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STRONG CONVEX NONLINEAR RELAXATIONS OF THE POOLING PROBLEM: EXTREME POINTS

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Abstract. We investigate new convex relaxations for the pooling problem, a classic nonconvex production planning problem in which products are mixed in intermediate pools in order to meet quality targets at their destinations. In this technical report, we characterize the extreme points of the convex hull of our nonconvex set, and show that they are not finite, i.e., the convex hull is not polyhedral. This analysis was used to derive valid nonlinear convex inequalities and show that, for a specific case, they characterize the convex hull of our set. The new valid inequalities and computational results are presented in [6].

1. Introduction. The pooling problem is a classic nonconvex nonlinear problem introduced by Haverly in 1978, see [4]. The problem consists in routing flow through a feed forward network from inputs through pools to output products. The material that is introduced at inputs has known quality for certain attributes. The task is to find a flow distribution that respects quality restrictions on the output products. As is standard in the pooling problem, we assume linear blending, i.e., the attributes at a node are mixed in the same proportion as the incoming flows. As the quality of the attributes in the pools is dependent on the decisions determining amount of flow from inputs to the pools, the resulting constraints include bilinear terms.

There are many applications of the pooling problem, including petroleum refining, wastewater treatment, and general chemical engineering process design [1, 3, 5, 9]. This is confirmed by an interesting analysis performed by Ceccon et al. [2] whose method allows to recognize pooling problem structures in general mixed integer nonlinear programming problems.

The aim of this work is to strengthen the relaxation of the strongest known formulation, i.e., the so-called pq -formulation proposed in [8, 10]. By focusing on a single output product, a single attribute, and a single pool, and aggregating variables, we derive a structured nonconvex 5-variable set that is a relaxation of the original feasible set. The description of this set contains one bilinear term which captures some of the nonconvex essence of the problem. In this paper, we analyze the extreme points of the relaxation and provide a complete list of all possible and in general infinitely many extreme points. The relaxation is thus not a polyhedron.

Valid convex inequalities for this set directly translate to valid inequalities for the original pooling problem. In [6], we derive valid linear and nonlinear convex inequalities for the set. For three cases determined by the parameters of the set, we demonstrate that a subset of these inequalities define the convex hull of the set. Finally, we conduct an illustrative computational study that demonstrates that these inequalities can indeed improve the relaxation quality over the pq -formulation, particularly on instances in which the underlying network is sparse, which are precisely the instances in which pq -formulation relaxation has the largest gap to the optimal value.

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2. Mathematical Formulation and Relaxation. There are multiple formulations for the pooling problem, primarily differing in the modeling of the concentrations of attributes throughout the network. We base our work on the state-of-the-art *pq-formulation*.

We are given a directed graph $G = (V, A)$ where V is the set of vertices that is partitioned into inputs I , pools L , and outputs J , i.e., $V = I \cup L \cup J$. For a node $u \in V$, the sets $I_u \subseteq I$, $L_u \subseteq L$, $J_u \subseteq J$ denote the inputs, pools, and outputs, respectively, that are directly connected to u . Arcs $(i, j) \in A$ link inputs to pools, pools to outputs, and inputs directly to outputs, i.e., $A \subseteq (I \times L) \cup (L \times J) \cup (I \times J)$. In particular, pool-to-pool connections are not considered.

The *pq*-formulation of the pooling problem uses the following decision variables:

- x_{ij} is the flow on $(i, j) \in A$;
- $q_{i\ell}$ is the proportion of flow to pool $\ell \in L$ that comes from input $i \in I_\ell$;
- $w_{i\ell j}$ is the flow from $i \in I$ through pool $\ell \in L_i$ to output $j \in J_\ell$.

With these definitions, the *pq*-formulation of the pooling problem is:

$$\begin{aligned}
(1a) \quad & \min \quad \sum_{(i,j) \in A} c_{ij} x_{ij} \\
(1b) \quad & \text{s.t.} \quad \sum_{\ell \in L_i} x_{i\ell} + \sum_{j \in J_i} x_{ij} \leq C_i && \text{for all } i \in I \\
(1c) \quad & \sum_{j \in J_\ell} x_{\ell j} \leq C_\ell && \text{for all } \ell \in L \\
(1d) \quad & \sum_{\ell \in L_j} x_{\ell j} + \sum_{i \in I_j} x_{ij} \leq C_j && \text{for all } j \in J \\
(1e) \quad & \sum_{i \in I_\ell} q_{i\ell} = 1 && \text{for all } \ell \in L \\
(1f) \quad & w_{i\ell j} = q_{i\ell} x_{\ell j} && \text{for all } i \in I_\ell, \ell \in L_j, j \in J \\
(1g) \quad & x_{i\ell} = \sum_{j \in J_\ell} w_{i\ell j} && \text{for all } i \in I_\ell, \ell \in L \\
(1h) \quad & \sum_{i \in I_j} \bar{\gamma}_{ijk} x_{ij} + \sum_{\ell \in L_j} \sum_{i \in I_\ell} \bar{\gamma}_{ijk} w_{i\ell j} \leq 0 && \text{for all } j \in J, k \in K \\
(1i) \quad & \sum_{i \in I_\ell} w_{i\ell j} = x_{\ell j} && \text{for all } j \in J_\ell, \ell \in L \\
(1j) \quad & \sum_{j \in J_\ell} w_{i\ell j} \leq C_\ell q_{i\ell} && \text{for all } i \in I_\ell, \ell \in L \\
(1k) \quad & 0 \leq x_{ij} \leq C_{ij} && \text{for all } (i, j) \in A \\
(1l) \quad & 0 \leq q_{i\ell} \leq 1 && \text{for all } i \in I_\ell, \ell \in L.
\end{aligned}$$

The objective (1a) is to minimize the production cost, where c_{ij} is the cost per unit flow on arc (i, j) . Inequalities (1b)–(1d) represent capacity constraints on inputs, pools, and outputs, respectively, where here $C_i, i \in I$, $C_\ell, \ell \in L$, and $C_j, j \in J$ are given capacity limits. Equations (1e) enforce that the proportions at each pool sum up to one. Equations (1f) and (1g) define the auxiliary variables $w_{i\ell j}$ and link them to the flow variables. (1h) formulates the quality constraints for each attribute k in the set of attributes K . The coefficients $\bar{\gamma}_{ijk}$ represent the excess of attribute quality k of the material from input i with respect to the upper quality bound at output j .

The upper quality bound is met when there is no excess, i.e., the total excess is not positive. For brevity, we do not include lower bounds on attribute quality at the final products, but these can be easily added. Inequalities (1i) and (1j) are redundant in the formulation but are not when the nonconvex constraints (1f) are not enforced as is done in a relaxation-based solution algorithm. These two constraints constitute the difference between the q - and the pq -formulation and are responsible for the strong linear relaxation of the latter. Finally, (1k) limits the flow on each arc (i, j) to a given capacity C_{ij} .

A linear programming relaxation of the pq -formulation is obtained by replacing the constraints (1f) with the McCormick inequalities derived using the bounds (1k) and (1l):

$$(2a) \quad w_{ilj} \leq x_{lj}, \quad w_{ilj} \leq C_{lj}q_{il}, \quad \text{for all } i \in I_\ell, \ell \in L_j, j \in J$$

$$(2b) \quad w_{ilj} \geq 0, \quad w_{ilj} \geq C_{lj}q_{il} + x_{lj} - C_{lj}, \quad \text{for all } i \in I_\ell, \ell \in L_j, j \in J.$$

We refer to the relaxation obtained by replacing (1f) with (2) as the *McCormick relaxation*. Our goal is to derive tighter relaxations of the pooling problem by considering more of the problem structure.

3. Strong Convex Nonlinear Relaxations. To derive a stronger relaxation of the pooling problem, we seek to identify a relaxed set that contains the feasible region of the pooling problem, but includes some of the key nonconvex structure. First, we consider only one single attribute $k \in K$ and relax all constraints (1h) concerning the other attributes. Next, we consider only one output $j \in J$, and remove all nodes and arcs which are not in a path to output j . In particular, this involves all other outputs. Then, we focus on pool $\ell \in L$ with the intention to split flows into two categories: the flow through pool ℓ and aggregated flow on all paths not passing through pool ℓ , also called “by-pass” flow. Finally, we aggregate all the flow from the inputs to pool ℓ .

As a result, we are left with five decision variables:

1. the total flow through the pool, i.e., the flow x_{lj} from pool ℓ to output j
2. the total flow z_{lj} over the by-pass, i.e., the flow to output j that does not pass through pool ℓ

$$z_{lj} := \sum_{i \in I_j} x_{ij} + \sum_{\ell' \in L_j | \ell' \neq \ell} x_{\ell'j}$$

3. the contribution $u_{k\ell j}$ of the flow through pool ℓ to the excess of attribute k at output j , i.e.,

$$u_{k\ell j} := \sum_{i \in I_\ell} \gamma_{kij} w_{ilj}$$

4. the contribution $y_{k\ell j}$ of by-pass flow to the excess of attribute k at output j , i.e.,

$$y_{k\ell j} := \sum_{i \in I_j} \gamma_{kij} x_{ij} + \sum_{\ell' \in L_j | \ell' \neq \ell} \sum_{i \in I_{\ell'}} \gamma_{kij} w_{i\ell'j}$$

5. the attribute quality $t_{k\ell j}$ of the flow through pool ℓ , i.e.,

$$t_{k\ell} := \sum_{i \in I_\ell} \gamma_{kij} q_{il}.$$

With these decision variables, the quality constraint associated with attribute k of output j and the capacity constraint associated with output j from (1) can be written

as:

$$(3a) \quad y_{k\ell j} + u_{k\ell j} \leq 0, \quad \text{for all } k \in K, j \in J$$

$$(3b) \quad z_{\ell j} + x_{\ell j} \leq C_j, \quad \text{for all } j \in J.$$

A key property of these new decision variables is the relation between the flow and quality in the pool with the excess of the attribute contributed by the flow through the pool

$$(4) \quad u_{k\ell j} = x_{\ell j} t_{k\ell} \quad \text{for all } \ell \in L, j \in J,$$

which is valid because using (1f) and (1i)

$$u_{k\ell j} = \sum_{i \in I_\ell} \gamma_{kij} w_{i\ell j} = \sum_{i \in I_\ell} \gamma_{kij} q_{i\ell} x_{\ell j} = \sum_{i \in I_\ell} \gamma_{kij} q_{i\ell} \sum_{i' \in I_\ell} w_{i'\ell j} = t_{k\ell} x_{\ell j}.$$

In order to derive bounds on the new decision variables we define the parameters $\underline{\gamma}_{k\ell}$ and $\bar{\gamma}_{k\ell}$ representing bounds on the excess of attribute k over inputs that are connected to pool ℓ , and $\underline{\beta}_{k\ell j}$ and $\bar{\beta}_{k\ell j}$ representing bounds on the excess of attribute k over inputs that are connected to output j via a by-pass flow :

$$\underline{\gamma}_{k\ell} = \min_{i \in I_\ell} \gamma_{ki} \quad \underline{\beta}_{k\ell j} = \min\{\gamma_{ki} : i \in I_j \cup \bigcup_{\ell' \in L \setminus \{\ell\}} I_{\ell'}\}$$

$$\bar{\gamma}_{k\ell} = \max_{i \in I_\ell} \gamma_{ki} \quad \bar{\beta}_{k\ell j} = \max\{\gamma_{ki} : i \in I_j \cup \bigcup_{\ell' \in L \setminus \{\ell\}} I_{\ell'}\}.$$

We thus have,

$$(5a) \quad t_{k\ell} \in [\underline{\gamma}_{k\ell}, \bar{\gamma}_{k\ell}] \quad \text{for all } k \in K, \ell \in L$$

$$(5b) \quad \underline{\beta}_{k\ell j} z_{\ell j} \leq y_{k\ell j} \leq \bar{\beta}_{k\ell j} z_{\ell j}, \quad \text{for all } k \in K, \ell \in L, j \in J.$$

Despite the many relaxations performed in deriving this set, the nonconvex relation (4), which relates the contribution of the excess from the pool to the attribute quality of the pool and the quantity passing through the pool, still preserves a key nonconvex structure of the problem.

With these variables and constraints we now formulate the relaxation of the pooling problem that we want to study. To simplify notation, we drop the fixed indices ℓ, j , and k . Gathering the constraints (3), (4), and (5), together with nonnegativity on the z and x variable, we define the set T as those $(x, u, y, z, t) \in \mathbb{R}^5$ that satisfy:

$$(6) \quad u = xt$$

$$(7) \quad y + u \leq 0$$

$$(8) \quad z + x \leq C$$

$$(9) \quad y \leq \bar{\beta}z$$

$$(10) \quad y \geq \underline{\beta}z$$

$$z \geq 0, x \in [0, C], t \in [\underline{\gamma}, \bar{\gamma}].$$

We can assume, without loss of generality, that $C = 1$ by scaling the variables x, u, y , and z by C^{-1} .

Due to the nonlinear equation $u = xt$, T is a nonconvex set unless x or t is fixed. Using the bounds $0 \leq x \leq 1$ and $\underline{\gamma} \leq t \leq \bar{\gamma}$, the constraint $u = xt$ can be relaxed by the McCormick inequalities [7]:

$$\begin{aligned} (11) \quad & u - \underline{\gamma}x \geq 0 \\ (12) \quad & \bar{\gamma}x - u \geq 0 \\ (13) \quad & u - \underline{\gamma}x \leq t - \underline{\gamma} \\ (14) \quad & \bar{\gamma}x - u \leq \bar{\gamma} - t. \end{aligned}$$

Equations (11)–(14) provide the best possible convex relaxation of the feasible points of $u = xt$ given that x and t are in the bounds mentioned above. However, replacing the nonconvex constraint $u = xt$ with these inequalities is not sufficient to define $\text{conv}(T)$.

Note that (11)–(14) imply the bounds $0 \leq x \leq 1$ and $\underline{\gamma} \leq t \leq \bar{\gamma}$. Also the bound constraint $z \geq 0$ is implied by (9) and (10). Thus, we define the standard relaxation of the set T by

$$R^0 := \{(x, u, y, z, t) : (7)\text{--}(14)\}.$$

Every convex set is described completely by its extreme points and rays. The set T is bounded and so has no extreme rays.

3.1. Extreme Points Analysis. In this section, we provide a complete list of the extreme points of $\text{conv}(T)$. Recall that a point $p \in T$ is extreme if it can not be represented as convex combination of two distinct points from the set, i.e., if there are not two other points $p_1, p_2 \in T$ with $p_1 \neq p_2$ and a $\lambda \in (0, 1)$ with $p = \lambda p_1 + (1 - \lambda)p_2$. The set of extreme points of $\text{conv}(T)$ is denoted by $\text{ext}(\text{conv}(T))$. Note that $\text{ext}(\text{conv}(T)) \subset T$.

The following lemma states that extreme points either transport no material at all ($z + x = 0$) or that the capacity of the output is fully used ($z + x = 1$).

LEMMA 1. *If $p = (x, t, z, y, u) \in \text{ext}(\text{conv}(T))$, then $z + x \in \{0, 1\}$.*

Proof. Suppose there was a $p = (x, t, z, y, u) \in \text{ext}(\text{conv}(T))$ with $0 < z + x < 1$. Then $p \in T$ and there exists an $\epsilon > 0$ such that scaling all variable except t with $(1 + \epsilon)$ and scaling them with $(1 - \epsilon)$ yields two feasible points $p_+ \in T$ and $p_- \in T$. Since $p = 0.5p_+ + 0.5p_-$, p is not extreme which is a contradiction. \square

When there is no flow though the network, the concentration in the pool can take arbitrary values in the bounds. The result are two extreme points for this case.

THEOREM 2. *The points $p = (x, t, z, y, u) \in \text{ext}(\text{conv}(T))$ with $z + x = 0$ are $(0, \underline{\gamma}, 0, 0, 0)$ and $(0, \bar{\gamma}, 0, 0, 0)$.*

Proof. Since extreme points are in T , the condition $z + x = 0$ implies $z = x = u = y = 0$. The only variable that is not fixed is t which can vary freely in its bound interval $[\underline{\gamma}, \bar{\gamma}]$. Hence the two extreme points. \square

By Lemma 1, all remaining extreme points fulfill $z + x = 1$ and Lemma 3 reveals the structure of them.

LEMMA 3. *If $p = (x, t, z, y, u) \in \text{ext}(\text{conv}(T))$ and $z + x = 1$, then either*

- $x = 1$,
- $z = 1$, or
- $y + u = 0$.

Proof. Let $p = (x, t, z, y, u) \in \text{ext}(\text{conv}(T))$ with $x < 1$, $z < 1$, and $y + u < 0$. Let K such that $y = Kz$. Define

$$\begin{aligned} p_+ &= (x(1 + \epsilon), t, 1 - x(1 + \epsilon), K(1 - x(1 + \epsilon)), tx(1 + \epsilon)) \\ p_- &= (x(1 - \epsilon), t, 1 - x(1 - \epsilon), K(1 - x(1 - \epsilon)), tx(1 - \epsilon)) \end{aligned}$$

Since $p \in T$, both p_+ and p_- , are in T and $p = 0.5p_+ + 0.5p_-$. Therefore, p is not extreme and not all three inequalities can be strict simultaneously. \square

The following two theorems characterize the extreme points with $z = 1$ and with $x = 1$.

THEOREM 4. *If $\underline{\beta} > 0$, then $\text{ext}(\text{conv}(T))$ has no extreme points with $z = 1$.*

If $\underline{\beta} \leq 0$, then the points $p = (x, t, z, y, u) \in \text{ext}(\text{conv}(T))$ with $z = 1$ are

- $(0, \underline{\gamma}, 1, \underline{\beta}, 0)$ and $(0, \bar{\gamma}, 1, \underline{\beta}, 0)$ and
- $(0, \underline{\gamma}, 1, \min(\bar{\beta}, 0), 0)$ and $(0, \bar{\gamma}, 1, \min(\bar{\beta}, 0), 0)$.

Proof. Since $z = 1$, we have $x = u = 0$, $y \in [\underline{\beta}, \bar{\beta}] \cap [-\infty, 0]$, and $t \in [\underline{\gamma}, \bar{\gamma}]$. This set becomes infeasible if $[\underline{\beta}, \bar{\beta}] \cap [-\infty, 0] = \emptyset$, i.e., if $\underline{\beta} > 0$. If $\underline{\beta} \leq 0$, the extreme points are the vertices of the hyperrectangle $\{0\} \times [\underline{\gamma}, \bar{\gamma}] \times \{1\} \times [\underline{\beta}, \min(\bar{\beta}, 0)] \times \{0\}$. \square

THEOREM 5. *If $\underline{\gamma} > 0$, then $\text{ext}(\text{conv}(T))$ has no extreme points with $x = 1$.*

If $\underline{\gamma} \leq 0$, then the points $p = (x, t, z, y, u) \in \text{ext}(\text{conv}(T))$ with $x = 1$ are

- $(1, \underline{\gamma}, 0, 0, \underline{\gamma})$ and
- $(1, \min(\bar{\gamma}, 0), 0, 0, \min(\bar{\gamma}, 0))$.

Proof. If $x = 1$, then $z = y = 0$, $u = t$. Since $t = u \leq 0$ and $t \in [\underline{\gamma}, \bar{\gamma}]$ the system is infeasible if $\underline{\gamma} > 0$ and there are not extreme points with $x = 1$. Otherwise, i.e., if $\underline{\gamma} \leq 0$, the extreme points with $x = 1$ are completely characterized by $t = \underline{\gamma}$ and $t = \min(\bar{\gamma}, 0)$. \square

The remaining extreme points fulfill $z + x = 1$ and $y + u = 0$. Using these two equations and propagating them through the defining inequalities of T , it is easy to see that the remaining extreme points have only two liberties and satisfy the following system which we denote by \tilde{T} :

$$(15) \quad -xt \leq \bar{\beta}(1 - x)$$

$$(16) \quad -xt \geq \underline{\beta}(1 - x)$$

$$x \in [0, 1]$$

$$t \in [\underline{\gamma}, \bar{\gamma}].$$

The remaining variables can be computed by substitution and other choices as x and t as variables describing the two liberties are possible. All extreme points of $\text{conv}(\tilde{T})$ are extreme points of $\text{conv}(T)$.

To attack \tilde{T} , we fix the variable t to $t = \alpha$ and define the set

$$T_\alpha := \{(x, t, z, y, u) \in T \mid z + x = 1, y + u = 0, t = \alpha \in [\underline{\gamma}, \bar{\gamma}]\}.$$

It is clear that $\text{conv}(\tilde{T}) = \text{conv}(\{T_\alpha \mid \alpha \in [\underline{\gamma}, \bar{\gamma}]\})$. Now, it is not clear anymore that all extreme points of T_α are extreme points of $\text{conv}(\tilde{T})$; some might actually lie in the interior of $\text{conv}(\tilde{T})$. We know, however, that the extreme point of T with $z + x = 1$ and $y + u = 0$ are in $\cup_{\alpha \in [\underline{\gamma}, \bar{\gamma}]} \text{ext}(T_\alpha)$.

THEOREM 6. The extreme points of T_α , $\alpha \notin \{\underline{\beta}, \overline{\beta}\}$, are completely characterized by

- $x = \max(0, \frac{\underline{\beta}}{\underline{\beta}-\alpha})$ and $x = \min(1, \frac{\overline{\beta}}{\overline{\beta}-\alpha})$ if $\alpha < \underline{\beta} < \overline{\beta}$
- $x = 0$ and $x = \min(1, \frac{\underline{\beta}}{\underline{\beta}-\alpha}, \frac{\overline{\beta}}{\overline{\beta}-\alpha})$ if $\underline{\beta} < \alpha < \overline{\beta}$
- $x = \max(0, \frac{\overline{\beta}}{\overline{\beta}-\alpha})$ and $x = \min(1, \frac{\underline{\beta}}{\underline{\beta}-\alpha})$ if $\underline{\beta} < \overline{\beta} < \alpha$

Proof. The set T_α has only one degree of freedom and every $p \in T_\alpha$ is of the form

$$p = (x, \alpha, 1 - x, -x\alpha, x\alpha)$$

for some x .

Working with (15), we get

$$x(\overline{\beta} - \alpha) \leq \overline{\beta} \quad \iff \quad x \begin{cases} \leq \frac{\overline{\beta}}{\overline{\beta}-\alpha} & \text{if } \overline{\beta} - \alpha > 0 \\ \geq \frac{\overline{\beta}}{\overline{\beta}-\alpha} & \text{if } \overline{\beta} - \alpha < 0 \end{cases}$$

For $\overline{\beta} - \alpha = 0$, the system is infeasible if $\overline{\beta} < 0$ and feasible with $x \in [0, 1]$ if $\overline{\beta} \geq 0$. (In any case, $\alpha = \overline{\beta}$ does not yield new extreme points for $\text{conv}(T)$, since the extreme points in this case are on the line between two previously known extreme points.)

Similar for (16)

$$x(\underline{\beta} - \alpha) \geq \underline{\beta} \quad \iff \quad x \begin{cases} \geq \frac{\underline{\beta}}{\underline{\beta}-\alpha} & \text{if } \underline{\beta} - \alpha > 0 \\ \leq \frac{\underline{\beta}}{\underline{\beta}-\alpha} & \text{if } \underline{\beta} - \alpha < 0 \end{cases}$$

Here, for $\underline{\beta} - \alpha = 0$, the system is infeasible if $\underline{\beta} > 0$ and feasible with $x \in [0, 1]$ if $\underline{\beta} \leq 0$. (Also in this case we don't get new extreme points for $\text{conv}(T)$.)

With the condition $\alpha \notin \{\underline{\beta}, \overline{\beta}\}$, we get three cases:

<p>case $\alpha < \underline{\beta} < \overline{\beta}$:</p> $x \leq \frac{\overline{\beta}}{\overline{\beta}-\alpha}$ $x \geq \frac{\underline{\beta}}{\underline{\beta}-\alpha}$	<p>case $\underline{\beta} < \alpha < \overline{\beta}$:</p> $x \leq \frac{\overline{\beta}}{\overline{\beta}-\alpha}$ $x \leq \frac{\underline{\beta}}{\underline{\beta}-\alpha}$	<p>case $\underline{\beta} < \overline{\beta} < \alpha$:</p> $x \geq \frac{\overline{\beta}}{\overline{\beta}-\alpha}$ $x \leq \frac{\underline{\beta}}{\underline{\beta}-\alpha}$
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which completes the proof. \square

Theorems 2, 4 and 5 provide a discrete set of extreme points of $\text{conv}(T)$ and Theorem 6 provides a continuous set of points that might or might not be extreme for $\text{conv}(T)$.

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