperrectangle [x, b] that are adjacent to *b*, while v^1, \ldots, v^n are the *n* vertices of the hyperrectangle [a, x] that are adjacent to *a*.

For any two z, y define $J(z, y) = \{j | z_j > y_j\}.$

Proposition 4 (i) Let P be a polyblock with proper vertex set $T \subset [a, b]$, let $x \in [a, b]$, be such that $T_* := \{z \in T \mid z \ge x\} \neq \emptyset$. For every $z \in T_*$ and every $i = 1, \ldots, n$ define $z^i = z + (x_i - z_i)e^i$. Then the vertex set of the polyblock $P \setminus (x, b]$ is

$$T' = (T \setminus T_*) \cup \{z^i | z \in T_*, z_i > x_i, i \in \{1, \dots, n\}\},$$
(2)

where the improper elements are those z^i such that $J(z, y) = \{i\}$ for some $y \in T_*$.

(ii) Let Q be a copolyblock with proper vertex set $T \subset [a, b]$, let $x \in [a, b]$, be such that $T_* := \{z \in T \mid z \leq x\} \neq \emptyset$. For every $z \in T_*$ and every $i = 1, \ldots, n$ define $z^i = z + (x_i - z_i)e^i$. Then the vertex set of the copolyblock $Q \setminus [a, x)$ is

$$T' = (T \setminus T_*) \cup \{z^i | z \in T_*, z_i < x_i, i \in \{1, \dots, n\}\},$$
(2*)

where the improper elements are those z^i such that $J(y, z) = \{i\}$ for some $y \in T_*$.

Proof We prove (i). Since $[a, z] \cap (x, b] = \emptyset$ for every $z \in T \setminus T_*$, it follows that $P \setminus (x, b] = P_1 \cup P_2$, where P_1 is the polyblock with vertex $T \setminus T_*$ and $P_2 = (\bigcup_{z \in T_*} [a, z]) \setminus (x, b] = \bigcup_{z \in T_*} ([a, z] \setminus (x, b])$. Noting that $[a, b] \setminus (x, b]$ is a polyblock with vertices given by (1), we can then write $[a, z] \setminus (x, b] = [a, z] \cap ([a, b] \setminus (x, b]) = [a, z] \cap (\bigcup_{i=1,\dots,n} u^i) = \bigcup_{i=1,\dots,n} [a, z] \cap [a, u^i] = \bigcup_{i=1,\dots,n} [a, z \wedge u^i]$, hence $P_2 = \bigcup \{[a, z \wedge u^i] \mid z \in T_*, i = 1, \dots, n\}$, which shows that the vertex set of $P \setminus (x, b]$ is the set T' given by (2).

It remains to show that every $y \in T \setminus T_*$ is proper, while a z^i with $z \in T_*$ is improper if and only if $J(z, y) = \{i\}$ for some $y \in T_*$.

Since every $y \in T \setminus T_*$ is proper in T, if $z' \ge y$ for some $z' \in T'$, then z' must be some z^i with $z \in T_*$, $i \in \{1, \ldots, n\}$. But then $z \ge z \wedge u^i = z^i \ge y$, conflicting with y being proper in T. Therefore, every $y \in T \setminus T_*$ is proper. On the other hand, if $z^i \le y$ for some $y \in T \setminus T_*$ then $x_i = z_i^i \le y_i$, while $x_j \le z_j = z_j^i \le y_j \ \forall j \ne i$, hence $x \le y$, i.e. $y \in T_*$, conflicting with $y \notin T_*$. Consequently, if z^i is improper then $z^i \le y^l$ for some $(y, l) \ne (z, i), y \in T_*$, $i, l \in \{1, \ldots, n\}$. We cannot have $y = z, l \ne i$ for then the relation $z^i \le z^l$ would imply $z_l = z_l^i \le z_l^l = x_l$, conflicting with (2). So $y \ne z$ and $z_j^i \le y_j^l \ \forall j = 1, \ldots, n$. Remembering that

$$z_j^i = \begin{cases} x_i \le z_i & \text{for } j = i \\ z_j & \text{for } j \neq i \end{cases} \quad y_j^l = \begin{cases} x_l \le y_l & \text{for } j = l \\ y_j & \text{for } j \neq l \end{cases}$$

we then infer $l \neq i$. In fact if l = i, then $z_j \leq y_j \forall j \neq i$, hence, since $z \not\leq y$ (z being proper), $z_i > y_i \geq x_i$, contradicting (2). Thus, $y \neq z$ and $l \neq i$. Since $z_j^i \leq y_j^l \forall j = 1, \ldots, n$, we must then have $z_j \leq y_j \forall j \notin \{i, l\}$, while for $j = l : z_l^i \leq y_l^l$, i.e. $z_l \leq x_l \leq y_l$. Hence, $z_j \leq y_j \forall j \neq i$, and again since $z \not\leq y$, we derive $z_i > y_i$ and $J(z, y) = \{i\}$. Thus any improper z^i must satisfy $J(z, y) = \{i\}$ for some $y \in T_*$. Conversely, if $J(z, y) = \{i\}$ for some $y \in T_*$ then $z_j \leq y_j \ \forall j \neq i$, hence $z^i \leq y^i$, i.e. z^i is improper. This completes the proof of the Proposition. \Box

Remark 1 When T_* is a singleton, T' is exactly the proper vertex set of $P \setminus (x, b]$.

3 Basic properties

In this section we discuss some properties of problem (DM/A) relevant to optimization. Similar properties can be established for problem (DM/B), consisting of minimizing, instead of maximizing, f(x) over $G \cap H \cap Z$.

Observe that a basic property of convex sets that has been used in almost every study of convex optimization (though sometimes indirectly or in some equivalent form) is the separation theorem which states that a convex closed set can always be separated from a point outside by a halfspace containing that point but disjoint from the convex set.

We now prove a similar (but not quite the same) *separation property* for normal (conormal) closed sets.

Let $G \subset [a, b]$ be a normal closed set. For any $v \in [a, b]$ define $\pi_G(v)$ to be the last point of G on the halfline from a through v, i.e.

$$\pi_G(v) = a + \lambda(v - a), \text{ with } \lambda = \sup\{\alpha \ge 0 \mid a + \alpha(v - a) \in G\}.$$
 (3)

Clearly, if $v \in G$ then $\pi_G(v) = v$.

Proposition 5 If $v \in [a, b] \setminus G$ then $G \cap (\pi_G(v), b] = \emptyset$

Proof If there were $x \in G$ such that $x > \pi_G(v)$ then $[a, x] \subset G$ by normality of G, so that one would have $a + \alpha(v - a) \in G$ for some $\alpha > \lambda$, contradicting (3). \Box

This Proposition says essentially that a normal closed set can be separated from a point outside by a cone congruent to the orthant of the space (more precisely, a translate of this orthant).

On the basis of this property, a polyblock approximation method has been developed [3] for solving canonical monotonic optimization problems (CM/A). We now extend this method to the discrete optimization problem (DM/A). First observe the following.

Proposition 6 Let $\tilde{G} = (G \cap S)^{\uparrow}$. Problem (DM/A) is equivalent to

$$\max\{f(x)|\ x\in \tilde{G}\cap H\}\tag{4}$$

Proof Since the feasible set of (DM/A) is contained in the feasible set of (4), the optimal value of (DM/A) cannot exceed that of problem (4). Conversely, if \bar{x} solves (4) then $\bar{x} \in \tilde{G}$, and by Proposition 1 $\bar{x} \in G \cap S$, hence \bar{x} is feasible to (DM/A) and consequently, the optimal value of (4) cannot ecceed that of (DNO). Therefore, the two problems (DM/A) and (4) have the same optimal value. \Box

Solving problem (DM/A) is thus reduced to solving (4) which is a monotonic optimization problem without explicit discrete constraint. The difficulty, now, is how to handle the polyblock \tilde{G} which is defined only implicitly as the normal hull of $G \cap S$. In a sense the discrete condition has been incorporated in this normal hull.

It turns out, fortunately, that a separation property for $G = (G \cap S)^{\dagger}$ can be derived from the corresponding property of $G \cap S$. First, without loss of generality we can assume that

$$a_i = \min\{x_i \mid x \in S\} \quad i = 1, \dots, n \tag{5}$$

Now we introduce the operation $\lfloor \rfloor_S$ by defining for any $v \in (a, b]$:

$$\lfloor v \rfloor_S = \tilde{v}, \text{ with } \tilde{v}_i = \max_{y \in S} \{ y_i | y_i < v_i \} \quad (i = 1, \dots, n).$$
(6)

A frequently encountered special case is when $S = S_1 \times \cdots \times S_n$, and every S_i is a finite set of real numbers. In this case

$$\tilde{v}_i = \max\{\xi | \xi \in S_i, \xi < v_i\}, \quad i = 1, \dots, n,$$
(7)

so $\tilde{v} \in S$. (For example, if each S_i is the set of integers, then \tilde{v}_i is the largest integer still less than v_i).

Note that $\tilde{v} = \lfloor v \rfloor_S$ is uniquely defined for every $v \in (a, b]$. We shall refer to $\lfloor v \rfloor$ as the *S*-adjustment of v.

For our purpose the most useful property of S-adjustment is the following.

Proposition 7 If $[x, b] \cap (G \cap S) = \emptyset$ and $\tilde{v} = \lfloor x \rfloor_S$ then $(\tilde{v}, b] \cap G \cap S = \emptyset$.

Proof Suppose there is $y \in (\tilde{v}, b] \cap G \cap S$. Since $y \in (\tilde{v}, b]$ we have $y_i > \tilde{v}_i$ for every $i = 1, \ldots, n$. On the other hand, since $y \in G \cap S$ while $[x, b] \cap G \cap S = \emptyset$, there is at least one $i \in \{1, \ldots, n\}$ such that $y_i < x_i$. From the definition of \tilde{v} it then follows that $\tilde{v}_i \geq y_i$, a contradiction. \Box

Proposition 8 Let P be a polyblock containing $\tilde{G} \cap H$, let v be a proper vertex of P such that $v \in H \setminus \tilde{G}$. Define $x = \pi_G(v)$, and

$$\tilde{v} = \begin{cases} x & \text{if } x \in S \\ \lfloor x \rfloor_S & \text{if } x \notin S. \end{cases}$$
(8)

Then $(\tilde{v}, b] \cap \tilde{G} = \emptyset$, i.e. the cone $\{x \mid x \geq \tilde{v}\}$ separates v from \tilde{G} .

Proof If $x \in S$ so that $\tilde{v} = x$ then $(\tilde{v}, b] \cap G = \emptyset$ from the property of $x = \pi_G(v)$, hence $(\tilde{v}, b] \cap \tilde{G} = \emptyset$. If $x \notin S$, then, since $[x, b] \cap G \cap S = \emptyset$, it follows from Proposition 7 that $(\tilde{v}, b] \cap G \cap S = \emptyset$, i.e. $G \cap S \subset [a, b] \setminus (\tilde{v}, b]$, hence $\tilde{G} \subset [a, b] \setminus (\tilde{v}, b]$, and so $(\tilde{v}, b] \cap \tilde{G} = \emptyset$. \Box

In the next section we exploit this separation property to devise a polyblock approximation method for solving (DM/A).

4 The Discrete Polyblock Algorithm

Observe that if g(a) > 0 i.e. $a \notin G$ then, since g(x) is increasing, it follows that $g(x) > 0 \ \forall x \in [a, b]$ and the problem is infeasible. Similarly, if h(b) < 0, i.e. $b \notin H$ then $h(x) < 0 \ \forall x \in [a, b]$, and the problem is infeasible. Therefore, without loss of generality we can assume that

$$a \in G, \quad b \in H.$$
 (9)

Before proceeding to the solution of the problem it is useful to reduce the size of the rectangle [a, b] if possible. For this let

$$\begin{split} \beta_i &= \sup\{\beta > 0: \ a + \beta e^i \in G\}, \quad b' = a + \sum_{i=1}^n \beta_i e^i, \\ \alpha_i &= \sup\{\alpha > 0: \ b' - \alpha e^i \in H\}, \quad a' = b' - \sum_{i=1}^n \alpha_i e^i. \end{split}$$

Then clearly $G \cap H \subset [a', b']$. Further, by resetting $G \leftarrow G \cap [a', b'], H \leftarrow H \cap [a', b']$, we have a box [a, b] which is generally a tighter approximation of $G \cap H$ than the original one.

To solve (DM/A) we now construct a sequence of polyblocks, $P_0 \supset P_1 \supset \cdots$ together with a sequence of numbers $\gamma_0 \leq \gamma_1 \leq \cdots$, such that:

(i) $\gamma_k = f(\hat{x}^k)$, for some $\hat{x}^k \in G \cap H \cap S$, if $\gamma_k > -\infty$; (ii) $P_k \supset G \cap H \cap S_{\gamma_k}$ where $S_{\gamma_k} = \{x \in S \mid f(x) > \gamma_k\}$.

We start with an initial polyblock $P_0 \supset G \cap H \cap S$, e.g. $P_0 = [a, b]$, with vertex set $T_0 = \{b\}$, and $\gamma_0 = -\infty$. At iteration $k = 0, 1, \ldots$, let P_k be the current polyblock, T_k its vertex set, γ_k the current best value, and \hat{x}^k the current best solution, satisfying (i) and (ii). Reduce T_k using the following rules:

- Drop any improper $v \in T_k$;
- Drop any $v \in T_k \setminus H$;
- Drop any $v \in T_k$ such that $f(v) \leq \gamma_k$.

Let \tilde{T}_k be the set that remains from T_k after this pruning operation. Reset $T_k \leftarrow \tilde{T}_k$. If $T_k = \emptyset$ the procedure terminates: the current best feasible solution is optimal (if $\gamma_k > 0$), or the problem is infeasible (if $\gamma_k = -\infty$). If $T_k \neq \emptyset$ let P_k be the polyblock with vertex set T_k and select

$$v^k \in T_k$$

(e.g. $v^k \in \operatorname{argmax} \{f(x) | x \in T_k\}$. Two cases can be distinguished:

<u>Case 1</u>: $v^k \in G \cap S$. Since $v^k \in H$, then $v^k \in G \cap H \cap S_{\gamma_k}$ and v^k is a feasible solution of (DM/A) with objective function value no less than γ_k . We set $\hat{x}^{k+1} = v^k, \gamma_{k+1} = f(v^k)$, and define P_{k+1} as the polyblock with vertex set

 $T_{k+1} = T_k \setminus \{v^k\}$. Also in this case define $\tilde{v}^k = v^k$.

<u>Case 2</u>: $v^k \notin G \cap S$. Then we find $x^k = \pi_G(v^k)$, set $\tilde{v}^k = x^k$ if $x^k \in S_{\gamma_k}$, $\tilde{v}^k = \lfloor x^k \rfloor_{S_{\gamma_k}}$ if $x^k \notin S_{\gamma_k}$. Let $T_{k,*} = \{z \in T_k | z \ge \tilde{v}^k\}$, and compute

$$T_{k+1} = (T_k \setminus T_{k,*}) \cup \{z^{k,i} | z \in T_{k,*}, z_i > \tilde{v}_i^k, i = 1, \dots, n\}$$
(10)

where $z^{k,i} = z + (\tilde{v}_i^k - z_i)e^i$. Define P_{k+1} as the polyblock with vertex set T_{k+1} .

Furthermore, if a new feasible solution has appeared that has a better objective function value than γ_k , then let \hat{z}^{k+1} be the best among them, and set $\gamma_{k+1} =$ $f(\hat{z}^{k+1})$; otherwise, set $\hat{z}^{k+1} = \hat{z}^k, \gamma_{k+1} = \gamma_k$.

Proposition 9 Let $\gamma_k = f(\hat{x}^{k+1})$, where \hat{x}^{k+1} is the new current best feasible solution. The polyblock P_{k+1} still contains $G \cap H \cap S_{\gamma_k}$ and $P_{k+1} \subset P_k \setminus (\tilde{v}^k, b]$. (So conditions (i),(ii) still hold for $k \leftarrow k+1$.)

Proof This is obvious in case 1, because $f(x) \leq f(v^k) \ \forall x \leq v^k$ while $(v^k, b] \cap P_k = \emptyset$ $(v^k \text{ is a proper vertex of } P_k)$. In case 2, if $v^k \in G \setminus S$, then, since $P_k \supset G \cap H \cap S_{\gamma_k}$ whereas $[v^k, b] \cap P_k = \{v^k\}$ because v^k is a proper vertex of P_k , we must have $[v^k, b] \cap G \cap S_{\gamma_k} = \emptyset$ (note that $v^k \notin S$ and $[v^k, b] \subset H$ because $v^k \in H$). Therefore, by Proposition 7, $(\tilde{v}^k, b] \cap G \cap S_{\gamma_k} = \emptyset$, and consequently, $P_{k+1} \supset G \cap H \cap S_{\gamma_k} \supset$ $G \cap H \cap S_{\gamma_{k+1}}$. On the other hand, if $v^k \notin G$, then Proposition 8 implies that $(\tilde{v}^k, b] \cap G \cap S_{\gamma_k} = \emptyset$, and again $P_{k+1} \supset G \cap H \cap S_{\gamma_k} \supset G \cap H \cap S_{\gamma_{k+1}}$. That $P_{k+1} \subset P_k \setminus (\tilde{v}^k, b]$ follows from Proposition 4.

Thus, P_{k+1} and γ_{k+1} will still satisfy (i), (ii) (for $k \leftarrow k+1$). We can then go to iteration k+1.

In a formal way we can state

Algorithm 1. (Discrete Polyblock Algorithm)

Initialization. Take an initial polyblock $P_0 \supset G \cap H$, with proper vertex set T_0 . Let \hat{x}^0 be the best feasible solution available (the current best feasible solution), $\gamma_0 = f(\hat{x}^0)$. If no feasible solution is available, let $\gamma_0 = -\infty$. Set k = 0.

Step 1. From T_k remove: all $z \in T_k \setminus H$ and all $z \in T_k$ such that $f(z) \leq \gamma_k$. Let T_k be the resulting set. Reset $T_k \leftarrow T_k$.

Step 2. If $T_k = \emptyset$, terminate: if $\gamma_k = -\infty$, the problem is infeasible; if $\gamma_k > \infty$ $-\infty$, \hat{x}^k is an optimal solution.

Step 3. If $T_k \neq \emptyset$, select $v^k \in T_k$.

If $v^k \in G \cap S$ define $T_{k+1} = T_k \setminus \{v^k\}, \ \hat{x}^{k+1} = v^k, \ \gamma_{k+1} = f(\hat{x}^{k+1})$, increment k and return to Step 1.

Step 4. If $v^k \in G \setminus S$, compute $\tilde{v}^k = \lfloor v^k \rfloor_{S_{\gamma_k}}$ (using formula (6) for $S \leftarrow S_{\gamma_k}$). If $v^k \notin G$ compute $x^k = \pi_G(v^k)$ and define $\tilde{v}^k = x^k$ if $x^k \in S_{\gamma_k}$, $\tilde{v}^k = \lfloor x^k \rfloor_{S_{\gamma_k}}$ if $x^k \notin S_{\gamma_k}$.

Step 5. Let $T_{k,*} = \{z \in T_k | z \ge \tilde{v}^k\}$. Compute

$$T'_{k} = (T_{k} \setminus T_{k,*}) \cup \{ z^{k,i} | \ z \in T_{k,*}, z_{i} > \tilde{v}_{i}^{k}, i = 1, \dots, n \}$$
(11)

where $z^{k,i} = z + (\tilde{v}_i^k - z_i)e^i$. Let T_{k+1} be the set obtained from T'_k by removing every z^i such that $\{j \mid z_j > y_j\} = \{i\}$ for some $y \in T_{k,*}$. Step 6. Determine the new current best feasible solution \hat{x}^{k+1} and $\gamma_{k+1} = f(\hat{x}^{k+1})$. Increment k and return to Step 1.

Theorem 1 Algorithm 1 is finite.

Proof For every i = 1, ..., n the set $X_i = \{\xi \in \mathbb{R} : \xi = x_i, x \in S\}$ is finite, hence the set $X = \prod_{i=1}^n X_i$ is also finite. At each iteration k a point $y^k \in X \cap P_k$ is generated (namely $y^k = v^k$ in Step 3 and $y^k = \tilde{v}^k$ in Step 4) such that the rectangle $(y^k, b]$ contains no point of P_l with l > k, hence no y^l with l > k. Therefore, there can be no repetition in the sequence $\{y^0, y^1, \ldots, y^k, \ldots\} \subset X$. The finiteness of Xthen implies that of the algorithm. \Box

Remark 2 If in Step 3 we always select

$$v^{k} \in \operatorname{argmax}\{f(v) \mid v \in T_{k}\} \subset \operatorname{argmax}\{f(x) \mid x \in P_{k}\}$$
(12)

then the value $f(v^k)$ gives an upper bound of the optimal value of (DM/A), so if it so happens that $v^k \in G \cap Z$ then v^k is an optimal solution of (DM/A).

Remark 3 A similar discrete copolyblock algorithm can be developed for discrete monotonic minimization problem (DM/B): $\min\{f(x) \mid x \in G \cap H \cap S\}$. The roles of G and H will then be interchanged, the operation $x = \pi_G(v)$ will be replaced by $x = \rho_H(v)$ (the last point of H on the halfline from v through b), and the operation $\lfloor v \rfloor$ by

$$[v] = \tilde{v}, \text{ with } \tilde{v}_i = \min\{y_i \mid y \in S, y_i > v_i\}.$$

5 Alternative Branch and Bound Algorithm

Algorithm 1 can be interpreted as a branh and bound algorithm in which a node z of the branch and bound tree represents a box $[\bar{a}, z]$ and branching is performed by splitting a node into n descendants while the bound over a node z is taken to be f(z). A positive feature of this algorithm is that the bound computation is straightforward. However, since each node has n descendants, storage problems may arise with the growth of the number of iterations. Therefore, for large scale problems an alternative rectangular branch and bound algorithm in a more conventional format such as the following one may be more efficient.

The initial rectangle of the branch and bound tree is [a, b]. Branching is performed by rectangular subdivision and for each generated subrectangle $M = [p, q] \subset [a, b]$ an upper bound $\mu(M)$ and a lower bound $\nu(M)$ are computed for $\max\{f(x) : x \in G \cap H \cap S \cap M\}$ by applying a number of iterations of Algorithm 1 for the latter problem. **BRANCHING.** Let M = [p, q] be a candidate for subdivision, such that $p, q \in X$, where $X = \prod_{i=1}^{n} X_i$ denotes the set defined in the proof of Theorem 1. Compute $\delta(M) = \max_{i=1,\dots,n} (q_i - p_i) = q_{i_M} - p_{i_M}$ and divide M into two boxes

$$M_{+} = \{ x \in M | x_{i_{M}} \ge p_{i_{M}} + \lfloor \delta(M)/2 \rfloor_{X_{i}} \}, M_{-} = \{ x \in M | x_{i_{M}} \le p_{i_{M}} + \lfloor \delta(M)/2 \rfloor_{X_{i}} \}$$

where $\lfloor \delta/2 \rfloor_{X_i}$ denotes the largest element of X_i still not exceeding $\delta/2$. Clearly, if $r_{i_M} = p_{i_M} + \lfloor \delta(M)/2 \rfloor_{X_i}$ then $M_- = [p, q - r_{i_M} e^{i_M}], M_+ = [p + r_{i_M} e^{i_M}, q]$ with $q - r_{i_M} e^{i_M} \in X, p + r_{i_M} e^{i_M} \in X.$

For the initial box [a, b] if for every i = 1, ..., n we let $\hat{a}_i = \min_{x \in S \cap M} x_i$, $\dot{b}_i = \max_{x \in S \cap M} x_i$, and set $[a, b] \leftarrow [\hat{a}, \hat{b}]$ then $a, b \in X$ and every subbox $M = [p, q] \subset [a, b]$ generated by the above subdivision rule will satisfy $p, q \in X$.

BOUNDING. Given a partition set M = [p, q], compute $\mu(M)$ such that

$$\mu(M) \ge \gamma(M) := \max\{f(x) : x \in G \cap H \cap S \cap M\}.$$

Let CBS denote the current best solution, i.e. the best <u>feasible</u> solution to problem (DM/A) known thus far, and CBV the current best value, i.e. the objective function value at CBS.

First observe that if $p \notin G$ (g(p) > 0) or $q \notin H$ (h(q) < 0) then $\mu(M) = -\infty$ (because *M* contains no feasible point); if $q \in G \cap H$ then $\mu(M) = f(q)$. If none of these cases occurs, reduce the box *M* by computing

$$\beta_i = \sup\{\beta > 0 \mid p + \beta e^i \in G \cap S, \ p_i + \beta \le q_i\}, \quad q' = p + \sum_{i=1}^n \beta_i e^i$$
(13)
$$\alpha_i = \sup\{\alpha > 0 \mid q' - \alpha e^i \in H \cap S, \ p_i \le q'_i - \alpha\}, \quad p' = q' - \sum_{i=1}^n \alpha_i e^i.$$
(14)

and setting $[p,q] \leftarrow [p',q']$. Then compute $\mu(M)$ using either of the following mehods.

Method I

Step 0. Let L = (user supplied) maximal number of iterations to be executed. Set $v^1 = q, T_1 = \{v^1\}$. Set l = 1 (iteration counter for the bounding subroutine).

Step 1. Compute x^l = intersection of the surface g(x) = 0 with the segment joining p and v^l (this can be done because $g(p) \le 0$, g(q) > 0), then compute $\tilde{v}^l = \lfloor v^l \rfloor_S$. Let $T_{l,*} = \{z \in T_l | z \ge \tilde{v}^l\}$ and compute

$$T'_{l} = (T_{l} \setminus T_{l,*}) \cup \{z^{i} | z \in T_{l,*}, z_{i} > \tilde{v}^{l}_{i}, i = 1, \dots, n\}$$

where $z^i = z + (\tilde{v}_i^l - z_i)e^i$. If \tilde{v}^l is feasible to (DM/A), use it to update CBS and CBV.

Step 2. Let T_{l+1} be the set that remains from T'_l after removing all $z \notin H$, all z such that $f(z) \leq \text{CBV}$ and all improper elements. If $T_{l+1} = \emptyset$, set $\mu(M) = \text{CBV}$. Otherwise, compute

$$v^{l+1} \in \operatorname{argmax} \{ f(z) \mid z \in T_{l+1} \}$$

If l = L, set $\mu(M) = f(z^{l+1})$, $v(M) = v^{l+1}$, $x(M) = x^{l+1}$. Otherwise, set $l \leftarrow l+1$ and return to Step 1.

Method II

Consider a grid $U = \{c^0, c^1, \dots, c^n\} \subset \{x \in \mathbb{R}^n_+ | \sum_{i=1}^n x_i = 1\}$. For example, let U consist of the following points

$$c^{0} = e/n$$
 (barycentre of unit simplex)
 $c^{k} = \frac{(n+1)e - ne^{k}}{n^{2}}$ $k = 1, \dots, n$
 $(c^{k} \text{ is barycentre of simplex spanned by } c^{0}, e^{i}, i \neq k).$

For each k = 0, 1, ..., n, let $x^k = \pi(c^k) := p + \lambda_k c^k$, with $\lambda_k = \sup\{\alpha \mid p + \alpha c^k \in G\}$. Construct a set T by proceeding as follows:

Step 0. Let $T = \{u^1, ..., u^n\}$ with $u^i = q + (x_i^0 - q_i)e^i$ i = 1, ..., n. Set k = 1. Step k. Compute $x^k = \pi(c^k)$, let $T_* = \{z \in T | z \ge x^k\}$, and compute

$$T' = (T \setminus T_*) \cup \{z^i | z \in T_*, z_i > x_i^k, i = 1, \dots, n\}$$

where $z^i = z + (x_i^k - z_i)e^i$. From T' remove all z^i for which there exists $y \in T_*$ such that $\{j \mid z_j > y_j\} = \{i\}$. Reset T equal to the set of remaining elements of T'. If k < n, let $k \leftarrow k + 1$ and go back to Step k. If k = n, stop.

If T is the last set obtained by the above procedure then an upper bound is taken to be

$$\mu(M) = \max\{f(z) \mid z \in T\}$$

while a lower bound is given by

$$\nu(M) = \max\{f(x^k) | k = 0, 1, \dots, n\}$$

The more dense the grid U the tighter the upper bound is, but also the more costly the computation is. Therefore a reasonable trade-off should be resolved between the denseness of the grid and the quality of the bound.

Algorithm 2.(Branch and Bound Discrete Polyblock Algorithm)

Initialization. Start with $\mathcal{P}_1 = \mathcal{S}_1 = \{M_1 = [a, b]\}$ (supposed to have been reduced). Let $CBS = \bar{x}$ be the best feasible solution available, $CBV = f(\bar{x})$ (if no feasible solution is available, set $CBV = +\infty$). Set k = 1.

Step 1. For each box $M = [p,q] \in \mathcal{P}_k$ compute $\mu(M)$ (using Method I or II) and update CBS and CBV whenever possible.

Step 2. Delete every $M \in S_k$ such that $\mu(M) \leq \text{CBV}$. Let \mathcal{R}_k be the collection of remaining members of S_k . If $\mathcal{R}_k = \emptyset$, then terminate: $\bar{x} = \text{CBS}$ is an optimal

solution if $CBV < +\infty$, or the problem is infeasible otherwise.

Step 3. Select $M_k \in \mathcal{R}_k$. Choose $j_k \in \operatorname{argmax}_i \{q_i - p_i\}$ and divide M_k into two subboxes via the hyperplane $y_{j_k} = (p_{j_k}^k + q_{j_k}^k)/2$. Let \mathcal{P}_{k+1} be the partition of M_k . Step 4. Set $\mathcal{S}_{k+1} = (\mathcal{R}_k \setminus \{M_k\}) \cup \mathcal{P}_{k+1}$. Set $k \leftarrow k+1$ and go back to Step 1.

Proposition 10 Algorithm 2 terminates after finitely many iterations, yielding an optimal solution of (FP) or establishing that the problem is infeasible.

Proof The set X defined in the proof of Theorem 1 is finite. But, according to the subdivision rule when branching, every box M is of the form M = [p, q] with $p \in X, q \in X$. Therefore, the total number of nodes of the branch and bound tree is finite, which implies finiteness of the algorithm itself. \Box

6 Application: A discrete location problem

Consider the following discrete location (DL) problem:

Given *m* points $a^i \in \mathbb{R}^n$, (i = 1, ..., m) together with *m* positive numbers $\alpha_i (i = 1, ..., m)$, and a finite set $S \subset \mathbb{R}^n$, find an $x \in S$ such that $||x - a^i|| > \alpha_i$ for every i = 1, ..., m.

This problem is encountered in various applications. For example, if a^i , $i = 1, \ldots, m$, are the locations of m obnoxious facilities and $\alpha_i > 0$ is the radius of the polluted region of facility i then an optimal solution of the above problem is a location $x \in S$ outside all polluted regions.

To solve this problem we replace it by the following problem

maximize z subject to

$$||x - a^i|| \ge \alpha_i \quad i = 1, \dots, m$$
 (P)
 $x \in S \subset \mathbb{R}^n_+, \ z \in \mathbb{R}_+.$

Clearly if the optimal value of problem (P) is positive then any optimal solution \bar{x} of it solves (DL); otherwise, (DL) is infeasible.

Since $||x - a||^2 = ||x||^2 + ||a||^2 - 2\langle a, x \rangle$ problem (P) can be rewritten as

$$maximize \ z \quad \text{s.t.} \tag{15}$$

$$||x||^{2} + ||a^{i}||^{2} - (z + 2\langle a^{i}, x \rangle + \alpha_{i}) \ge 0 \quad i = 1, \dots, m$$
(16)

$$x \in S, \ z \in \mathbb{R}_+ \tag{17}$$

The set of constraints (16) can be transformed into a single constraint as follows

$$\|x\|^{2} + \|a^{i}\|^{2} - (z + 2\langle a^{i}, x \rangle + \alpha_{i}) \geq 0 \quad i = 1, ..., m$$

$$\Leftrightarrow \min_{i=1,...,m} \{\|x\|^{2} + \|a^{i}\|^{2} - (z + 2\langle a^{i}, x \rangle + \alpha_{i})\} \geq 0$$

$$\Leftrightarrow \|x\|^{2} - z - \max_{i=1,...,m} \{2\langle a^{i}, x \rangle + \alpha_{i} - \|a^{i}\|^{2}\}] \geq 0$$

$$\Leftrightarrow \|x\|^{2} - \varphi(x) \geq z$$
(18)

where

$$\varphi(x) = \max_{i=1,\dots,m} (2\langle a^i, x \rangle + \alpha_i - \|a^i\|^2)$$
(19)

Finally, problem (P), and hence, problem (DL), reduces to the following

$$\max\{\|x\|^2 - \varphi(x)\| \ x \in S\}$$
(20)

where $\varphi(x)$ is defined by (19). If (DL) is feasible, the optimal value of the latter problem is positive, and any optimal solution of it solves (DL).

Now without loss of generality we can assume that all a^i as well as the set S are contained in a box $[0,b] \subset \mathbb{R}^n_+$. Then both functions $||x||^2$ and $\varphi(x)$ are increasing, so that in particular, $0 \leq \varphi(b) - \varphi(x) \leq \varphi(b) - \varphi(0) \quad \forall x \in [0,b]$. Therefore, the problem (20) can be written as

$$\max\{\|x\|^2 + t - \varphi(b)\| t + \varphi(x) \le \varphi(b), \ x \in S, \ 0 \le x \le b, 0 \le t \le c_1\}$$

where $c_1 = \varphi(b) - \varphi(0)$. This is a discrete monotonic optimization problem and can be solved by the proposed algorithm. We refer the interested reader to [8], where some preliminary computational experience with the implementation of this mehod has been reported.

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