

# SUBMODULARITY AND VALID INEQUALITIES IN NONLINEAR OPTIMIZATION WITH INDICATOR VARIABLES

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**ABSTRACT.** We propose a new class of valid inequalities for mixed-integer nonlinear optimization problems with indicator variables. The inequalities are obtained by lifting polymatroid inequalities in the space of the 0–1 variables into conic inequalities in the original space of variables. The proposed inequalities are shown to describe the convex hull of the set under study under appropriate submodularity conditions. Moreover, the inequalities include the perspective reformulation and pairwise inequalities for quadratic optimization with indicator variables as special cases. Finally, we use the proposed methodology to derive ideal formulations of other mixed-integer sets with indicator variables.

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## 1. INTRODUCTION

Given a ground set  $N = \{1, \dots, n\}$ , a set function  $f : 2^N \rightarrow \mathbb{R}$  is submodular if

$$\rho_j(S) \geq \rho_j(T) \quad \forall j \in N \text{ and } \forall S \subseteq T \subseteq N \setminus \{j\},$$

where  $\rho_j(S) = f(S \cup \{j\}) - f(S)$  is the increment function. Submodularity plays a key role in combinatorial optimization [10], as submodular minimization problems can be solved in polynomial time [11, 14], and exploiting submodularity is also key to devising strong formulations for 0–1 optimization problems [6, 15]. However, despite recent works on using submodularity to derive strong formulations in mixed-integer nonlinear optimization [1, 4, 5], it is still unknown how to systematically exploit submodularity in the presence of both continuous and discrete variables. Our goal in this paper is precisely to show how to derive strong formulations when the continuous and discrete variables are linked by indicator constraints.

**Notation** For a set  $S \subseteq N$ , define  $x_S$  as the indicator vector of  $S$ , and define  $S_x$  as the support set of a vector  $x \in \{0, 1\}^N$ . For a set  $X \subseteq \mathbb{R}^N$ , let  $\text{conv}(X)$  denote the closure of the convex hull of  $X$ . We adopt the convention that  $a/0 = \infty$  if  $a > 0$  and  $a/0 = 0$  if  $a = 0$ .

## 2. VALID INEQUALITIES

Consider the set

$$X = \{x \in \{0, 1\}^N, y \in \mathbb{R}^N, t \in \mathbb{R} : f(x, y) \leq t, y_i(1 - x_i) = 0 \forall i \in N\}$$

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where  $f : [0, 1]^N \times \mathbb{R}^N \rightarrow \mathbb{R} \cup \{\infty\}$  is a function under study. For  $\alpha \in \mathbb{R}^n$ , define the set function  $g_\alpha : 2^N \rightarrow \mathbb{R} \cup \{\infty, -\infty\}$  as

$$g_\alpha(S) = \min_{y \in \mathbb{R}^S} \alpha'y + f(x_S, y). \quad (1)$$

Define  $A \subseteq B \subseteq \mathbb{R}^N$  as

$$B = \{\alpha \in \mathbb{R}^N : |g_\alpha(S)| < \infty \forall S \in N\}$$

$$A = \{\alpha \in B : g_\alpha \text{ is submodular}\}.$$

Finally, let  $v = ((1), \dots, (n))$  be a permutation of  $N$ , let  $N_i^v = \{(1), \dots, (i)\}$  and let  $\pi_i^v(\alpha) = g_\alpha(N_i^v) - g_\alpha(N_{i-1}^v)$ . Observe that  $\pi^v(\alpha)$  is an extreme point of the extended polymatroid associated with the submodular function  $g_\alpha$  [8].

**Proposition 1.** *For any  $\alpha \in A$ , the inequality*

$$-\alpha'y + g_\alpha(\emptyset) + \sum_{i=1}^n \pi_i^v(\alpha)x_{(i)} \leq t \quad (2)$$

is valid for  $\text{conv}(X)$ .

*Proof.* For any  $\alpha \in A$  and  $(x, y, t) \in X$ , we find

$$t + \alpha'y \geq f(x, y) + \alpha'y \geq g_\alpha(S_x) \geq g_\alpha(\emptyset) + \sum_{i=1}^n \pi_i^v(\alpha)x_{(i)},$$

where the last inequality follows from the fact that polymatroid inequalities describe of the convex lower envelope of the submodular function  $g_\alpha$  [13].  $\square$

Define  $\phi^v : [0, 1]^N \times \mathbb{R}^N \rightarrow \mathbb{R}$  as

$$\phi^v(x, y) = \max_{\alpha \in A} -\alpha'y + g_\alpha(\emptyset) + \sum_{i=1}^n \pi_i^v(\alpha)x_{(i)}$$

and let

$$\phi(x, y) = \max\{\phi^v(x, y) : v \text{ is a permutation of } N\}.$$

Obviously, the convex inequality

$$\phi(x, y) \leq t \quad (3)$$

is valid for  $\text{conv}(X)$ .

**Theorem 1.** *If  $b \in A$ , then the optimization problem*

$$z^* = \min_{x, y, t} a'x + b'y + t \text{ s.t. } \phi(x, y) \leq t, f(x, y) \leq t, x \in [0, 1]^N, y \in \mathbb{R}^N \quad (4)$$

has an optimal solution  $(x^*, y^*, t^*)$  integral in  $x^*$ .

*Proof.* Consider the relaxation

$$\hat{z} = \min a'x + b'y + t \quad (5a)$$

$$\text{s.t. } -b'y + g_b(\emptyset) + \sum_{i=1}^n \pi_i^v(b)x_{(i)} \leq t \quad \text{for all permutations } v \text{ of } N \quad (5b)$$

$$x \in [0, 1]^N, y \in \mathbb{R}^N, t \in \mathbb{R}. \quad (5c)$$

The terms involving the continuous variables cancel out, and problem (5) reduces to optimizing a linear function over the polymatroid associated with the submodular function  $g_b$ , thus is equivalent to  $\min_{x \in \{0,1\}^N} \sum_{i \in S_x} a_i + g_b(S_x)$  [13] and has an integral optimal solution  $x^*$  with objective value  $\hat{z} \leq z^*$ . Note that any point  $(x^*, y)$  with  $y \in \mathbb{R}^N$  is optimal for relaxation (5), but may be unfeasible for problem (4). Letting  $y^*$  be an optimal solution of (1) corresponding to  $S_{x^*}$ , we find that  $a'x^* + b'y^* + f(x^*, y^*) = \sum_{i \in S_{x^*}} a_i + g_b(S_{x^*}) = \hat{z}$ . Setting  $t^* = f(x^*, y^*)$  we find that  $(x^*, y^*, t^*)$  is feasible for (5), thus  $\hat{z} = z^*$  and  $(x^*, y^*, t^*)$  is optimal for (5).  $\square$

**Corollary 1.** *If  $A = B$  and function  $f$  is convex, then*

$$\text{conv}(X) = \{x \in [0, 1]^N, y \in \mathbb{R}^N, t \in \mathbb{R} : \phi(x, y) \leq t, f(x, y) \leq t\}.$$

**Theorem 2.** *If  $g(\emptyset) = 0$ , then the function  $\phi(x, y)$  is positively homogeneous of degree 1.*

*Proof.* When  $g(\emptyset) = 0$ , we find that for  $\lambda \geq 0$ ,

$$\begin{aligned} \phi^v(\lambda x, \lambda y) &= \max_{\alpha \in A} -\alpha'(\lambda y) + \sum_{i=1}^n \pi_i^v(\alpha)(\lambda x_{(i)}) \\ &= \lambda \max_{\alpha \in A} -\alpha'y + \sum_{i=1}^n \pi_i^v(\alpha)x_{(i)} = \lambda \phi^v(x, y). \end{aligned}$$

Moreover,

$$\begin{aligned} \phi(\lambda x, \lambda y) &= \max\{\phi^v(\lambda x, \lambda y) : v \text{ is a permutation of } N\} \\ &= \lambda \max\{\phi^v(x, y) : v \text{ is a permutation of } N\} = \lambda \phi(x, y), \end{aligned}$$

and the proof is complete.  $\square$

It follows from Theorem 2 that the set

$$K = \{x \in \mathbb{R}_+^N, y \in \mathbb{R}^N, t \in \mathbb{R} : \phi(x, y) - g(\emptyset) \leq t\}$$

is a cone, thus the proposed valid inequalities are amenable to conic optimization techniques.

### 3. SPECIAL CASES

In this section we describe special cases of the proposed inequalities. Specifically, in Section 3.1 we re-derive the valid inequalities proposed in [3] using the methodology described in Section 2. In Sections 3.2 and 3.3 we use the proposed methodology to derive (for the first time) the convex hull descriptions of other mixed-integer sets.

**3.1. Quadratic function with negative correlations.** Consider the set

$$X_q = \{x \in \{0, 1\}^2, y \in \mathbb{R}_+^2, t \in \mathbb{R} : (y_1 - y_2)^2 \leq t, y_i(1 - x_i) = 0, i = 1, 2\}.$$

In this case, we have

$$f(x, y) = \begin{cases} \infty & \text{if } y_1 \leq 0 \text{ or } y_2 \leq 0 \\ (y_1 - y_2)^2 & \text{otherwise.} \end{cases}$$

We find that

$$g_\alpha(N) = \min_y \alpha_1 y_1 + \alpha_2 y_2 + (y_1 - y_2)^2 > -\infty$$

if  $\alpha_1 + \alpha_2 \geq 0$  (otherwise,  $y_1 = y_2 \rightarrow \infty$  results in arbitrarily low values). Moreover, for  $\alpha_1 + \alpha_2 \geq 0$ , we find  $g_\alpha(S)$  is given by

$$\begin{aligned} g_\alpha(\emptyset) &= \emptyset, \\ g_\alpha(\{1\}) &= -\frac{\alpha_1^2}{4} \text{ if } \alpha_1 \leq 0 \text{ and } g_\alpha(\{1\}) = 0 \text{ otherwise,} \\ g_\alpha(\{2\}) &= -\frac{\alpha_2^2}{4} \text{ if } \alpha_2 \leq 0 \text{ and } g_\alpha(\{2\}) = 0 \text{ otherwise,} \\ g_\alpha(\{1, 2\}) &= \begin{cases} -\frac{\alpha_1^2}{4} & \text{if } \alpha_1 \leq 0 \\ -\frac{\alpha_2^2}{4} & \text{if } \alpha_2 \leq 0 \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

In particular,  $g_\alpha$  is submodular for any  $\alpha_1 + \alpha_2 \geq 0$ . Now let  $v = (1, 2)$  be the permutation corresponding to the natural ordering of the variables, and consider the inequality

$$\phi^v(x, y) = \max_{\alpha_1 + \alpha_2 \geq 0} -\alpha_1 y_1 - \alpha_2 y_2 + g_\alpha(\{1\})x_1 + (g_\alpha(\{1, 2\}) - g_\alpha(\{1\}))x_2. \quad (6)$$

Observe that if  $y_i < 0$ , then  $\phi^v(x, y) = \infty$  by letting  $\alpha_i \rightarrow \infty$ , thus we assume  $y_1, y_2 \geq 0$ . Moreover, if  $\alpha_1, \alpha_2 \geq 0$ , then the optimal solution of (6) corresponds to setting  $\alpha_1 = \alpha_2 = 0$  with objective value 0, thus we can assume that either  $\alpha_1 \leq 0$  or  $\alpha_2 \leq 0$  without loss of generality.

- First suppose  $\alpha_1 \leq 0$  in an optimal solution. Then

$$\phi_1^v(x, y) = \max_{\substack{\alpha_1 + \alpha_2 \geq 0 \\ \alpha_1 \leq 0}} -\alpha_1 y_1 - \alpha_2 y_2 - \frac{\alpha_1^2}{4} x_1.$$

Clearly  $\alpha_2 = -\alpha_1$  in any optimal solution, and the problem reduces to

$$\phi_1^v(x, y) = \max_{\alpha_2 \geq 0} \alpha_2 (y_1 - y_2) - \frac{\alpha_2^2}{4} x_1.$$

If  $y_2 \geq y_1$ , the optimal solution corresponds to setting  $\alpha_2 = 0$  with objective value 0. Otherwise, the optimal solution corresponds to  $\alpha_2 = \frac{2(y_1 - y_2)}{x_1}$  with objective value  $\phi^v(x, y) = \frac{(y_1 - y_2)^2}{x_1}$ .

- The case where  $\alpha_1 \geq 0$  and  $\alpha_2 \leq 0$  is symmetric, and we find that if  $y_2 \geq y_1$ , then  $\phi_2^v(x, y) = \frac{(y_1 - y_2)^2}{x_2}$  and  $\phi_2^v(x, y) = 0$  otherwise.

Letting  $\phi^v(x, y) = \max\{\phi_1^v(x, y), \phi_2^v(x, y)\}$ , one obtains the convex hull of  $X_q$ .

**Proposition 2** (Atamtürk and Gómez [3]). *Bound constraints  $0 \leq x \leq 1$ ,  $0 \leq y$ , and inequality*

$$t \geq \phi^v(x, y) = \begin{cases} \frac{(y_1 - y_2)^2}{x_1} & \text{if } y_1 \geq y_2 \\ \frac{(y_1 - y_2)^2}{x_2} & \text{if } y_2 \geq y_1. \end{cases} \quad (7)$$

*describe  $\text{conv}(X_q)$ .*

We point out that inequalities (7) were further generalized in [7] and used in signal estimation problems with sparsity.

**3.2. Conic quadratic function with negative correlations.** Given  $\sigma \geq 0$ , consider the set

$$X_{cq} = \left\{ x \in \{0, 1\}^2, y \in \mathbb{R}_+^2, t \in \mathbb{R} : \sqrt{\sigma^2 + (y_1 - y_2)^2} \leq t, y_i(1 - x_i) = 0, i = 1, 2 \right\}.$$

We find that  $g_\alpha(N) > -\infty$  if  $\alpha_1 + \alpha_2 \geq 0$  (otherwise,  $y_1 = y_2 \rightarrow \infty$  results in arbitrarily low values) and  $\alpha_i \geq -1$ ,  $i = 1, 2$  (otherwise  $y_i \rightarrow \infty$  results in arbitrarily low values). Moreover, if  $\alpha_1 + \alpha_2 \geq 0$ ,  $\alpha_1 \geq -1$  and  $\alpha_2 \geq -1$ , we find (from KKT conditions) that  $g_\alpha(S)$  is given by

$$\begin{aligned} g_\alpha(\emptyset) &= \sigma, \\ g_\alpha(\{1\}) &= \sigma \sqrt{1 - \alpha_1^2} \text{ if } \alpha_1 \leq 0 \text{ and } g_\alpha(\{1\}) = \sigma \text{ otherwise,} \\ g_\alpha(\{2\}) &= \sigma \sqrt{1 - \alpha_2^2} \text{ if } \alpha_2 \leq 0 \text{ and } g_\alpha(\{2\}) = \sigma \text{ otherwise,} \\ g_\alpha(\{1, 2\}) &= \begin{cases} \sigma \sqrt{1 - \alpha_1^2} & \text{if } \alpha_1 \leq 0 \\ \sigma \sqrt{1 - \alpha_2^2} & \text{if } \alpha_2 \leq 0 \\ \sigma & \text{otherwise.} \end{cases} \end{aligned}$$

In particular,  $g_\alpha$  is submodular for any  $\alpha \in B$ . Now let  $v = (1, 2)$  be the permutation corresponding to the natural ordering of the variables, and consider the inequality

$$\phi^v(x, y) = \max_{\substack{\alpha_1 + \alpha_2 \geq 0 \\ \alpha_1, \alpha_2 \geq -1}} -\alpha_1 y_1 - \alpha_2 y_2 + \sigma + g_\alpha(\{1\})x_1 + (g_\alpha(\{1, 2\}) - g_\alpha(\{1\}))x_2.$$

Using a similar argument as in Section 3.1, we may assume  $y_1, y_2 \geq 0$  and either  $\alpha_1 \leq 0$  or  $\alpha_2 \leq 0$ .

First suppose  $\alpha_1 \leq 0$  in an optimal solution. Then

$$\phi_1^v(x, y) = \max_{\substack{\alpha_1 + \alpha_2 \geq 0 \\ -1 \leq \alpha_1 \leq 0}} -\alpha_1 y_1 - \alpha_2 y_2 + \sigma + \sigma \left( \sqrt{1 - \alpha_1^2} - 1 \right) x_1.$$

Clearly  $\alpha_2 = -\alpha_1$  in any optimal solution, and the problem reduces to

$$\phi_1^v(x, y) = \sigma(1 - x_1) + \max_{0 \leq \alpha_2 \leq 1} \alpha_2(y_1 - y_2) + \sigma x_1 \sqrt{1 - \alpha_2^2}. \quad (8)$$

If  $y_2 \geq y_1$ , the optimal solution corresponds to setting  $\alpha_2 = 0$  with objective value  $\sigma$ . Otherwise, by taking derivatives with respect to  $\alpha_2$ , we find that

$$\begin{aligned} 0 &= (y_1 - y_2) - \frac{\sigma x_1}{\sqrt{1 - \alpha_2^2}} \alpha_2 \\ \implies \alpha_2^2 &= \frac{(y_1 - y_2)^2}{(\sigma x_1)^2} (1 - \alpha_2^2) \\ \implies \alpha_2^2 &= \frac{\frac{(y_1 - y_2)^2}{(\sigma x_1)^2}}{1 + \frac{(y_1 - y_2)^2}{(\sigma x_1)^2}} = \frac{(y_1 - y_2)^2}{(\sigma x_1)^2 + (y_1 - y_2)^2} \\ \implies \alpha_2 &= \frac{y_1 - y_2}{\sqrt{(\sigma x_1)^2 + (y_1 - y_2)^2}}. \end{aligned}$$

Observe that since  $\alpha_2 \leq 1$ , we can ignore the upper bound. Replacing  $\alpha_2$  with its optimal value in (8), we find

$$\phi_1^v(x, y) = \sigma(1 - x_1) + \sqrt{(\sigma x_1)^2 + (y_1 - y_2)^2}.$$

The case where  $\alpha_2 \leq 0$  is symmetric; we find that

$$\phi_2^v(x, y) = \sigma(1 - x_2) + \sqrt{(\sigma x_2)^2 + (y_1 - y_2)^2}$$

if  $y_2 \geq y_1$  and  $\phi_2^v(x, y) = 0$  otherwise. Letting  $\phi^v(x, y) = \max\{\phi_1^v(x, y), \phi_2^v(x, y)\}$ , we obtain from Corollary 1:

**Proposition 3.** *Bound constraints  $0 \leq x \leq 1$ ,  $0 \leq y$ , and inequality*

$$t \geq \phi^v(x, y) = \begin{cases} \sigma(1 - x_1) + \sqrt{(\sigma x_1)^2 + (y_1 - y_2)^2} & \text{if } y_1 \geq y_2 \\ \sigma(1 - x_2) + \sqrt{(\sigma x_2)^2 + (y_1 - y_2)^2} & \text{if } y_2 \geq y_1. \end{cases}$$

*describe  $\text{conv}(X_{cq})$ .*

**3.3. Fractional function: quadratic over nondecreasing supermodular.** Given a nondecreasing nonnegative supermodular function  $h : 2^N \rightarrow \mathbb{R}_+$ , consider the set

$$X_f = \left\{ x \in \{0, 1\}^N, y \in \mathbb{R}^N, t \in \mathbb{R} : \frac{\sum_{i \in N} y_i^2}{h(S_x)} \leq t, y_i(1 - x_i) = 0, i \in N \right\}.$$

In particular, if  $h(S) = |S|$ , then function  $f(x, y) = \frac{\sum_{i \in N} y_i^2}{\sum_{i \in N} x_i}$  can be interpreted as an average; alternatively, if  $h(S) = 1$  for all  $S \subseteq N$ , then set  $X_f$  corresponds to the mixed-integer epigraph of a separable quadratic function, the convex hull of which is described by the well-known perspective reformulation [2, 9, 12], i.e., by bound constraints and inequality  $\sum_{i \in N} \frac{y_i^2}{x_i} \leq t$ .

We find that  $g_\alpha(N)$  is given by

$$g_\alpha(S) = -\frac{h(S)}{4} \sum_{i \in S} \alpha_i^2.$$

Function  $g_\alpha$  can easily be verified to be submodular for all  $\alpha \in \mathbb{R}^N$ : letting  $S \subseteq T \subseteq N \setminus \{j\}$ , we find that

$$\begin{aligned}
\rho_j(T) &= -\frac{h(T \cup \{j\})}{4} \sum_{i \in T} \alpha_i^2 - \frac{h(T \cup \{j\})}{4} \alpha_j + \frac{h(T)}{4} \sum_{i \in T} \alpha_i^2 \\
&= -\frac{h(T \cup \{j\})}{4} \alpha_j^2 - \frac{h(T \cup \{j\}) - h(T)}{4} \sum_{i \in S} \alpha_i^2 - \frac{h(T \cup \{j\}) - h(T)}{4} \sum_{i \in T \setminus S} \alpha_i^2 \\
&\leq -\frac{h(S \cup \{j\})}{4} \alpha_j^2 - \frac{h(T \cup \{j\}) - h(T)}{4} \sum_{i \in S} \alpha_i^2 && (h \text{ is nondecreasing}) \\
&\leq -\frac{h(S \cup \{j\})}{4} \alpha_j^2 - \frac{h(S \cup \{j\}) - h(S)}{4} \sum_{i \in S} \alpha_i^2 && (h \text{ is supermodular}) \\
&= \rho_j(S).
\end{aligned}$$

Now let  $v = (1, \dots, n)$  be the permutation of  $N$  corresponding to the natural order of the variables (for simplicity), and consider the inequality

$$\begin{aligned}
\phi^v(x, y) &= \max_{\alpha \in \mathbb{R}^N} -\alpha' y + \sum_{i=1}^n \left( -\frac{h(N_i^y)}{4} \sum_{j=1}^i \alpha_j^2 + \frac{h(N_{i-1}^y)}{4} \sum_{j=1}^{i-1} \alpha_j^2 \right) x_i \\
&= \max_{\alpha \in \mathbb{R}^N} -\alpha' y + \sum_{i=1}^n \left( -\frac{h(N_i^y)}{4} \alpha_i^2 - \frac{h(N_i^y) - h(N_{i-1}^y)}{4} \sum_{j=1}^{i-1} \alpha_j^2 \right) x_i. \quad (9)
\end{aligned}$$

Taking derivatives with respect to  $\alpha_k$  and setting to 0, we obtain

$$\begin{aligned}
0 &= -y_k - \frac{h(N_k^y) x_k}{2} \alpha_k - \sum_{\ell=k+1}^n \frac{(h(N_\ell^y) - h(N_{\ell-1}^y)) x_\ell}{2} \alpha_k \\
\implies \alpha_k &= \frac{-2y_k}{h(N_k^y) x_k + \sum_{\ell=k+1}^n (h(N_\ell^y) - h(N_{\ell-1}^y)) x_\ell}.
\end{aligned}$$

Substituting  $\alpha$  with their optimal values in (9), we find that

$$\begin{aligned}
\phi^v(x, y) &= \sum_{i=1}^n \frac{2y_i^2}{h(N_i^y) x_i + \sum_{\ell=i+1}^n (h(N_\ell^y) - h(N_{\ell-1}^y)) x_\ell} \\
&\quad - \sum_{i=1}^n h(N_i^y) \left( \frac{y_i}{h(N_i^y) x_i + \sum_{\ell=i+1}^n (h(N_\ell^y) - h(N_{\ell-1}^y)) x_\ell} \right)^2 x_i \\
&\quad - \sum_{i=1}^n (h(N_i^y) - h(N_{i-1}^y)) \sum_{j=1}^{i-1} \left( \frac{y_j}{h(N_j^y) x_j + \sum_{\ell=j+1}^n (h(N_\ell^y) - h(N_{\ell-1}^y)) x_\ell} \right)^2 x_j \\
&= \sum_{i=1}^n \frac{y_i^2}{h(N_i^y) x_i + \sum_{\ell=i+1}^n (h(N_\ell^y) - h(N_{\ell-1}^y)) x_\ell}. \quad (10)
\end{aligned}$$

Observe that if  $h$  is a constant function, inequalities (10) reduces to the perspective reformulation. In general, inequalities (10) are sufficient to describe  $\text{conv}(X_f)$ .

**Proposition 4.** *Bound constraints  $0 \leq x \leq 1$  and inequalities*

$$\sum_{i=1}^n \frac{y_{(i)}^2}{h(N_i^v)x_{(i)} + \sum_{\ell=i+1}^n (h(N_\ell^v) - h(N_{\ell-1}^v))x_{(\ell)}} \leq t \quad \text{for all permutations } v \text{ of } N$$

*describe  $\text{conv}(X_f)$ .*

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