



Convergent Outer Approximation Algorithms for Solving Unary Programs

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Abstract. Interesting cutting plane approaches for solving certain difficult multiextremal global optimization problems can fail to converge. Examples include the concavity cut method for concave minimization and Ramana’s recent outer approximation method for unary programs which are linear programming problems with an additional constraint requiring that an affine mapping becomes unary. For the latter problem class, new convergent outer approximation algorithms are proposed which are based on sufficiently deep l_∞ -norm or quadratic cuts. Implementable versions construct optimal simplicial inner approximations of Euclidean balls and of intersections of Euclidean balls with halfspaces, which are of general interest in computational convexity. Computational behavior of the algorithms depends crucially on the matrices involved in the unary condition. Potential applications to the global minimization of indefinite quadratic functions subject to indefinite quadratic constraints are shown to be practical only for very small problem sizes.

Key words: Unary programs, Indefinite quadratic optimization under indefinite quadratic constraints, Outer approximation, Cutting plane methods

1. Introduction

Let

$$\mathcal{S}_n := \{S \in \mathbb{R}^{n \times n} : S \text{ symmetric}\}$$

and

$$\mathcal{U}_n := \{U \in \mathcal{S}_n : \exists v \in \mathbb{R}^n \text{ with } U = vv^T\}$$

denote the space of real symmetric $n \times n$ matrices and the set of *unary* $n \times n$ matrices, respectively.

Moreover, let $U : \mathbb{R}^d \rightarrow \mathcal{S}_n$ be an affine mapping defined by

$$U(z) = U^0 + \sum_{i=1}^d z_i U^i, \tag{1.1}$$

where $z = (z_1, \dots, z_d) \in \mathbb{R}^d$ and $U^i \in \mathcal{S}_n, i = 0, \dots, d$.

Given $U^i \in \mathcal{S}_n$, $i = 0, \dots, d$ and $h \in \mathbb{R}^d$, $A \in \mathbb{R}^{m \times d}$, $b \in \mathbb{R}^m$, we call the optimization problem

$$\begin{aligned} \min h^T z \\ \text{s.t. } Az \leq b \\ U(z) \in \mathcal{U}_n \end{aligned} \quad (1.2)$$

in $z \in \mathbb{R}^d$ a *unary program* (UP).

Throughout this article we will assume that the polyhedron defined by $Az \leq b$ is *bounded*, i.e. a polytope.

Our interest in problem (1.2) and the content of the present paper are motivated from interesting observations and algorithmic ideas proposed in the dissertation of Ramana (1993: ch. 7). Notice that Problem (1.2) can also be formulated as a semidefinite program with an additional rank constraint (for related discussion, see, e.g., Fujie and Kojima, 1995; Poljak et al., 1995; Ramana, 1993; Shor, 1987; Vandenberg and Boyd, 1996). A first interesting observation made in Ramana (1993) (without detailed proof) is that an arbitrary all-quadratic global optimization problem, which consists in minimizing an indefinite quadratic objective function subject to a finite number of indefinite quadratic constraints, can be transformed into an equivalent (UP) of the form (1.2). Such indefinite all-quadratic optimization problems arise from various important applications; for a survey we refer to Al-Khayyal et al. (1945). A second observation is based on eigenvalue inequalities due to Weyl: Given an optimal vertex solution \bar{z} of the LP-relaxation $\min\{h^T z : Az \leq b\}$ of (1.2) satisfying $U(\bar{z}) \notin \mathcal{U}_n$, and given the eigenvalues of $U(\bar{z})$, a linear constraint $\ell(z) \leq 0$ can be constructed satisfying $\ell(\bar{z}) > 0$ but $\ell(z) \leq 0 \forall z : U(z) \in \mathcal{U}_n$. Therefore, by successively adding such valid cuts $\ell(z) \leq 0$ to LP-relaxations of (1.2), one obtains an outer approximation (or cutting plane) algorithmic approach for solving (1.2), several variants of which are proposed in Ramana (1993). A serious deficiency of this algorithmic approach, however, consists in the fact that cuts can eventually become very shallow such that convergence of the sequence of outer approximation to an optimal solution of (1.2) cannot be guaranteed. A similar deficiency has been observed in other cutting plane methods for certain global optimization problems (cf. Horst and Tuy, 1996: ch. 3).

It is the purpose of the present paper to overcome the above deficiency by proposing alternative outer approximation algorithms for solving (1.2) which are convergent in the sense that every accumulation point of the sequence of outer approximations is an optimal solution of (1.2). Using the observation that in Problem (1.2) with (1.1) it suffices to consider matrices $U^i \in \mathcal{S}_n$, $i = 1, \dots, d$, which form an orthonormal system with respect to the inner product.

$$\cdot : \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times n} \rightarrow \mathbb{R} : \Leftrightarrow A \cdot B = \text{tr}(A^T B) = \sum_{i,j=1}^n A_{ij} B_{ij}, \quad (1.3)$$

where

$$A = (A_{ij})_{n \times n}, \quad B = (B_{ij})_{n \times n} \in \mathcal{S}_n,$$

we first derive valid l_∞ -norm and quadratic cuts. These are reverse convex constraints which, for each optimal solution \bar{z} of an LP-relaxation of (1.2) satisfying $U(\bar{z}) \notin \mathcal{U}_n$, cut a sufficiently large ball (with respect to the l_∞ -norm or to the Euclidean norm) centered at \bar{z} out of the polyhedron defined by relaxed constraints without affecting unarity in such a way that convergent outer approximation schemes result. In case of the l_∞ -norm, the balls can be built up by successive cutting planes. In case of the Euclidean norm, we propose an optimal inner approximation by regular simplices which leads to a convergent cutting plane algorithm. Suitable additional cuts can be derived in order to speed up convergence.

The paper is organized as follows. The next section demonstrates how indefinite all-quadratic optimization problems can be transformed into an equivalent unary program of the form (1.2), where the matrices corresponding to the matrices U^i in (1.1) form an orthonormal system with respect to the inner product (1.3). Section 3 puts together some preliminaries underlying the basic idea of the outer approximation approaches and discusses briefly Ramana's algorithm. In Section 4, the above mentioned quadratic cuts are derived along with convergence properties of corresponding outer approximation schemes. Section 5 presents a convergent cutting plane algorithm which uses the l_∞ -norm, and Section 6 discusses implementable algorithms for the case of Euclidean balls. The final Sections 7 and 8 contain some preliminary numerical results obtained with a number of randomly generated examples and a brief conclusion, respectively, which shows, in particular, that practical application to all-quadratic optimization problems is limited to very small problem sizes.

2. Unary programs and all-quadratic optimization problems

In this section, it is shown that an optimization problem with arbitrary quadratic objective function and p arbitrary quadratic inequalities in n variables is equivalent to an unary program in $\binom{n+1}{2} + n$ variables. By reasons which will become evident in Section 4, we choose a transformation which yields an unary program, where the matrices corresponding to the matrices U^i , $i = 1, \dots, d$, in (1.1) form an orthonormal system (ONS) with respect to the inner product (1.3). Consider the all-quadratic optimization problem (AQP)

$$\begin{aligned} \min x^T Q^0 x + (d^0)^T x \\ \text{s.t. } x^T Q^i x + (d^i)^T x + c^i \leq 0, \quad i = 1, \dots, p, \end{aligned} \quad (2.1)$$

where the Q^i are symmetric real $n \times n$ matrices, $d^i \in \mathbb{R}^n$, $i = 0, \dots, p$, and $c^i \in \mathbb{R}$, $i = 1, \dots, p$. Notice that the matrices Q^i can be negative semidefinite or indefinite, cases in which we are particularly interested in.

Let e_i denote the i -th unit vector in \mathbb{R}^{n+1} , and let $E_{ij} = e_i e_j^T$ be the elementary matrix with entry 1 at position (i, j) , entries 0 else. Consider the (UP)

$$\begin{aligned} & \min h^T z \\ & \text{s.t. } Az \leq b, \\ & U(z) \in \mathcal{U}_{n+1}, \quad z \in \mathbb{R}^{\binom{n+1}{2}+n} \end{aligned} \quad (2.2)$$

in the variable $z = (z_{11}, \dots, z_{1n}, z_{1,n+1}, z_{22}, \dots, z_{2,n+1}, \dots, z_{nn}, z_{n,n+1})^T$, where

$$\begin{aligned} h_{ij} &= \sqrt{2}Q_{ij}^0, \quad 1 \leq i < j \leq n; \quad h_{ii} = Q_{ii}^0, \quad h_{i,n+1} = \frac{1}{\sqrt{2}}d_i^0, \quad i = 1, \dots, n, \\ A_{\ell,ij} &= \sqrt{2}Q_{ij}^\ell, \quad 1 \leq i < j \leq n, \quad \ell = 1, \dots, p; \quad A_{\ell,ii} = Q_{ii}^\ell, \\ A_{\ell,(i,n+1)} &= \frac{1}{\sqrt{2}}d_i^\ell, \quad i = 1, \dots, n, \quad \ell = 1, \dots, p; \quad b_\ell = -c^\ell, \quad \ell = 1, \dots, p, \end{aligned}$$

and

$$U : \mathbb{R}^{\binom{n+1}{2}+n} \rightarrow \mathcal{S}_{n+1} : \Leftrightarrow$$

$$U(z) = \sum_{1 \leq i < j \leq n+1} z_{ij} U^{ij} + \sum_{i=1}^n z_{ii} U^{ii} + U^0 \quad (2.3)$$

with $U^{ij} = \frac{1}{\sqrt{2}}(E_{ij} + E_{ji})$, $U^{ii} = E_{ii}$, and $U^0 = E_{n+1,n+1}$. Equivalence between the (AQP) (2.1) and the (UP) (2.2) holds in the sense of the following result.

PROPOSITION 2.1. *Let x^* be an optimal solution of Problem (2.1) and let z^* be an optimal solution of Problem (2.2). If we set*

$$\begin{aligned} \bar{z}_{ij} &= \sqrt{2}x_i^* x_j^*, \quad 1 \leq i < j \leq n; \\ \bar{z}_{ii} &= x_i^* x_i^*, \quad 1 \leq i \leq n; \quad \bar{z}_{i,n+1} = \sqrt{2}x_i^*, \quad 1 \leq i \leq n, \end{aligned}$$

and

$$\bar{x}_i = \frac{1}{\sqrt{2}}z_{i,n+1}^*, \quad 1 \leq i \leq n,$$

then \bar{z} is a feasible solution of Problem (2.2), \bar{x} is a feasible solution of Problem (2.1), and

$$(\bar{x})^T Q^0 \bar{x} + (d^0)^T \bar{x} = (x^*)^T Q^0 x^* + (d^0)^T x^* = h^T \bar{z} = h^T z^*. \quad (2.4)$$

Proof. Straightforward calculation shows that

$$U(\bar{z}) = \begin{pmatrix} x^* \\ 1 \end{pmatrix} ((x^*)^T, 1),$$

and hence $U(\bar{z}) \in \mathcal{U}_{n+1}$.

Let A_ℓ denote the ℓ -th row of the matrix A , $\ell = 1, \dots, p$. Then we have

$$\begin{aligned} A_\ell \bar{z} &= \sum_{1 \leq i < j \leq n} A_{\ell,ij} \bar{z}_{ij} + \sum_{i=1}^n A_{\ell(i,n+1)} \bar{z}_{i,n+1} = \sum_{i,j=1}^n Q_{ij}^\ell x_i^* x_j^* + \sum_{i=1}^n d_i^\ell x_i^* \\ &= (x^*)^T Q^\ell x^* + (d^\ell)^T x^* \leq -c^\ell = b^\ell \end{aligned}$$

i.e., \bar{z} is a feasible solution of Problem (2.2). Similar direct calculations show that

$$h^T \bar{z} = (x^*)^T Q^0 x^* + (d^0)^T x^*,$$

and hence, since \bar{z} satisfies the constraints of (2.2), and z^* is an optimal solution of (2.2), we have

$$h^T z^* \leq (x^*)^T Q^0 x^* + (d^0)^T x^*.$$

Analogously, one easily obtains that \bar{x} is feasible for (2.1) and $h^T z^* = (\bar{x})^T Q^0 \bar{x} + (d^0)^T \bar{x}$, which implies that

$$h^T z^* \geq (x^*)^T Q^0 x^* + (d^0)^T x^*. \quad \square$$

Notice that additional linear constraints in (2.1) can be transformed into equivalent linear constraints to be added to (2.2) in a straightforward way. Boundedness of $\{z \in \mathbb{R}^d : Az \leq b\}$ is not necessarily guaranteed in the (UP) (2.2) arising from (2.1). But if bounds $\bar{\ell} \leq x \leq \bar{L}$ for the variable $x \in \mathbb{R}^n$ of (2.1) are known (which is often the case in applications), then we obtain the additional constraints $\bar{\ell} \leq z \leq \bar{L}$ in (2.2), where the components of the vectors $\bar{\ell}, \bar{L} \in \mathbb{R}^d$, $d = \binom{n+1}{2} + n$, are given by

$$\begin{aligned} l_{ii} &:= \min\{\bar{l}_i \bar{l}_i, \bar{L}_i \bar{L}_i\}, \quad 1 \leq i \leq n; \quad L_{ii} := \max\{\bar{l}_i \bar{l}_i, \bar{L}_i \bar{L}_i\}, \quad 1 \leq i \leq n; \\ l_{ij} &:= \sqrt{2} \min\{\bar{l}_i \bar{l}_j, \bar{l}_i \bar{L}_j, \bar{L}_i \bar{l}_j, \bar{L}_i \bar{L}_j\}, \quad 1 \leq i < j \leq n; \\ L_{ij} &:= \sqrt{2} \max\{\bar{l}_i \bar{l}_j, \bar{l}_i \bar{L}_j, \bar{L}_i \bar{l}_j, \bar{L}_i \bar{L}_j\}, \quad 1 \leq i < j \leq n; \\ l_{i,n+1} &:= \sqrt{2} \bar{l}_i, \quad 1 \leq i \leq n; \quad L_{i,n+1} := \sqrt{2} \bar{L}_i, \quad 1 \leq i \leq n, \end{aligned}$$

respectively.

Notice that a short formulation of Proposition 2.1 using semidefinite programming notation is available along the lines given, e.g., in Fujie and Kojima (1995), Poljak et al. (1995), Ramana (1993), and Vandenberg and Boyd (1996).

3. Preliminaries and Ramana's approach

The following results taken from Ramana (1993) are needed for the cutting plane algorithms which we will discuss in this and subsequent sections.

Let $n \geq 2$.

LEMMA 3.1. *Let $U \in \mathcal{S}_n$, and let $\lambda_1(U) \leq \lambda_2(U) \leq \dots \leq \lambda_n(U)$ denote its eigenvalues. Then the following assertions are equivalent:*

- (i) $U \in \mathcal{U}_n$;
- (ii) $\lambda_i(U) = 0, \quad i = 1, \dots, n-1$;
- (iii) $\lambda_1(U) \geq 0$ and $\lambda_{n-1}(U) \leq 0$;
- (iv) $\lambda_1(U) \geq 0$ and $\text{tr}(U) \leq \lambda_n(U)$.

Proof. The above equivalences follow readily from the well-known facts that a matrix U is unary if and only if it is positive semidefinite and $\text{rank}(U) = 1$, and that $\text{tr}(U) = \sum_{i=1}^n \lambda_i(U)$. \square

LEMMA 3.2 (Weyl). *Let $E, F \in \mathcal{S}_n$ with eigenvalues indexed in an increasing order as above. Then, for $k \in \{1, \dots, n\}$, we have*

$$\lambda_1(F) + \lambda_k(E) \leq \lambda_k(F + E) \leq \lambda_k(E) + \lambda_n(F)$$

Proof. See, e.g., Horn & Johnson (1985). \square

COROLLARY 3.1. *Let $U : \mathbb{R}^d \rightarrow \mathcal{S}_n$ be an affine matrix mapping defined by*

$$U(z) = U^0 + \sum_{i=1}^d z_i U^i, \quad z \in \mathbb{R}^d,$$

where $U^i \in \mathcal{S}_n, i = 0, \dots, d$. Then, for every $y \in \mathbb{R}_+^d$ and $k \in \{1, \dots, n\}$,

$$\lambda_k(U(y)) \leq \lambda_k(U^0) + \sum_{i=1}^d y_i \lambda_n(U^i)$$

and

$$\lambda_k(U(y)) \geq \lambda_k(U^0) + \sum_{i=1}^d y_i \lambda_1(U^i).$$

Proof. Apply twice Weyl's inequality (Lemma 3.2) and use that $\lambda_i(\mu U) = \mu \lambda_i(U) \forall \mu \geq 0$. \square

Next, consider the LP-relaxation

$$\begin{aligned} \min \quad & h^T z \\ \text{s.t.} \quad & Az \leq b \end{aligned} \tag{3.1}$$

of (UP) (1.2) which arises from (1.2) when the unary condition $U \in \mathcal{U}_n$ is omitted. Given a vertex optimal solution \bar{z} of (3.1) and the affine matrix mapping U defined in (1.1), then $\lambda_1(U(\bar{z})) = 0$ and $\lambda_{n-1}(U(\bar{z})) = 0$ implies that \bar{z} is an optimal solution of (UP) because of Lemma 3.1. Otherwise, one must have $\lambda_1(U(\bar{z})) < 0$ or $\lambda_{n-1}(U(\bar{z})) > 0$ (or both). In this case, however, Corollary 3.1 allows one to construct an additional linear constraint $\ell(z) \leq 0$ which, when added to the constraints of (3.1), is violated by \bar{z} but satisfied by all feasible solutions of (1.2). Continuing in this way, one obtains a polyhedral outer approximation (or cutting plane) approach which, in each iteration requires only solving linear programs and eigenvalue calculation. Each vertex optimal solution z^k of such a linear program is the unique solution of a nonsingular $d \times d$ system of linear equations binding at z^k , which – following the standard terminology in simplex algorithms – will be called a nonsingular basic system corresponding to z^k . Simplex-type algorithms provide such a system automatically. Based on the above arguments, Ramana (1993) proposed the following approach:

ALGORITHM 1**Initialization:**

Set $P^0 \leftarrow \{z \in \mathbb{R}^d : Az \leq b\}$, stop \leftarrow false, $k \leftarrow 0$

While stop = false **do**

Solve the LP $\min\{h^T z : z \in P^k\}$ to obtain a vertex optimal solution z^k and a corresponding nonsingular basic system $B^k z \leq r^k$ satisfying $B^k z^k = r^k$; compute the eigenvalues $\lambda_i(U(z^k))$

if $\lambda_1(U(z^k)) \geq 0$ and $\lambda_{n-1}(U(z^k)) \leq 0$ **then**

z^k is optimal solution of (UP),

set stop \leftarrow true

else

if $\lambda_{n-1}(U(z^k)) > 0$ **then**

set $(a^1)_i^k \leftarrow \lambda_1(U^0 - U((B^k)^{-1}e_i))$, $i = 1, \dots, d$,

$(\beta^1)^k \leftarrow -\lambda_{n-1}(U(z^k))$, and

$P^k \leftarrow P^k \cap \{z \in \mathbb{R}^d : -((a^1)^k)^T B^k z \leq -((a^1)^k)^T B^k z^k + (\beta^1)^k\}$

end if

if $\lambda_1(U(z^k)) < 0$ **then**

set $(a^2)_i^k \leftarrow \lambda_n(U^0 - U((B^k)^{-1}e_i))$, $i = 1, \dots, d$,

$(\beta^2)^k \leftarrow \lambda_1(U(z^k))$, and

$P^k \leftarrow P^k \cap \{z \in \mathbb{R}^d : ((a^2)^k)^T B^k z \leq ((a^2)^k)^T B^k z^k + (\beta^2)^k\}$

end if

set $P^{k+1} \leftarrow P^k$, $k \leftarrow k + 1$

end if

end while

It is easy to see that the cuts constructed in Algorithm 1 are valid (for details, see Ramana, 1993), i.e., $z^k \notin P^{k+1}$ but $F := \{z \in \mathbb{R}^d : Az \leq b, U(z) \in \mathcal{U}_n\} \subset P^{k+1}$. However, convergence of the algorithm in the sense that every accumulation point z^* of the sequence $\{z^k\}_{k \in \mathbb{N}}$ satisfies $z^* \in F$ cannot be guaranteed, since $((a^j)^k)^T B^k$ ($j = 1, 2; k \in \mathbb{N}$) might fail to be bounded. For a related convergence theory of cutting plane algorithms in global optimization, we refer to Horst & Tuy (1996).

4. Valid cuts for convergent outer approximation algorithms

A first step towards convergent outer approximation algorithms for solving (UP) or (AQP) via the corresponding (UP) consists in requiring that in the affine matrix mapping (1.1)

$$U : \mathbb{R}^d \rightarrow \mathfrak{S}_n : \Leftrightarrow U(z) = U^0 + \sum_{i=1}^d z_i U^i$$

the matrices $U^i, i = 1, \dots, d$, form an orthonormal system (ONS) with respect to the inner product (1.3).

LEMMA 4.1. *Each (UP) of the form (1.2) with $U(z)$ defined by (1.1) can be transformed into an equivalent (UP) where the matrices $U^i, i = 1, \dots, d$, form an ONS.*

Proof. Let in the original problem $U(z) = \sum_{i=1}^{\bar{d}} z_i \bar{U}^i$ where $\bar{U}^i \in \mathfrak{S}_n, i = 1, 2, \dots, \bar{d}$, are arbitrary. Determine a maximal linearly independent subset

$$\{\bar{U}^{i_j} : j = 1, \dots, d\} \subset \{\bar{U}^i : i = 1, \dots, \bar{d}\}$$

(so that the two linear spaces generated by the \bar{U}^{i_j} respectively the \bar{U}^i have equal dimension). Remove from the original (UP) all variables $z_i, i \in \{1, \dots, \bar{d}\} \setminus \{i_j, j = 1, \dots, d\}$ along with the corresponding components of the vector h and the corresponding columns of the matrix A . Use the Gram–Schmidt procedure to generate from $\{\bar{U}^{i_j} : j = 1, \dots, d\}$ a corresponding ONS $\{U^j : j = 1, \dots, d\}$. The final transformation of the remaining entries of h and A , respectively, is straightforward via the homeomorphism which maps the \bar{U}^{i_j} onto the $U^j, j = 1, \dots, d$. \square

Notice that the transformation presented in Section 2 which links the all-quadratic problem (2.1) to an equivalent unary program (2.2) yields an ONS U^{ij} in (2.3).

LEMMA 4.2. *Let $E_{ij} = e_i e_j^T \in \mathbb{R}^{(n+1) \times (n+1)}, i, j = 1, \dots, n+1$. Then the matrices*

$$\begin{aligned} U^{ii} &= E_{ii}, \quad i = 1, \dots, n; \\ U^{ij} &= \frac{1}{\sqrt{2}}(E_{ij} + E_{ji}), \quad 1 \leq i < j \leq n+1 \end{aligned}$$

form an ONS with respect to the inner product defined in (1.3).

Proof. Lemma 4.2 can be verified by straightforward calculation. \square

Next, let $\|A\|_F = \sqrt{A \cdot A}$, $A \in \mathfrak{S}_n$, denote the norm induced by the inner product (1.3) (the so-called Frobenius norm), and let $\|\cdot\|_2$ and $\|\cdot\|_\infty$ denote the Euclidean norm and the maximum norm, respectively, in \mathbb{R}^d .

LEMMA 4.3. *Let $\{U^i; i = 1, \dots, d\} \subset \mathfrak{S}_n$ form an ONS with respect to the inner product \cdot . Then*

$$\left\| \sum_{i=1}^d (z - \bar{z})_i U^i \right\|_F = \|z - \bar{z}\|_2 \quad \forall z, \bar{z} \in \mathbb{R}^d. \quad (4.1)$$

Proof. We have

$$\begin{aligned} \left\| \sum_{i=1}^d (z - \bar{z})_i U^i \right\|_F^2 &= \text{tr} \left(\left(\sum_{i=1}^d (z - \bar{z})_i U^i \right)^T \left(\sum_{i=1}^d (z - \bar{z})_i U^i \right) \right) \\ &= \sum_{i,j=1}^d (z - \bar{z})_i (z - \bar{z})_j \text{tr}((U^i)^T U^j) \\ &= \sum_{i=1}^d (z - \bar{z})_i^2 = \|z - \bar{z}\|_2^2 \end{aligned}$$

since $\text{tr}((U^i)^T U^j) = U^i \cdot U^j = \delta_{ij}$. \square

Lemma 4.3 combined with Weyl's inequality (Lemma 3.2) allows one to derive bounds on the distance of eigenvalues of $U(z)$ and $U(\bar{z})$.

PROPOSITION 4.1. *Let $\{U^i : i = 1, \dots, d\} \subset \mathfrak{S}_n$ form an ONS with respect to the inner product \cdot , and let $U : \mathbb{R}^d \rightarrow \mathfrak{S}_n$ be an affine matrix mapping of the form*

$$z \rightarrow U(z) = U^0 + \sum_{i=1}^d z_i U^i, \quad U^0 \in \mathfrak{S}_n.$$

Assume that the eigenvalues of the matrices involved are indexed in an increasing order. Then, for each $z, \bar{z} \in \mathbb{R}^d$, we have

$$\lambda_{n-1}(U(z)) \geq \lambda_{n-1}(U(\bar{z})) - \|z - \bar{z}\|_2, \quad (4.2)$$

and

$$\lambda_1(U(z)) \leq \lambda_1(U(\bar{z})) + \|z - \bar{z}\|_2. \quad (4.3)$$

Proof. Since the Frobenius norm is an upper bound for the spectral radius, one obtains by means of Lemma 3.2:

$$\begin{aligned}
\lambda_{n-1}(U(z)) &= \lambda_{n-1}(U(z - \bar{z}) + U(\bar{z}) - U^0) \\
&= \lambda_{n-1}\left(\sum_{i=1}^d (z - \bar{z})_i U^i + U(\bar{z})\right) \\
&\geq \lambda_{n-1}(U(\bar{z})) + \lambda_1\left(\sum_{i=1}^d (z - \bar{z})_i U^i\right) \\
&\geq \lambda_{n-1}(U(\bar{z})) - \left\|\sum_{i=1}^d (z - \bar{z})_i U^i\right\|_F \\
&= \lambda_{n-1}(U(\bar{z})) - \|z - \bar{z}\|_2.
\end{aligned}$$

Similarly, inequality (4.3) follows from

$$\begin{aligned}
\lambda_1(U(z)) &= \lambda_1(U(z - \bar{z}) + U(\bar{z}) - U^0) = \lambda_1\left(\sum_{i=1}^d (z - \bar{z})_i U^i + U(\bar{z})\right) \\
&\leq \lambda_1(U(\bar{z})) + \lambda_n\left(\sum_{i=1}^d (z - \bar{z})_i U^i\right) \\
&\leq \lambda_1(U(\bar{z})) + \left\|\sum_{i=1}^d (z - \bar{z})_i U^i\right\|_F \\
&= \lambda_1(U(\bar{z})) + \|z - \bar{z}\|_2. \quad \square
\end{aligned}$$

Notice that Proposition 4.1 can also be derived from the Hoffman–Wielandt (1953) inequality.

Similar bounds with respect to the maximum norm follow by using

$$\|z\|_2^2 = \sum_{i=1}^d |z_i|^2 \leq \sum_{i=1}^d \|z\|_\infty^2 = d \|z\|_\infty^2.$$

COROLLARY 4.1. *Under the assumption of Proposition 4.1 there holds*

$$\lambda_{n-1}(U(z)) \geq \lambda_{n-1}(U(\bar{z})) - \sqrt{d} \|z - \bar{z}\|_\infty \quad (4.4)$$

and

$$\lambda_1(U(z)) \leq \lambda_1(U(\bar{z})) + \sqrt{d} \|z - \bar{z}\|_\infty. \quad (4.5)$$

Let now again $\bar{z} \in \mathbb{R}^d$ be an optimal solution of an LP-relaxation of the (UP) (1.2) satisfying $U(\bar{z}) \notin \mathcal{U}_n$. Then it follows from Proposition 4.1 and Lemma 3.1 (iii)

that

$$\ell_{1,\bar{z}}(z) := \max\{\lambda_{n-1}(U(\bar{z})), -\lambda_1(U(\bar{z}))\} - \|z - \bar{z}\|_2 \leq 0 \quad (4.6)$$

is a valid cut, i.e., we have $\ell_{1,\bar{z}}(\bar{z}) > 0$ but $\ell_{1,\bar{z}}(z) \leq 0 \forall z : U(z) \in \mathcal{U}_n$. Likewise, Corollary 4.1 yields a similar valid cut

$$\ell_{2,\bar{z}}(z) := \frac{1}{\sqrt{d}}(\max\{\lambda_{n-1}(U(\bar{z})), -\lambda_1(U(\bar{z}))\}) - \|z - \bar{z}\|_\infty \leq 0. \quad (4.7)$$

Next, we show that an outer approximation algorithm for solving (1.2) which uses either (4.6) or (4.7) is convergent. Notice, however, that both cuts are nonlinear so that an algorithm which uses one of them directly induces difficult subproblems. Ways to overcome these difficulties will be discussed in the following sections.

PROPOSITION 4.2. *Let $\{z^k\}_{k \in \mathbb{N}}$ be a sequence of points in $\{z \in \mathbb{R}^d : Az \leq b\}$ satisfying either*

$$\ell_{1,z^k}(z^i) \leq 0, k, i \in \mathbb{N}, i > k \quad (4.8)$$

or

$$\ell_{2,z^k}(z^i) \leq 0, k, i \in \mathbb{N}, i > k. \quad (4.9)$$

Then every accumulation point z^* of $\{z^k\}_{k \in \mathbb{N}}$ satisfies $U(z^*) \in \mathcal{U}_n$.

Proof. We prove the result for ℓ_{1,z^k} ; the proof for ℓ_{2,z^k} is similar: Let $\{z^{k_q}\}_{q \in \mathbb{N}}$ be a subsequence of $\{z^k\}_{k \in \mathbb{N}}$ satisfying $z^{k_q} \rightarrow z^*(q \rightarrow \infty)$. From (4.8) follows that

$$\ell_{1,z^{k_q}}(z^{k_{q+1}}) \leq 0,$$

which, in view of (4.6), implies

$$\max\{\lambda_{n-1}(U(z^{k_q})), -\lambda_1(U(z^{k_q}))\} \rightarrow 0 \quad (q \rightarrow \infty),$$

since $\|z^{k_{q+1}} - z^{k_q}\|_2 \rightarrow 0$ ($q \rightarrow \infty$).

From this ensues

$$\lambda_1(U(z^*)) = \lambda_{n-1}(U(z^*)) = 0$$

by continuity of the eigenvalue functionals $\lambda_1, \lambda_{n-1} : \mathfrak{S}_n \rightarrow \mathbb{R}$. But this is equivalent to $U(z^*) \in \mathcal{U}_n$ because of Lemma 3.1. \square

5. Implementable algorithm using the ℓ_∞ -norm

Consider the (UP) (1.2) with $\{z \in \mathbb{R}^d : Az \leq b\}$ not empty and bounded. Assume that $\{U^i : i = 1, \dots, d\}$ forms an ONS with respect to the inner product \cdot defined in (1.3), and let $n \geq 2, d \geq 2$. The following algorithm is based on the cut (4.7) and uses the fact that the ℓ_∞ -unit ball is the intersection of $2d$ hyperplanes.

ALGORITHM 2**Initialization:**

Set $P^0 \leftarrow \{z \in \mathbb{R}^d : Az \leq b\}$, and solve the LP $\min\{h^T z : z \in P^0\}$ to obtain an optimal solution z^0 ; set $\mu_{P^0} \leftarrow h^T z^0$, $\mu^0 \leftarrow \mu_{P^0}$, $\mathcal{P} \leftarrow \{P^0\}$, $stop \leftarrow false$, $k \leftarrow 0$

While $stop = false$ **do**

if $\lambda_1(U(z^k)) \geq 0$ and $\lambda_{n-1}(U(z^k)) \leq 0$ **then**

z^k is optimal solution of (UP),

set $stop \leftarrow true$

else

set $\varepsilon^k \leftarrow \frac{1}{\sqrt{d}} \max\{-\lambda_1(U(z^k)), \lambda_{n-1}(U(z^k))\}$

for $j = 1$ **until** 2

for $i = 1$ **until** d

set $P_{ij}^k \leftarrow P^k \cap \{z \in \mathbb{R}^d : (-1)^j z_i \leq (-1)^j z_i^k - \varepsilon^k\}$

if $P_{ij}^k \neq \emptyset$ **then**

solve the LP $\min\{h^T z : z \in P_{ij}^k\}$ to obtain an optimal solution z_{ij}^k

and optimal objective function value $\mu_{P_{ij}^k}$; set $\mathcal{P} \leftarrow \mathcal{P} \cup \{P_{ij}^k\}$

end if

end for

end for

set $\mathcal{P} \leftarrow \mathcal{P} \setminus \{P^k\}$

if $\mathcal{P} \neq \emptyset$ **then**

set $\mu^{k+1} \leftarrow \min\{\mu_P : P \in \mathcal{P}\}$, and choose z^{k+1} and $P^{k+1} \in \mathcal{P}$ such

that $z^{k+1} \in P^{k+1}$ and $\mu^{k+1} = h^T z^{k+1} = \mu_{P^{k+1}}$; set

$k \leftarrow k + 1$

else

Problem (UP) has no feasible point, set $stop \leftarrow true$

end if

end if

end while

REMARK 5.1. The set \mathcal{P} is a collection of polytopes, and the number of inequalities describing a polytope $P \in \mathcal{P}$ can be bounded by $m + 2d$, since for i, j fixed the halfspaces defined by $(-1)^j z_i \leq (-1)^j z_i^k - \varepsilon^k$ are parallel for all $k \in \mathbb{N}$.

PROPOSITION 5.1.

- (i) *If Algorithm 2 terminates at a point z^k , then z^k is an optimal solution of Problem (UP).*
- (ii) *Otherwise, every accumulation point of the sequence $\{z^k\}_{k \in \mathbb{N}}$ is an optimal solution of Problem (UP).*

Proof. We first show by induction that, at each iteration k , the current partition \mathcal{P} satisfies

$$\bigcup_{P \in \mathcal{P}} P \supset F, \quad (5.1)$$

where F denotes the feasible set of Problem (UP).

This implies assertion (i), and moreover, that $\mu^k \leq \min\{h^T z : z \in F\}$. For $k = 0$, we have $\mathcal{P} = \{P^0\}$, $P^0 = \{z \in \mathbb{R}^d : Az \leq b\}$, and hence (5.1). Assume that (5.1) holds at the beginning of iteration k . Then it suffices to show that

$$\bigcup_{\substack{i=1, \dots, d \\ j=1, 2}} P_{ij}^k \supset F \cap P^k.$$

Let $z \in F \cap P^k$. From Corollary 4.1 we know that

$$\lambda_{n-1}(U(z)) \geq \lambda_{n-1}(U(z^k)) - \sqrt{d}\|z - z^k\|_\infty$$

and

$$\lambda_1(U(z)) \leq \lambda_1(U(z^k)) + \sqrt{d}\|z - z^k\|_\infty.$$

But $\lambda_{n-1}(U(z)) = \lambda_1(U(z)) = 0$, since $z \in F$ (cf. Lemma 3.1), and hence

$$\|z - z^k\|_\infty = \max_{i=1, \dots, d} |z_i - z_i^k| \geq \frac{1}{\sqrt{d}} \max\{-\lambda_1(U(z^k)), \lambda_{n-1}(U(z^k))\} = \varepsilon^k.$$

It follows that there exist $i_0 \in \{1, \dots, d\}$, $j_0 \in \{1, 2\}$ such that $(-1)^{j_0}(z_{i_0}^k - z_{i_0}) \geq \varepsilon^k$. This implies $z \in P_{i_0 j_0}^k$, since $z \in P^k$.

Next, let z^* be an accumulation point of the sequence $\{z^k\}_{k \in \mathbb{N}}$, and let $\{z^{k_q}\}_{q \in \mathbb{N}}$ be a subsequence such that $z^{k_q} \rightarrow z^*$ ($q \rightarrow \infty$). It suffices to show that $z^* \in F$, since this implies $h^T z^* \geq \min\{h^T z : z \in F\}$, where equality must hold because of $h^T z^{k_q} = \mu^{k_q} \leq \min\{h^T z : z \in F\}$. By passing to a subsequence, if necessary, we can assume that $P^{k_{q+1}} \subset P^{k_q}$, $q \in \mathbb{N}$. This implies, by construction,

$$\|z^{k_{q+1}} - z^{k_q}\|_\infty \geq \varepsilon^{k_q} = \frac{1}{\sqrt{d}} \max\{-\lambda_1(U(z^{k_q})), \lambda_{n-1}(U(z^{k_q}))\} \quad \forall q \in \mathbb{N}.$$

Passing to the limit $q \rightarrow \infty$ and using continuity of the eigenvalue functionals yields $\lambda_1(U(z^*)) = \lambda_{n-1}(U(z^*)) = 0$, i.e., $z^* \in F$ (cf. Lemma 3.1). \square

6. Implementable algorithms using the Euclidean norm

Geometrically, the inequalities (4.6) and (4.7) tell us that, for each optimal solution \bar{z} of an LP-relaxation of the (UP), satisfying $U(\bar{z}) \notin \mathcal{U}_n$, one can cut a ball out

of the polyhedron defined by relaxed constraints without affecting unarity. This can be done by linear cuts in case of the ℓ_∞ -norm (Algorithm 2). In case of the Euclidean norm (inequality (4.6)), we propose inner approximation of the ball by a regular d -dimensional simplex (d -simplex) with vertices at the boundary of the ball. This choice is motivated by the two facts, that, on one hand, a d -simplex is the d -polytope with minimal number of facets, and, on the other hand, that among the d -simplices contained in a given ball, only the regular ones are largest (with respect to volume) (for a proof see Slepan, 1969).

Let B^d denote the Euclidean unit ball centered at the origin, and let $S = [v_0, \dots, v_d]$ be a regular d -simplex with all vertices on the boundary of B^d . Then it is known that the edge-length of S is given by

$$\|v_i - v_j\|_2 = \sqrt{\frac{2(d+1)}{d}}, \quad i, j \in \{0, \dots, d\}, \quad i \neq j \quad (6.1)$$

(cf. Sommerville, 1929; Gritzmann et al., 1995). Moreover, it is elementary to show that we have $0 = \frac{1}{d+1} \sum_{i=0}^d v_i$, and that the radius of the largest Euclidean ball which can be inscribed into S is

$$r = \frac{1}{d}, \quad (6.2)$$

where the number r is also the distance of each facet of S from the origin. We also use the fact that, for $j = 0, \dots, d$, the vertex v_j is orthogonal to the facet $S_j = [v_0, \dots, v_{j-1}, v_{j+1}, \dots, v_d]$, and hence the hyperplane H_{S_j} generated by S_j can be described by

$$H_{S_j} = \{x \in \mathbb{R}^d : v_j^T(v_i - x) = 0\}, \quad i \in \{0, \dots, d\} \setminus \{j\}. \quad (6.3)$$

Next we show that the following vectors v_0, \dots, v_d are vertices of a regular d -simplex S with circumsphere B^d . Set

$$\begin{aligned} v_0 &= \sqrt{a_0} e_d \\ v_i &= \sqrt{a_{2i}} e_{d-1} - \sum_{j=1}^i \sqrt{a_{2j-1}} e_{d-(j-1)}, \quad i = 1, \dots, d-1, \\ v_d &= -\sqrt{a_{2(d-1)}} e_1 - \sum_{j=1}^{d-1} \sqrt{a_{2j-1}} e_{d-(j-1)}, \end{aligned} \quad (6.4)$$

where

$$\begin{aligned} a_0 &= 1, \\ a_i &= \begin{cases} a_{i-1} / \left(d - \frac{i-1}{2}\right)^2, & i \text{ odd} \\ a_{i-2} - a_{i-1}, & i \text{ even,} \end{cases} \end{aligned} \quad (6.5)$$

and $e_i \in \mathbb{R}^d$ is the i -th unit vector.

LEMMA 6.1. *Let $a_0, \dots, a_{2(d-1)}$ be defined as above. Then we have*

$$a_{2i} = \frac{d+1}{d} \cdot \frac{d-i}{d-i+1}, i = 1, \dots, d-1. \quad (6.6)$$

Proof. The assertion is obviously correct for $i = 0$. Assume that it holds for $i = j-1, j \geq 1$. Then we have, in view of (6.5):

$$\begin{aligned} \frac{d-j+1}{d-j} a_{2j} &= \frac{d-j+1}{d-j} (a_{2j-2} - a_{2j-1}) \\ &= \frac{d-j+1}{d-j} (a_{2j-2} - a_{2j-2}/(d-j+1)^2) \\ &= \frac{d-j+1}{d-j} \frac{(d-j+1)^2 - 1}{(d-j+1)^2} a_{2j-2} \\ &= \frac{d-j+2}{d-j+1} a_{2j-2} = \frac{d+1}{d} \end{aligned}$$

which is the desired result for $i = j$.

PROPOSITION 6.1. *The simplex $S = [v_0, \dots, v_d]$ constructed as above satisfies*

(i) $\|v_i\|_2 = 1, \quad i \in \{0, \dots, d\},$

(ii) $\|v_i - v_j\|_2 = \sqrt{\frac{2(d+1)}{d}}, \quad i, j \in \{0, \dots, d\}, i \neq j.$

Proof. From (6.5) we have

$$a_{2i} = 1 - \sum_{j=1}^i a_{2j-1}, \quad i = 0, \dots, d-1, \quad (6.7)$$

and hence

$$\|v_i\|_2^2 = a_{2i} + \sum_{j=1}^i a_{2j-1} = 1, \quad i = 0, \dots, d-1.$$

Assertion (i) follows, since $\|v_d\|_2 = \|v_{d-1}\|_2$.

Lemma 6.1 and (6.7) yield

$$\|v_{d-1} - v_d\|_2^2 = 4a_{2(d-1)} = 2 \frac{d - (d-1) + 1}{d - (d-1)} a_{2(d-1)} = 2 \frac{d+1}{d},$$

and, for $i, j \in \{0, \dots, d\}$, $i < j$, $i < d - 1$:

$$\begin{aligned}
\|v_i - v_j\|_2^2 &= a_{2j} + \sum_{l=i+2}^j a_{2l-1} + (\sqrt{a_{2i}} + \sqrt{a_{2i+1}})^2 \\
&= 1 - \sum_{l=1}^j a_{2l-1} + \sum_{l=i+2}^j a_{2l-1} + (\sqrt{a_{2i}} + \sqrt{a_{2i+1}})^2 \\
&= 1 - \sum_{l=1}^{i+1} a_{2l-1} + a_{2i} + a_{2i+1} + 2\sqrt{a_{2i}}\sqrt{a_{2i+1}} \\
&= 2a_{2i} + 2\sqrt{a_{2i}}\sqrt{\frac{a_{2i}}{(d-i)^2}} \\
&= 2a_{2i} + 2a_{2i}\frac{1}{d-i} \\
&= 2\frac{(d-i+1)}{d-i}a_{2i} = 2\frac{(d+1)}{d}. \quad \square
\end{aligned}$$

Given the above regular simplicial inner approximation of an Euclidean ball and the simple representation (6.3) of the hyperplanes generated by its facets, an implementable outer approximation algorithm for solving Problem (UP) can be formulated along lines which are very similar to Algorithm 2 and its discussion: Substitute the unit ball B^d by the ball $\{z \in \mathbb{R}^d : \|z - z^k\|_2 \leq \varepsilon^k\}$ where z^k is an optimal solution to an LP-relaxation of Problem (UP) satisfying $U(z^k) \notin \mathcal{U}_n$, and $\varepsilon^k = \max\{-\lambda_1(U(z^k)), \lambda_{n-1}(U(z^k))\}$, and replace the above simplex vertices v_i by $\varepsilon^k v_i + z^k$.

Finally, in Algorithm 2 replace ε^k accordingly, and, in the loop generating the sets $P_{i_j}^k$, replace these by

$$P_i^k \leftarrow P^k \cap \{z \in \mathbb{R}^d : v_i^T z \leq v_i^T (\varepsilon^k v_1 + z^k)\}, \quad \text{if } i = 0,$$

and by

$$P_i^k \leftarrow P^k \cap \{z \in \mathbb{R}^d : v_i^T z \leq v_i^T (\varepsilon^k v_0 + z^k)\}, \quad \text{if } 1 \leq i \leq d.$$

Convergence of the resulting algorithm can be proved very similarly to the proof of Proposition 5.1 by using

$$\frac{\varepsilon^{k_q}}{d} \leq \|z^{k_{q+1}} - z^{k_q}\|_2 \quad (6.8)$$

for the correspondent subsequence, which holds because of (6.2). Details are given in Raber (1996).

Improved cuts can be constructed by exploiting the following two observations. The first observation will allow us to construct an additional linear cut in each

iteration whereas the second observation aims at improving the above simplex with respect to the depth of the cuts induced by its facets.

Let \bar{z} be an optimal vertex solution of an LP-relaxation of (UP), $\varepsilon = \max\{-\lambda_1(U(\bar{z})), \lambda_{n-1}(U(\bar{z}))\}$ and let $Bz \leq r$ denote a corresponding subsystem with $B \in \mathbb{R}^{d \times d}$ regular satisfying $B\bar{z} = r$. Then the set $C = \{z \in \mathbb{R}^d : Bz \leq r\}$ describe a cone vertexed at \bar{z} and containing $P = \{z \in \mathbb{R}^d : Az \leq b\}$ (C is the smallest of such cones and uniquely determined when \bar{z} is a nondegenerate vertex). Each of the d extremal directions $w^i (i = 1, \dots, d)$ of C is a nontrivial solution of the system

$$B_\ell w^i = 0, \quad \ell = 1, \dots, i-1, i+1, \dots, d,$$

$$B_i w^i \leq 0,$$

where B_ℓ denotes the ℓ -th row of B . Let $\bar{w}^1, \dots, \bar{w}^d$ denote the intersection points of the rays

$$\{w \in \mathbb{R}^d : w = \bar{z} + \lambda w^i, \lambda \geq 0\}, \quad i = 1, \dots, d$$

respectively, with the ball

$$B_{\bar{z}} := \{z \in \mathbb{R}^d : \|z - \bar{z}\|_2 \leq \varepsilon\},$$

and let

$$H = \{z \in \mathbb{R}^d : a^T z = b\}$$

denote the unique hyperplane satisfying $\bar{w}^i \in H, i = 1, \dots, d, \|a\|_2 = 1$, and $a^T \bar{z} > b$. Then it follows from (4.6) that

$$P \cap \{z \in \mathbb{R}^d : a^T z \leq b\} \supset \{z \in P : U(z) \in \mathcal{U}_n\},$$

i.e.,

$$a^T z \leq b \tag{6.9}$$

is a valid cut.

Notice that, similarly to Ramana's original approach, a cutting plane algorithm which uses the above cut alone can fail to converge. However, convergence can be accelerated when one uses it as additional cut in each iteration of the above convergent outer approximation approach. Here, two variants are conceivable: Variant 1 adds the cut (6.9) to the list of cutting planes defining each polytope P^k . Variant 2 depends on the following condition:

Let \bar{P}_0 be a polytope obtained by a partitioning procedure which uses the above simplicial inner approximation. Then we generate the next polytopes

$$\bar{P}_i = \bar{P}_{i-1} \cap \{z \in \mathbb{R}^d : (a^i)^T z \leq b^i\}, \quad i = 1, \dots, r+1$$

by $r + 1$ successive cuts (6.9) of the form $(a^i)^T z \leq b^i$, $i = 1, \dots, r + 1$, where r is the largest number such that

$$\min_{i=0, \dots, r-1} \{\|z_{\bar{p}_r} - z_{\bar{p}_i}\|_2 - \varepsilon(z_{\bar{p}_i})d\} \geq 0$$

holds with $z_{\bar{p}_i}$ optimal solution of $\min\{h^T z : z \in \bar{P}_i\}$, and

$$\varepsilon(z_{\bar{p}_i}) = \max\{-\lambda_1(U(z_{\bar{p}_i})), \lambda_{n-1}(U(z_{\bar{p}_i}))\}.$$

The polytope \bar{P}_{r+1} is then partitioned according to the above outlined variant of Algorithm 2 (simplicial inner approximation), and we restart with $\bar{P}_0 = \bar{P}_{r+1}$.

Next, we consider the cut (6.9), and observe that

$$P \subset \{z \in \mathbb{R}^d : a^T z \leq a^T \bar{z}\}.$$

Therefore, when using the cut (6.9), it suffices to construct a simplicial inner approximation \hat{S} of

$$B_{\bar{z}} \cap \{z \in \mathbb{R}^d : a^T z \leq a^T \bar{z}\}.$$

Let $d \geq 3$. The simplex \hat{S} which we propose will be the convex hull of a regular $(d - 1)$ -simplex $\bar{S} \subset \bar{H} := \{z \in \mathbb{R}^d : a^T z = a^T \bar{z}\}$ and the intersection point of the ray $\{z \in \mathbb{R}^d : z = \bar{z} - \lambda a, \lambda \geq 0\}$ with the boundary of $B_{\bar{z}}$. For simplicity of the presentation we construct \hat{S} first for the case where $B_{\bar{z}} = B^d$ (the Euclidean unit ball) and $\bar{H} = \{z \in \mathbb{R}^d : -e_d^T z = 0\}$. After this, we will show how this ‘standard’ simplex can be transformed to the general case of $B_{\bar{z}}$ and \bar{H} defined above.

It is clear from our previous construction that the vertices v_0, \dots, v_{d-1} of our regular $(d - 1)$ -simplex $\bar{S} = [v_0, \dots, v_{d-1}]$ are given by the formula (6.4), (6.5) where d has to be replaced throughout by $d - 1$. It is also clear from $\bar{H} = \{z \in \mathbb{R}^d : -e_d^T z = 0\}$ that the last vertex of \hat{S} is given by

$$v_d = e_d.$$

From Proposition 6.1 and the construction of v_d we see that

$$\|v_i\|_2 = 1, \quad i = 0, \dots, d$$

$$\|v_i - v_j\|_2 = \sqrt{\frac{2d}{d-1}}, \quad i, j = 0, \dots, d-1, i \neq j,$$

and

$$\|v_i - v_d\| = \sqrt{2}, \quad i = 0, \dots, d-1.$$

Next, in order to incorporate the simplex \hat{S} into a cutting plane approach, we have to derive an equivalent representation of the hyperplane $H_{\hat{S}_i}$ generated by the facets

$$\hat{S}_i := [v_0, \dots, v_{i-1}, v_{i+1}, \dots, v_d], \quad i = 0, \dots, d-1.$$

LEMMA 6.2. *We have*

$$H_{\hat{s}_i} = \{z \in \mathbb{R}^d : \hat{v}_i^T z = \hat{v}_i^T v_d\}, \quad i = 0, \dots, d-1,$$

where

$$\hat{v}_i := v_i - \frac{1}{d-1}e_d, \quad i = 0, \dots, d-1.$$

Proof. Since, for $i \in \{0, \dots, d-1\}$ we have

$$H_{\hat{s}_i} = \left\{ z \in \mathbb{R}^d : z = v_d + \sum_{j=0, j \neq i}^{d-1} \mu_j (v_j - v_d), \mu \in \mathbb{R}^d \right\}$$

it suffices to show that

$$\hat{v}_i^T (v_j - v_d) = 0, \quad j \in \{0, \dots, d-1\} \setminus \{i\}.$$

From $(v_j)_d = 0$, one obtains

$$\begin{aligned} \hat{v}_i^T (v_j - v_d) &= \left(v_i - \frac{1}{d-1}e_d \right)^T (v_j - e_d) \\ &= v_i^T v_j + \frac{1}{d-1}. \end{aligned}$$

But

$$v_i^T v_j = v_i^T v_0 = -\frac{1}{d-1}$$

because \bar{S} is a regular simplex with vertices at the boundary of the unit ball (cf. (6.2)). It follows that $\hat{v}_i \perp H_{\hat{s}_i}$. \square

Next, we show that the cuts given by $H_{\hat{s}_i}, i = 0, \dots, d-1$ are deeper than the cuts induced by the regular simplex.

PROPOSITION 6.2. *The Euclidean distance $\delta(0, H_{\hat{s}_i})$ of the hyperplane $H_{\hat{s}_i}$ defined in Lemma 6.2 to the origin is*

$$\delta(0, H_{\hat{s}_i}) = \frac{1}{\sqrt{d^2 - 2d + 2}} > \frac{1}{d}, \quad i = 0, \dots, d-1.$$

Proof. From

$$\|\hat{v}_i\|_2^2 = 1 + \frac{1}{(d-1)^2} = \frac{d^2 - 2d + 2}{(d-1)^2}$$

and Lemma 6.2, we see that

$$\|z\|_2 \geq \frac{1}{\|\hat{v}_i\|_2} |\hat{v}_i^T v_d| = \frac{1}{d-1} \cdot \frac{1}{\|\hat{v}_i\|_2} = \frac{1}{\sqrt{d^2 - 2d + 2}} \quad \forall z \in H_{\hat{S}_i},$$

and hence

$$\delta(0, H_{\hat{S}_i}) \geq \frac{1}{\sqrt{d^2 - 2d + 2}}.$$

Every affine combination $\sum_{j=0, j \neq i}^d \lambda_j v_j$, $\sum_{j=0, j \neq i}^d \lambda_j = 1$, lies in $H_{\hat{S}_i}$. Choosing

$$\lambda_j = \frac{d-1}{d^2 - 2d + 2}, \quad j = 0, \dots, d-1, \quad j \neq i,$$

and

$$\lambda_d = \frac{1}{d^2 - 2d + 2}$$

we obtain

$$\sum_{j=0, j \neq i}^d \lambda_j v_j = \sum_{j=0, j \neq i}^{d-1} \frac{d-1}{d^2 - d + 2} v_j + \frac{1}{d^2 - 2d + 2} v_d.$$

But $\sum_{j=0}^{d-1} v_j = 0$ since the origin is the barycenter of \bar{S} , and hence

$$\begin{aligned} \sum_{j=0, j \neq i}^d \lambda_j v_j &= -\frac{d-1}{d^2 - 2d + 2} v_i + \frac{1}{d^2 - 2d + 2} v_d \\ &= -\frac{d-1}{d^2 - 2d + 2} \left(v_i - \frac{1}{d-1} e_d \right) = -\frac{d-1}{d^2 - 2d + 2} \hat{v}_i \in H_{\hat{S}_i}. \end{aligned}$$

It follows that

$$\delta(0, H_{\hat{S}_i}) \leq \frac{d-1}{d^2 - 2d + 2} \|\hat{v}_i\|_2 = \frac{1}{\sqrt{d^2 + 2d + 2}},$$

which concludes the proof. \square

Next, we provide the transformation which maps the above constructed simplex \hat{S} (with respect to the unit ball B^d and the hyperplane $z_d = 0$) to a similar simplex \hat{S}' corresponding to the ball $B_{\bar{z}}$ and the hyperplane $\bar{H} = \{z \in \mathbb{R}^d : a^T z = a^T \bar{z}\}$. Construct an orthonormal basis $\{y_1, \dots, y_{d-1}\}$ of the linear subspace $\bar{H} - \{\bar{z}\}$ (for example, by means of the Gram–Schmidt method applied to the set of vectors spanning \bar{H}) and let

$$A = (y_1, \dots, y_{d-1}, -a)$$

be the matrix with columns $y_1, \dots, y_{d-1}, -a$. Clearly, the matrix A is orthogonal, and hence the transformation

$$T : \mathbb{R}^d \rightarrow \mathbb{R}^d : \Leftrightarrow T(z) = \varepsilon Az + \bar{z} \quad (6.10)$$

yields for any $z, \hat{z} \in \mathbb{R}^d$

$$\|T(z) - \bar{z}\|_2 = \varepsilon \|z\|_2 \text{ and } \|T(z) - T(\hat{z})\|_2 = \varepsilon \|z - \hat{z}\|_2.$$

Therefore, the desired simplex $\hat{S}^t = [v_0^t, \dots, v_d^t]$ is given by

$$v_i^t = T(v_i), i = 0, \dots, d. \quad (6.11)$$

One easily verifies that the hyperplanes $H_{\hat{S}_i^t}$ generated by the facets $\hat{S}_i^t = [v_0^t, \dots, v_{i-1}^t, v_{i+1}^t, \dots, v_d^t], i = 0, \dots, d-1$, are given by

$$H_{\hat{S}_i^t} = \{z \in \mathbb{R}^d : \hat{v}_i^t A^T z = \hat{v}_i^t (\varepsilon v_d + A^T \bar{z})\}. \quad (6.12)$$

Here is the algorithm which incorporates the above observations. Throughout, the points $v_i, i = 0, \dots, d$ are the vertices of the simplex constructed above with respect to B^d and the hyperplane $z_d = 0$.

In the following algorithm, we use again $\varepsilon(z) = \max\{-\lambda_1(U(z)), \lambda_{n-1}(U(z))\}$.

ALGORITHM 3

Initialization:

Set $P^0 \leftarrow \{z \in \mathbb{R}^d : Az \leq b\}$, and solve the LP $\min\{h^T z : z \in P^0\}$ to obtain an optimal vertex solution z^0 ; set $V_{P^0} \leftarrow \{z_{P^0}\}, \mu_{P^0} \leftarrow h^T z^0, \mu^0 \leftarrow \mu_{P^0}, \mathcal{P} \leftarrow \{P^0\}, stop \leftarrow false, k \leftarrow 0$

while $stop = false$ **do**

if $\lambda_1(U(z^k)) \geq 0$ **and** $\lambda_{n-1}(U(z^k)) \leq 0$ **then**

z^k is optimal solution of (UP),

set $stop \leftarrow true$

else

set $\varepsilon^k \leftarrow \max\{-\lambda_1(U(z^k)), \lambda_{n-1}(U(z^k))\}$; choose $B^k \in \mathbb{R}^{d \times d}$ regular and $r^k \in \mathbb{R}^d$ such that $B^k z \leq r^k$ is a subsystem of $Az \leq b$ and $B^k z^k = r^k$

for $i = 1$ **until** d

let $w_i^k \neq 0 \in \mathbb{R}^d$ be a solution of the linear system $B_\ell^k w_i^k = 0, \ell = 1, \dots, i-1, i+1, \dots, d, B_i^k w_i^k \leq 0$

set $\bar{w}_i^k \leftarrow z^k + \frac{\varepsilon^k}{\|w_i^k\|_2} w_i^k$

end for

determine $a^k \in \mathbb{R}^d, \|a^k\|_2 = 1$ and $b^k \in \mathbb{R}$ such that $\{\bar{w}_1^k, \dots, \bar{w}_d^k\} \subset$

$H^k := \{z \in \mathbb{R}^d : (a^k)^T z = b^k\}, (a^k)^T z^k > b^k;$

set $\bar{P}^k \leftarrow P^k \cap \{z \in \mathbb{R}^d : (a^k)^T z \leq b^k\}$

if $\bar{P}^k \neq \emptyset$ **then**
 solve the LP $\min\{h^T z : z \in \bar{P}^k\}$ to obtain an optimal vertex solution \bar{z}^k and the corresponding optimal value $\mu_{\bar{P}^k}$;
if $\min_{z \in V_{P^k}} \{\|\bar{z}^k - z\|_2 - \varepsilon(z)/\sqrt{d^2 - 2d + 2}\} < 0$ **then**
 determine an orthonormal basis y_1^k, \dots, y_{d-1}^k of the linear subspace $H^k - \{z^k\}$, and set
 $A_k \leftarrow (y_1^k, \dots, y_{d-1}^k, -a^k)$
for $i = 0$ **until** $d - 1$
 set $P_i^k \leftarrow \bar{P}^k \cap \{z \in \mathbb{R}^d : (v_i - \frac{1}{d-1}e_d)^T A_k^T \leq (v_i - \frac{1}{d-1}e_d)^T (\varepsilon^k v_d + A_k^T z^k)\}$
if $P_i^k \neq \emptyset$ **then**
 solve the LP $\min\{h^T z : z \in P_i^k\}$ to obtain an optimal vertex solution z_i^k and the corresponding optimal value $\mu_{P_i^k}$;
 set $\mathcal{P} \leftarrow \mathcal{P} \cup \{P_i^k\}$, $V_{P_i^k} \leftarrow \{z_i^k\}$
end if
end for
else
 $\mathcal{P} \leftarrow \mathcal{P} \cup \{\bar{P}^k\}$, $V_{\bar{P}^k} \leftarrow V_{P^k} \cup \{\bar{z}^k\}$
end if
end if
 $\mathcal{P} \leftarrow \mathcal{P} \setminus \{P^k\}$
if $\mathcal{P} \neq \emptyset$ **then**
 set $\mu^{k+1} \leftarrow \min\{\mu_P : P \in \mathcal{P}\}$, and choose z^{k+1} and $P^{k+1} \in \mathcal{P}$ such that z^{k+1} is a vertex of P^{k+1} and $\mu^{k+1} = h^T z^{k+1} = \mu_{P^{k+1}}$; set $k \leftarrow k + 1$
else
 Problem (UP) has no feasible point, set $stop \leftarrow true$
end if
end if
end while

Convergence of Algorithm 3 follows from the following property:

PROPOSITION 6.3. *If Algorithm 3 generates an infinite sequence $\{z^k\}_{k \in \mathbb{N}}$, then, for every accumulation point z^* of $\{z^k\}_{k \in \mathbb{N}}$, there exists a subsequence $\{z^{k_q}\}_{q \in \mathbb{N}}$ satisfying*

$$(i) \quad z^{k_q} \rightarrow z^* \text{ as } q \rightarrow \infty, \quad P^{k_q} \supset P^{k_{q+1}} \quad \forall q \in \mathbb{N},$$

$$(ii) \quad \|z^{k_{q+1}} - z^{k_q}\|_2 \geq \varepsilon(z^{k_q})/\sqrt{d^2 - 2d + 2} \quad \forall q \in \mathbb{N}.$$

Proof. Property (i) is obvious from the definition of an accumulation point and the construction of the polytopes. In order to prove (ii), we distinguish the following two cases for the subsequence $\{z^{k_q}\}$ satisfying (i).

CASE 1: $\forall i \geq 0 \exists q(i) > i : V_{P^{k_{q(i)}}} \not\supset V_{P^{k_i}}$.

This means that, while generating $P^{k_{q(i)}}$ from P^{k_i} one must have applied at least once the facial cuts induced by a simplex (the ‘ P_i^k -loop, $i = 1$ until $d - 1$ ’ in Algorithm 3). But then we know from Proposition 6.2 (taking into account the subsequent transformation) that

$$\|z^{k_{q(i)}} - z^{k_i}\|_2 \geq \varepsilon(z^{k_i})/\sqrt{d^2 - 2d + 2}.$$

Therefore, the sequence $\{z^{k_{q(i)}}\}_{i \in \mathbb{N}} \subset \{z^{k_q}\}_{q \in \mathbb{N}}$ satisfies property (ii).

CASE 2: $\exists i_0 \geq 0 \forall q \geq i_0 : V_{P^{k_q}} \supset V_{P^{k_{i_0}}}$.

This means that, for all $q \geq i_0$, the polytope $P^{k_{q+1}}$ is generated from the polytope P^{k_q} only by successive cuts of the form $(a^k)^T z \leq b^k$, and hence

$$\min_{z \in V_{P^{k_{q+1}}}} \{\|z^{k_{q+1}} - z\|_2 - \varepsilon(z)/\sqrt{d^2 - 2d + 2}\} \geq 0 \quad \forall q \geq i_0.$$

This implies in particular that, for all $q \geq i_0$, one has

$$z^{k_q} \in V_{P^{k_{q+1}}},$$

and hence

$$\begin{aligned} & \|z^{k_{q+1}} - z^{k_q}\|_2 - \varepsilon(z^{k_q})/\sqrt{d^2 - 2d + 2} \\ & \geq \min_{z \in V_{P^{k_{q+1}}}} \{\|z^{k_{q+1}} - z\|_2 - \varepsilon(z)/\sqrt{d^2 - 2d + 2}\} \geq 0. \end{aligned}$$

Therefore, the subsequence $\{z^{k_q}\}_{q \geq i_0} \subset \{z^{k_q}\}_{q \in \mathbb{N}}$ satisfies property (ii). \square

COROLLARY 6.1. *If Algorithm 3 generates an infinite sequence $\{z^k\}_{k \in \mathbb{N}}$, then every accumulation point z^* is an optimal solution of Problem (UP).*

Proof. In view of Proposition 6.3, the proof proceeds along the same lines of arguments as the proof of Proposition 5.1. \square

7. Preliminary numerical results

The algorithms of the preceding sections along with some variants involving additional cuts were encoded in C++ with management of partition sets by AVL-trees and use of the LP-subroutine E04NFF of the NAG-library.

Stopping criterion was $\max\{-\lambda_1(U(z)), \lambda_{n-1}(U(z))\} < \varepsilon$ with chosen tolerance $\varepsilon > 0$. Variant (V1) is Algorithm 2 with additional cuts of the form $(a^k)^T z \leq b^k$ as discussed with Algorithm 3. Variant (V2) is Variant (V1) with additional Ramana-cuts (cf. Algorithm 1) modified in the way that whenever $\lambda_1(U(z^k)) < 0$, we use the cut

$$0 \leq (w^k)^T U(z^k) w^k,$$

where w^k is a normalized eigenvector of $\lambda_1(U(z^k))$ (cf. Ramana, 1993).

Variant (V3) is Algorithm 3, and Variant (V4) is Algorithm 3 with additional modified Ramana-cuts as in (V2). A comprehensive study on numerical experiments with randomly generated testproblems run on a SUN Sparc 10 workstation is given in Raber (1996), from where we report some typical examples and main conclusions. In the following tables, we use the abbreviations V for the variant, NIT for the required number of iterations; MNPS and MNC denote the maximal number of occurring partition sets and of total linear constraints, respectively, and λ_1 , λ_{n-1} and T are the final values of $\lambda_1(U(z))$, $\lambda_{n-1}(U(z))$ and computing times (sec.), respectively.

A first observation is that the numerical performance of the approaches depends heavily on specific properties of each test problem. For example, all of the variants can perform very poorly when distinct multiple optimal solutions of Problem (UP) exist such that different convergent subsequences $\{z^{k_q}\}$ are generated, whereas unique optimal solutions might lead to quite satisfactory performances. As illustrative example, consider the (UP)

$$\begin{aligned} \min \quad & z_{11} + \frac{1}{\sqrt{2}}z_{12} + \frac{1}{\sqrt{2}}z_{13} + z_{22} + \frac{1}{\sqrt{2}}z_{23} \\ \text{s.t.} \quad & -z_{11} - z_{22} \leq 0.5 \\ & 0 \leq z_{ii} \leq 1 \quad i = 1, 2 \\ & 0 \leq z_{ij} \leq \sqrt{2} \quad 1 \leq i < j \leq 3 \\ & U(z) \in \mathcal{U}_3 \end{aligned} \tag{7.1}$$

with $U(z) = E_{33} + \sum_{i=1}^2 z_{ii} E_{ii} + \sum_{i=1}^2 \sum_{j=i+1}^3 z_{ij} \frac{1}{\sqrt{2}}(E_{ij} + E_{ji})$ arising from the simple quadratic problem

$$\begin{aligned} \min \quad & x_1^2 + x_1x_2 + x_2^2 + x_1 + x_2 \\ \text{s.t.} \quad & -x_1^2 - x_2^2 \leq 0.5 \\ & 0 \leq x_i \leq 1, i = 1, 2, \end{aligned} \tag{7.2}$$

having convex objective but a ‘reverse’ convex constraint. Problem (7.1) has the two optimal solutions $z^1 = (0.5, 0.0, 1.0, 0.0, 0.0)$ and $z^2 = (0.0, 0.0, 0.0, 0.5, 1.0)$, and for $\varepsilon = 0.1$, we obtain the poor performances shown in Table 1.

On the other hand, Problem (7.1) with objective function

$$z_{11} + \frac{1}{\sqrt{2}}z_{12} + \frac{1}{\sqrt{2}}z_{13} + z_{22}$$

which arises from (7.1) by omitting the last term $\frac{1}{\sqrt{2}}z_{23}$ of the objective (resp. from (7.2) by omitting the last term x_2) yields the results depicted in Table 2.

For unary problems not necessarily derived from all-quadratic optimization, it is clear that algorithmic performance does essentially also depend on the form of U^0 and the orthonormal basis U^i , $i = 1, \dots, d$.

Table 1. Problem (7.1) with $\varepsilon = 0.1$

V	NIT	MNPS	MNC	λ_1	λ_{n-1}	T
(V1)	3804	4167	39	0.08845	0.09883	100.26
(V2)	2947	3123	75	0.06801	0.09615	120.68
(V3)	179203	136062	127	0.09937	0.09979	7317
(V4)	8448	4191	206	0.09612	0.09746	550

Table 2. Modified problem (7.1)

ε	V	NIT	MNPS	MNC	λ_1	λ_{n-1}	T
0.1	(V1) and (V3)	9	1	19	-0.06449	0.0	0.14
0.1	(V2) and (V4)	5	1	21	-0.01019	0.04281	0.11
0.001	(V1) and (V3)	13	1	23	-0.00078	0.0	0.21
0.001	(V2) and (V4)	8	1	30	-2.6e-07	0.00015	0.17
0.000001	(V1) and (V3)	17	1	27	-9.6e-06	0.0	0.28
0.000001	(V2) and (V4)	9	1	33	-7.0e-09	5.2e-06	0.21

Table 3. Numerical results for $n = 7, d \leq n$

ε	d	V	NIT	MNPS	MNC	λ_1	λ_{n-1}	T
0.1	3	all	1	1	26	0.0	0.09236	0.03
0.1	4	(V1)	7	9	32	-0.08843	0.08267	0.20
0.1	4	(V2) and (V4)	3	1	34	0.0	0.05456	0.10
0.1	4	(V3)	5	2	33	-0.09423	0.08175	0.14
0.1	5	(V1)	1917	3276	55	-0.09378	0.09995	67.28
0.1	5	(V2)	28	22	54	0.0	0.09481	1.17
0.1	5	(V3)	1665	1223	85	-0.08985	0.09907	62.65
0.1	5	(V4)	13	1	58	0.0	0.07576	0.40
0.1	6	(V2)	16	6	62	0.0	0.09612	0.78
0.1	6	(V4)	13	1	62	0.0	0.09618	0.59
0.1	7	(V2)	21	27	61	0.0	0.09953	1.58
0.1	7	(V4)	18	7	66	-0.00176	0.05844	1.04
0.01	3	(V2) and (V4)	6	1	38	0.0	0.00305	0.13
0.01	4	(V2) and (V4)	7	1	43	0.0	0.00919	0.2
0.01	6	(V2)	39	21	72	0.0	1.5e-12	2.14
0.01	6	(V4)	16	1	68	0.0	1.5e-12	0.72

For example, for $U^0 = 0$, $U^i = E_{ii}$, $i = 1, \dots, d$, we obviously have $U(z) \in \mathcal{U}$ only on feasible points on the coordinate axes, and it would suffice to investigate the intersection points of the coordinate axes with the boundary of the polytope $\{z : Az \leq b\}$. Since, however, no practical application of unary programs with such simple matrices is known to us, in the numerical experiments in Raber (1996), we chose $n \in \mathbb{N}$ and used (similarly to the (UP) arising from quadratic problems)

$$\begin{aligned} U^0 &= E_{nn}, U^i = E_{ii}, 1 \leq i \leq \min\{n-1, d\}, \\ U^i &= \frac{1}{\sqrt{2}}(E_{\ell j} + E_{j\ell}), \quad \text{where } 1 \leq \ell < j \leq n, \min\{n-1, d\} \leq i \leq d \end{aligned} \tag{7.3}$$

such that an ONS results (which implies that we must have $d \leq \binom{n}{2} + n - 1$).

Typical results obtained for different problem sizes have been quite similar to the figures in Table 3 where we chose $n = 7$ and various dimensions $d \leq n$.

The variants (V2) and (V4) which use the additional modified Ramana cut always outperformed the variants (V1) and (V3), respectively, so that the latter approaches are not considered for $\varepsilon = 0.01$.

8. Conclusion

Previously proposed algorithms for solving unary programs cannot guarantee convergence to an optimal solution. The present article overcomes this drawback by presenting two convergent approaches which are based on sufficiently deep non-linear cuts and subsequent simplicial inner approximation. Numerical performance depends heavily on specific problem characteristics and on the form of the matrices defining the affine matrix mapping, and is not very encouraging when applied to unary programs arising from indefinite all-quadratic optimization problems. This is mainly due to the considerable increase of the number of variables from n to $d = \binom{n+1}{2} + n$. Further research should aim at the construction of deeper cuts and at new characterizations of unarity of the matrix mapping for the specific practically relevant matrices U^i . Another direction of ongoing research for solving indefinite all-quadratic problems attempts to construct partitioning methods in the original space combined with suitable relaxation techniques (cf. Al-Khayyal et al., 1945; Raber, 1996).

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