On regular simplex division in copositivity detection

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Abstract. Over the last decades checking copositivity of matrices by simplicial subdivision of the unit simplex has made a big progress. Recently it has been shown that surprisingly the use of regular simplicial subdivisions may have some advantage over traditional iterative bisection of simplices. In this contribution, we pose the question whether regular subdivisions may provide opportunities in copositivity testing.

INTRODUCTION

Copositivity plays an important role in combinatorial and quadratic optimization. Setting up a linear optimization problem over the copositive cone leads to exact reformulations of combinatorial problems, for example, maximum clique [1]. A symmetric $n \times n$ matrix A is certified to be noncopositive when $\exists x \in S_0,\ x^T Ax < 0$, with unit simplex

$$S_0 = \{x \in \mathbb{R}^n \mid \sum_{i=1}^{n} x_i = 1;\ x_i \geq 0,\ \ i = 1, \ldots, n\}. \tag{1}$$

A sub-simplex $S \subseteq S_0$ can be defined by a matrix of vertices V with vertex v_j as column of V. For S_0, V is the identity matrix $E = (e_1, \ldots, e_n)$. Given vertex matrix V, simplex S is defined by

$$x \in S \iff x = V\lambda;\ \sum_{i=1}^{n} \lambda_i = 1;\ \lambda_i \geq 0,\ \ i = 1, \ldots, n. \tag{2}$$

Computational procedures like the one in [2] can either certify that a matrix is not copositive, or prove it is so-called ϵ-copositive.

Definition 1 *Matrix A is certified ϵ-copositive for $\epsilon \geq 0$, if $\forall x \in S_0, x^T Ax \geq -\epsilon$.*

A related problem is the standard quadratic program

$$f^* := \min_{x \in S_0} f(x) := x^T Ax. \tag{3}$$

Clearly, if $f^* < 0$, then A is not copositive and if $f^* \geq -\epsilon$, A is ϵ-copositive.

Algorithm 1 uses a branch-and-bound method to perform an exhaustive search for $f(x) < 0,\ x \in S_0$. The working set Λ stores the pending simplices to be evaluated. A simplex from Λ is selected on line 8 to be divided. Points in each simplex are evaluated in procedure *EvalPointsInS()* (see lines 1 and 11) looking for a negative value of f. Each

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Algorithm 1 IsAϵ-copositive (A, ϵ)

Require: A: matrix, ϵ: accuracy.
1: **if** EvalPointsInS(S_0)<0 **then**
2:     **return** False
3: **if** Discard(S_0, ϵ) **then**
4:     **return** False
5: $\Lambda := \{S_0\}$ {Set of pending of evaluation sub-simplices}
6: $\Omega := \{\emptyset\}$ {Set of discarded sub-simplices}
7: **while** $\Lambda \neq \{\emptyset\}$ **do**
8:     $S \leftarrow \Lambda$ $\{\Lambda := \Lambda \setminus \{S\}\}$
9:     $S_1, \ldots, S_j$:=Divide (S)
10:     **for** $S_i,\ i = 1, \ldots, j$ **do**
11:         **if** EvalPointsInS(S_i)<0 **then**
12:             **return** False
13:         **if** Discard(S_i, ϵ)=False **then**
14:             $\Lambda \leftarrow S_i$ $\{\Lambda := \Lambda \cup \{S_i\}\}$
15: **return** True

simplex is checked to be ϵ-copositive and therefore it is discarded from the search (see lines 3 and 13). The Algorithm results in True when no negative point is found and A is proven to be ϵ-copositive.

ϵ-copositivity certification by simplicial refinement requires much more computation than verifying non-copositivity of a matrix. More recent implementations [3] that also include parallel computing show that verifying non-copositivity of matrices can be done for a dimension n up to several thousands. However, certifying ϵ-copositivity of a copositive matrix is limited to a size up to $n = 22$ in a reasonable time. In the implemented simplicial partitioning algorithms [2, 3] the edge (i, j) with the most negative value $v_i^T A v_j$ is subdivided aiming at finding a point x with negative value $f(x) = x^T A x$ quickly in the case of a non-copositive matrix. The question is whether one could find a way to make certification of ϵ-copositivity faster.

Moreover, it is known that branch and bound techniques like Algorithm 1 require an efficient management of memory storage of the underlying search tree and its nodes. A regular simplex can be determined by its centre and radius. Therefore, the regular simplex refinement [4] and a Depth-First search are candidates to reduce the use of memory and to facilitate the computational requirement. This contribution investigates how to apply the regular division to achieve the aim of efficient copositivity detection.

REGULAR SIMPLICES

A regular simplex Δ has a center c and a radius ρ which define its vertex matrix as

$$V = c\mathbf{1}^T + \rho D, \tag{4}$$

where $\mathbf{1}$ is the all ones vector and $D = (d_1, \ldots, d_n) = E - \frac{1}{n}\mathbf{1}\mathbf{1}^T$ is a symmetric matrix with the directions from the center towards the regular simplex vertices. Notice that the center of the unit simplex S_0 is $c = \frac{1}{n}\mathbf{1}$, whereas its radius, that is the step size relative to the deviation matrix D, is 1.

The vertices of an upside down, ∇ simplex are described by

$$V = c\mathbf{1}^T - \rho D. \tag{5}$$

POSITIVE SPHERES

Given a point c with $f(c) > 0$, a ball $B(c, \delta)$ around c on S_0 can be described where it is certified that $f(x) \geq 0$. For that we focus on $x = (c + h) \in S_0$, such that $\sum_j h_j = 0$. We can consider a point p in the ball $B(0, \delta)$ and project to $h = Dp$. Let $H = DAD$ and $g = DAc$ in order to simplify notation. We have that

$$f(x) = f(c + h) = f(c + Dp) = f(c) + 2g^T p + p^T H p. \tag{6}$$

Given that $f(c) > 0$, we now bound the other two terms from below. For the second term, the inner product with $||p|| \leq \delta$ is minimum for $p = -\delta\frac{g}{||g||}$, such that $g^T p \geq -\delta||g||$. For the third term, $p^T H p \geq \delta^2\mu_1$, where μ_1 is the minimum eigenvalue of H. In total, we are certain that $f(x)$ is nonnegative when δ is such that

$$f(x) \geq f(c) - 2\delta||g|| + \mu_1\delta^2 \geq 0. \tag{7}$$

In our search for a copositivity proof, this result can be used in several ways. First of all, given a regular simplex $\Delta(c, r)$, then a lower bound of f on $\Delta(c, r)$ is given by

$$LB(c, r) := f(c) - 2\delta||g|| + \mu_1\delta^2, \tag{8}$$

with $\delta = r\sqrt{\frac{n-1}{n}}$. If $LB(c, r) \geq 0$ then f is nonnegative on $\Delta(c, r)$.
Secondly, the lower bounding can also be used to derive a $\nabla(c, \rho)$ simplex around c, where it is certified that f has a nonnegative value. We have that typicially $f(c) > 0$ and $\mu_1 < 0$. Certain cases may apply. If $\mu_1 = 0$, we have $\delta = \frac{f(c)}{2||g||}$. If $\mu_1 > 0$, one may have $\mu_1 f(c) > ||g||^2$, where we know that f is positive everywhere on the unit simplex. Usually, $f(x)$ is nonnegative in a ball $B(c, \delta)$ for

$$\delta = \frac{||g|| - \sqrt{||g||^2 - \mu_1 f(c)}}{\mu_1}. \tag{9}$$

Considering c as the centroid of regular simplex Δ or ∇ with radius ρ, one proves the f is nonnegative for

$$\rho = \delta\sqrt{\frac{n}{n-1}}. \tag{10}$$

$e\nabla$ DIVISION: REMOVING A REGULAR ∇ SIMPLEX

From a $\Delta(c, r)$ simplex, the e∇ division removes a simplex $\nabla(c, \rho)$ where it is proven that $f(x) \geq 0$ using the positive sphere eq. (10) around c. The following cases may occur:

a) $\delta \geq r\sqrt{\frac{n-1}{n}}$. The ball B covers Δ and the simplex is discarded because $f(x) \geq 0$ over Δ.

b) $\delta > r\sqrt{\frac{n-2}{2n}}$. The ball B is not completely inside Δ (left image in Figure 1) and we generate n sub-simplices $\Delta(C_i, R_i)$ given by

$$C_i = c + (r - \mu)d_i \tag{11}$$

and

$$R_i = \mu \tag{12}$$

where $\mu = \frac{1}{2}\left(r - \sqrt{r^2 - 2(r^2\frac{n-1}{n} - \delta^2)}\right)$.

c) $\delta \leq r\sqrt{\frac{n-2}{2n}}$. The ball B does not cover the midpoints of the edges and may even be completely inside Δ (right image in Figure 1) and we generate n sub-simplices $\Delta(C_i, R_i)$ given by

$$C_i = c + \frac{\rho + r}{n}d_i \tag{13}$$

and

$$R_i = \frac{n-1}{n}r - \frac{1}{n}\rho \tag{14}$$

Notice that in case c) (right image in Figure 1) the ∇ simplex is inscribed in the ball B, but it is not in case b) (left image in Figure 1).

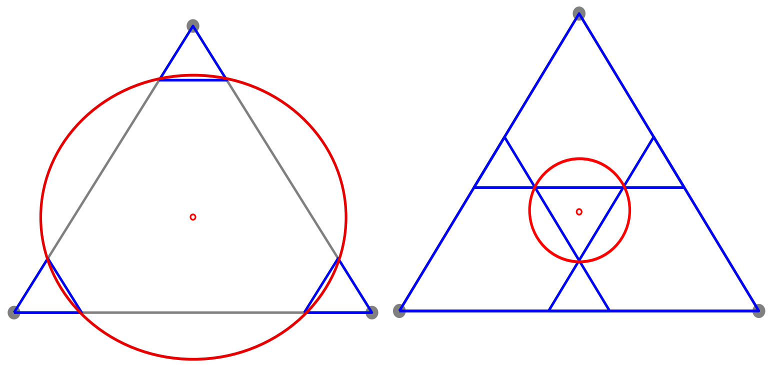

FIGURE 1. Examples of $e\nabla$ division for n=3.

Dealing with overlap in $e\nabla$ division

The division of a regular simplex using regular sub-simplices generates overlap for dimension $n > 3$ [5]. In the right image of Figure 1, the $e\nabla$ division with $\rho < r(n+1)$ generates ovelap among sbsimplices $\Delta(C_i, R_i)$. Using regular division, the area of S_0 discarded from the search is defined by the union of regular ϵ-copositive sub-simplices. A set Ω of discarded simplices can be applied in the Algorithm 1 to store ϵ-copositive sub-simplices. In case all siblings are proven to be ϵ-copositive, the parent simplex can be stored in Ω instead of them. Therefore, a new sub-simplex covered by a discarded sub-simplex is not evaluated. Given $\Delta_1 = \{c^{[1]}, r^{[1]}\}$ and $\Delta_2 = \{c^{[2]}, r^{[2]}\}$, Δ_2 is covered by Δ_1 if [5]:

$$c_j^{[2]} - c_j^{[1]} + \frac{r^{[1]} - r^{[2]}}{n} \geq 0 \quad j = 1, \ldots, n. \tag{15}$$

We will study the efficiency of the proposed $e\nabla$ division, taking into account the possible overlap of simplices in the simplicial refinement for copositive detection.

Conclusion

This work studies the use of regular simplicial subdivisions in copositivity detection. We study how regular simplex division could improve that process. The main advantage of using a regular space in this work is positive spheres, which allow to remove big noncopositivity areas before dividing the space.

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