SUBMODULAR FUNCTION MINIMIZATION AND POLARITY

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Abstract. Using polarity, we give an outer polyhedral approximation for the epigraph of set functions. For a submodular function, we prove that the corresponding polar relaxation is exact; hence, it is equivalent to the Lovász extension. The polar approach provides an alternative proof for the convex hull description of the epigraph of a submodular function. Preliminary computations show that the inequalities from outer approximations can be effective as cutting planes for solving submodular as well as non-submodular set function minimization problems.

Keywords: Polarity, Lovász extension, submodular functions, polymatroids, greedy algorithm, cutting planes.

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1. Introduction

Given a finite ground set $N$ and a rational valued set function $f : 2^N \to \mathbb{Q}$, we consider finding the minimum value of $f$:

$$\min_{S \subseteq N} f(S). \quad (1)$$

Throughout, by abuse of notation, we also use $f(x)$, where $x \in \{0,1\}^N$ is the indicator vector for the set of subsets of $N$. Introducing an auxiliary variable $z$ for the objective value, let us restate problem \(1\) as

$$\min \{ z : (x, z) \in Q_f \}, \quad (2)$$

where $Q_f$ is the convex hull of the epigraph of $f$, i.e.,

$$Q_f := \text{conv} \left\{ (x, z) \in \{0,1\}^N \times \mathbb{R} : f(x) \leq z \right\}.$$

In this paper, we give a polyhedral relaxation for $Q_f$ based on polarity. Whereas the Lovász extension \cite{Lovász} for a set function gives an inner piecewise polyhedral approximation of the convex hull of its epigraph, the polar relaxation is a polyhedral (hence convex) outer approximation.
A set function $f : 2^N \rightarrow \mathbb{Q}$ is submodular if

$$f(S \cup T) + f(S \cap T) \leq f(S) + f(T) \text{ for all } S, T \subseteq N.$$ 

For a submodular set function, we show that the corresponding polar relaxation is exact; hence, it is equivalent to the Lovász extension. The polar approach, thus, provides a new polyhedral proof of the convex hull description of the epigraph of a submodular function. Furthermore, through computational experiments, we show that the inequalities from outer approximations can be effective as cutting planes for solving submodular as well as non-submodular set function minimization problems.

A short literature review. Submodular set functions play an important role in many fields and have received much interest in the literature [7, 8, 25]. Combinatorial optimization problems such as the min-cut problem, entropy minimization, matroids, binary quadratic function minimization with a non-positive matrix, among many others, are special cases. Submodular functions can be minimized in polynomial time [11, 14, 22, 23]. For comprehensive reviews on this subject we refer the reader to [10, 13, 24]. While the majority of research on submodularity has been devoted to optimization on binary variables, submodularity has been useful for deriving strong inequalities for mixed 0–1 optimization as well [2, 3, 4, 26]. Unlike minimization, maximization of submodular functions is $NP$-hard (the max-cut problem is a special case). Most of the research for this case has been on approximation algorithms. The greedy algorithm and its extensions [9, 16, 19, 21] provide constant factor approximation. There is limited work on polyhedral analysis of submodular function maximization [1, 15, 18, 27].

Assumption and notation. Without loss of generality, we assume that $f(\emptyset) = 0$ as, otherwise, one can solve the equivalent minimization problem for $f' := f - f(\emptyset)$, i.e., with $f'(S) = f(S) - f(\emptyset)$ for all $S \subseteq N$. Let $\chi_S$ be the indicator vector for a set $S \subseteq N$ and $S_x$ be the support set of a binary vector $x \in \{0, 1\}^N$. For a vector $x \in \mathbb{R}^N$ and $S \subseteq N$, define $x(S) := \sum_{i \in S} x_i$.

2. Polar outer approximation

We start this section with a simple property of the facets of $Q_f$. We refer to the variable bounds $0 \leq x \leq 1$ as the trivial inequalities of $Q_f$.

Proposition 1. Any non-trivial facet-defining inequality $\pi x \leq \alpha z + \pi_0$ for $Q_f$ satisfies $\pi_0 \geq 0$ and $\alpha = 1$ (up to scaling).

Proof. Because $(0, 1)$ is a ray of $Q_f$, inequality is invalid unless $\alpha \geq 0$. However, any valid $\pi x \leq \pi_0$ is implied by the trivial inequalities $0 \leq x \leq 1$ as $\{(x, f(x)) : x \in \{0, 1\}^N \subseteq Q_f\}$. Thus, $\alpha > 0$ and by scaling may be assumed to be one. Furthermore, $\pi_0 \geq 0$ is necessary for validity, since otherwise inequality $\pi x \leq z + \pi_0$ is invalid for $(0, 0) \in Q_f$. □
For a set function $f$ with $f(\emptyset) = 0$, let the associated polyhedron be

$$P_f := \{ \pi \in \mathbb{R}^N : \pi(S) \leq f(S) \text{ for all } S \subseteq N \},$$

where $\pi(S)$ denotes $\sum_{i \in S} \pi_i$, $S \subseteq N$. Consider the polar of $P_f$

$$P_f^\circ := \{ (x, z) \in \mathbb{R}^N \times \mathbb{R} : \pi x \leq z, \text{ for all } \pi \in P_f \}.$$

The next proposition shows a polarity relationship between $P_f$ and the homogeneous ($\pi_0 = 0$) valid inequalities for $Q_f$.

**Proposition 2.** Inequality $\pi x \leq z$ is valid for $Q_f$ if and only if $\pi \in P_f$.

**Proof.** For $\pi \in P_f$, we have $\pi x = \pi(S_x) \leq f(S_x) \leq z$. Conversely, if $\pi \notin P_f$, then $\pi(S) > f(S)$ for some $S \subseteq N$; but then for $z = f(S)$, $\pi(S) = \pi(S) > z$, contradicting the validity of $\pi x \leq z$. \hfill \Box

We refer to inequalities of Proposition 2 as the polar inequalities. By Proposition 2 we have $Q_f \subseteq P_f^\circ$. Indeed, each facet of $P_f^\circ$ is a facet of $Q_f$ as well, as shown below.

**Proposition 3.** Inequality $\pi x \leq z$ is facet-defining for $Q_f$ if and only if $\pi$ is an extreme point of $P_f$.

**Proof.** From Proposition 2 if $\pi \notin P_f$, inequality $\pi x \leq z$ is invalid for $Q_f$. If $\pi \in P_f$ is not an extreme point, then $\pi = \lambda \pi^1 + (1 - \lambda) \pi^2$ for some $0 < \lambda < 1$ and distinct $\pi^1, \pi^2 \in P_f$ and $\pi x \leq z$ is implied by $\pi^1 x \leq z$ and $\pi^2 x \leq z$. Conversely, if $\pi$ is an extreme point of $P_f$, it is the unique solution to a set of $n$ linearly independent equations $\pi(S_i) = f(S_i)$ for $i = 1, \ldots, n$. Then, the corresponding linearly independent points $(\chi_{S_i}, f(S_i))$, $i = 1, \ldots, n$ of $Q_f$ and $(0, 0)$ are on the face $\{ x \in Q_f : \pi x = z \}$. Finally, as $(0, 1) \in Q_f$ but not on the face, the face is proper. \hfill \Box

The polar relaxation $P_f^\circ$ gives a (convex) polyhedral outer approximation for $Q_f$. It indeed gives all nontrivial homogeneous facets of $Q_f$. It is interesting to contrast it with the Lovász extension \cite{17} for a set function.

**Definition 1.** For a set function $f$, the Lovász extension $\hat{f} : [0, 1]^N \rightarrow \mathbb{R}$ is defined as

$$\hat{f}(x) := \sum_{i=1}^{n-1} (x_i - x_{i+1}) f(S_i) + x_n f(S_n),$$

where $1 \geq x_1 \geq \ldots \geq x_n \geq 0$ and $S_i = \{1, 2, \ldots, i\}$, $i \in N =: \{1, \ldots, n\}$.

Observe that $\hat{f}$ is homogeneous and $\hat{f}(\chi_S) = f(S)$, $\forall S \subseteq N$. It is easy to see that for a general set function, Lovász extension is a piecewise polyhedral inner approximation of $Q_f$. Thus, we have

$$\text{epi } \hat{f} \subseteq Q_f \subseteq P_f^\circ \cap [0, 1]^n \times \mathbb{R}.$$

\footnote{For the submodular case, $P_f$ is often referred to as the submodular polyhedron or the extended polymatroid.}
Example 1. In this example, we compare the polar outer approximation with the Lovász extension for a non-submodular set function. Consider the function \( f \) defined as
\[
\begin{align*}
\{ \emptyset \} & \rightarrow 0 \quad (A), \\
\{ 1 \} & \rightarrow -1 \quad (C), \\
\{ 2 \} & \rightarrow -1 \quad (B), \\
\{ 1, 2 \} & \rightarrow -1 \quad (D).
\end{align*}
\]
Function \( f \) is, in fact, supermodular.

The inequalities describing \( \text{epi} \hat{f}, Q_f, \) and \( P^\circ_f \), other than the bounds \( 0 \leq x \leq 1 \), are listed below and displayed in Figure 1.

\[
\begin{align*}
\text{epi} \hat{f} : & \quad \{ \begin{array}{l}
ACD: x \leq 1 \\
ABD: x \leq 2
\end{array} \quad \text{if } x \geq x_2 \\
Q_f : & \quad \{ \begin{array}{l}
ABC: x_1 - x_2 \leq 1 \\
BCD: -1 \leq z
\end{array}
\}
\]
\[
P^\circ_f : \quad \{ \begin{array}{l}
ABC: x_1 - x_2 \leq z
\end{array}
\}
\]

Observe that \( \text{epi} \hat{f} \) is non-convex and \( \text{epi} \hat{f} \subseteq Q_f \subseteq P^\circ_f \cap [0,1]^n \times \mathbb{R} \).

The submodular case. Lovász [17] has shown that \( \hat{f} \) is convex if and only if \( f \) is submodular, establishing the relationship between convexity and submodular set functions. Next we show that for a submodular function \( f \), all nontrivial facets of \( Q_f \) are homogeneous; consequently, the polar \( P^\circ_f \) gives an exact relaxation. So, for a submodular function \( f \), it holds
\[
\text{epi} \hat{f} = Q_f = P^\circ_f \cap [0,1]^n \times \mathbb{R}.
\]

Proposition 4. For a submodular function \( f \), any non-trivial facet-defining inequality
\[
\pi x \leq z + \pi_0 \quad (3)
\]
of \( Q_f \) satisfies \( \pi_0 \leq 0 \).

Proof. For contradiction, suppose \( \pi_0 > 0 \). Consider \( f' : 2^N \rightarrow \mathbb{R} \) defined as \( f'(\emptyset) = 0 \) and \( f'(S) = f(S) + \pi_0 \) for \( \emptyset \neq S \subseteq N \). Observe that \( f' \) is submodular as well. Since (3) is valid for \( Q_f \), \( \pi(S) \leq f(S) + \pi_0 \) for all \( S \subseteq N \) and hence, \( \pi \in P_{f'} \) and, by Proposition 2, inequality
\[
\pi x \leq z \quad (4)
\]
is valid for \( Q_{f'} \). Now, since (3) is facet-defining for \( Q_f \), (4) is facet-defining for \( Q_{f'} \). Hence, by Proposition 3, \( \pi \) is an extreme point of \( P_{f'} \). After permuting variables, if necessary, we may assume that \( \pi_1 = f'(S_1) = f(S_1) + \pi_0 \), and \( \pi_i = f'(S_i) - f'(S_{i-1}) = f(S_i) - f(S_{i-1}) \) for \( i = 2, \ldots, n \). Then, \( \gamma \in P_{f'} \) for \( \gamma_1 = \pi_1 - \pi_0 \), and \( \gamma_i = \pi_i \) for all \( i = 2, \ldots, n \). However, by Proposition 2, \( \gamma x \leq z \) is valid for \( Q_f \) and, together with \( x_1 \leq 1 \), it dominates inequality (3). \( \square \)
Remark 1. Note that if \( f(\emptyset) \neq 0 \), in order to define the inequalities for \( Q_f \), we may use the polyhedron \( P_{f'} \) for \( f' := f - f(\emptyset) \). In general, polar inequalities for \( Q_f \) take the form
\[
\pi x \leq z - f(\emptyset), \quad \pi \in P_{f-f(\emptyset)}.
\]
(5)

Remark 2. For a submodular function, \( P_f \) is an extended polymatroid and the polar inequalities reduce to the extended polymatroid inequalities. The separation problem for extended polymatroid inequalities is optimization of a linear objective over \( P_f \), which can be solved by the greedy algorithm of Edmonds [7]: Given \( \bar{x} \in \mathbb{R}^n_+ \) and \( \bar{z} \in \mathbb{R} \), checking whether \((\bar{x}, \bar{z})\) violates an extended polymatroid inequality is equivalent to solving the problem
\[
\zeta := \max \{ \pi \bar{x} : \pi \in P_f \}.
\]
(6)

For a nonincreasing order \( \bar{x}(1) \geq \bar{x}(2) \geq \cdots \geq \bar{x}(n) \), let \( S(i) = \{(1), (2), \ldots, (i)\} \) and \( \bar{\pi}(i) = f(S(i)) - f(S(i-1)) \) for \( 1 \leq i \leq n \). Then, \((\bar{x}, \bar{z})\) is violated by the corresponding extended polymatroid inequality if and only if \( \zeta = \bar{\pi} \bar{x} > \bar{z} \).

3. Inequalities for General Set Functions

Unlike the submodular case, homogeneous inequalities of the polar relaxation are not sufficient to describe \( Q_f \) for a general set function. One can, however, generate non-homogeneous inequalities by decomposing a set function into a sum of a submodular function and a supermodular function and utilizing inequalities for each.

It is well-known that for any set function \( f \), such a decomposition exists. For a strictly submodular \( h \) and sufficiently large \( \lambda > 0 \), the first term below is submodular, whereas the second term is supermodular:

\[
f = (f + \lambda h) + (-\lambda h).
\]

Although, in general, a submodular–supermodular decomposition may be difficult to compute, in many cases, such a decomposition is either readily available or easy to construct. Below we give a few examples that will also be used in the computations in Section 4:

- **Optimization with higher moments**: When random variables deviate significantly from the normal distribution, optimization of utility functions with higher moments, such as skewness and kurtosis, in addition to the expectation and standard deviation, are preferred for more accurate modeling:

\[
-\mu' x + \lambda_2 \left( \sum \sigma_i^2 x_i^2 \right)^{1/2} - \lambda_3 \left( \sum \gamma_i^3 x_i^3 \right)^{1/3} + \lambda_4 \left( \sum \kappa_i^4 x_i^4 \right)^{1/4}
\]

Here, the first term is modular, the second and fourth (even) terms submodular, and the third (odd) term is supermodular.

- **Quadratic optimization on binaries**: Let \( Q \) be a square matrix and \( Q^- \) and \( Q^+ \) be the square matrices with the negative and positive elements of \( Q \) and zeros elsewhere, respectively. Since \( g(x) = x'Q^-x \)
is submodular and \( -h(x) = x'Q^+x \) is supermodular \cite{20}, we have the corresponding submodular–supermodular decomposition:

\[
f(x) = x'Qx = x'Q^-x + x'Q^+x.
\]

- **Fractional linear functions:** Although not as immediate as in the cases above, a submodular-supermodular decomposition can be constructed for a fractional linear function with positive coefficients \( a, c > 0 \) as follows:

\[
f(x) := \frac{c'x}{1+ax} = \left( f(x) + \lambda \frac{ax}{1+ax} \right) - \left( \lambda \frac{ax}{1+ax} \right).
\]

Observe that \( h(x) = ax/(1+ax) \) is submodular as it is the composite of the univariate function \( x/(1+x) \), which is concave over nonnegative values and the modular function \( d'x \) \cite{1}. Han et al. \cite{12} show that \( f(x) \) is submodular if \( f(N) \leq r_{\text{min}} := \min_{i \in N} c_i/a_i \). Then letting \( \lambda \geq \lambda_{\text{min}} := (c(N) - r_{\text{min}}(1 + a(N)))^+ \) ensures that the first term \( f(x) + \lambda h(x) \) in the decomposition is always submodular: Observe that if all ratios \( c_i/a_i \) are equal, then \( f(x) \) is submodular and \( \lambda_{\text{min}} = 0 \) is sufficient. Otherwise, \( \lambda = \lambda_{\text{min}} \) implies \( f(N) + \lambda_{\text{min}}h(N) \leq r_{\text{min}} + \lambda_{\text{min}} \).

Writing \( f = g - h \) as the difference of two submodular functions, one can generate non-homogeneous inequalities using the polar inequalities for \( g \) and the submodular inequalities of Nemhauser and Wolsey \cite{20} pg 710 for \( h \):

\[
w \leq h(S) - \sum_{i \in S} \rho_i(N \setminus i)(1 - x_i) + \sum_{i \in N \setminus S} \rho_i(S)x_i \quad \text{for all } S \subseteq N, \quad (7)
\]

\[
w \leq h(S) - \sum_{i \in S} \rho_i(S \setminus i)(1 - x_i) + \sum_{i \in N \setminus S} \rho_i(\emptyset)x_i \quad \text{for all } S \subseteq N, \quad (8)
\]

where \( \rho_i(S) = h(S \cup i) - h(S) \). Submodular inequalities \[(7)-(8)\] are valid for the hypograph of \( h \), \( \text{hyp } h := \left\{ (x, w) \in \{0,1\}^N \times \mathbb{R} : h(x) \geq w \right\} \).

4. Computations

In this section we report on our computational experiments with using the inequalities from submodular–supermodular decompositions for non-submodular functions. In each experiment, we control the deviation of the set functions from submodularity. All computations are done with Gurobi version 9.0 with default solver options (except heuristics are turned off and single thread is used) on a Xeon workstation.

The first set of experiments are on binary quadratic optimization of the form: \( \min x'Qx + \Omega c'x : x \in \{0,1\}^n \). The data is generated following Carter \cite{6} : \( Q_{ij} \) is drawn from \( \text{Uniform}[-100\lambda, 100(1 - \lambda)] \) for \( i \neq j \) and \( Q_{ii} = 0 \); \( c_i \) is drawn from \( \text{Uniform}[-100(1 - \lambda)(n - 1), 100\lambda(n - 1)] \). The parameter \( \lambda \in [0,1] \) controls the distance from submodularity: for \( \lambda = 1 \), \( Q \) is nonpositive and the quadratic function is submodular, whereas for
Table 1. Binary quadratic optimization.

| $\lambda$ | 0.0 | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
|-----------|-----|-----|-----|-----|-----|-----|
| gap (%)   | 0.7 | 1.3 | 1.8 | 20.5| 19.0| 44.3|
| cgap (%)  | 0.7 | 0.9 | 0.2 | 2.9 | 0.1 | 0.0 |
| time (sec.) | 0.2 | 0.2 | 0.1 | 0.2 | 0.1 | 0.1 |
| ctime (sec.) | 0.2 | 0.2 | 0.0 | 0.2 | 0.0 | 0.0 |
| #nodes    | 797.4| 881.2| 297.6| 258.6| 257.0| 257.0|
| # cnodes  | 797.4| 641.4| 140.0| 156.8| 30.4 | 5.0 |
| # cuts    | 0.0 | 1.4 | 2.2 | 10.2| 5.0 | 3.0 |

$\lambda = 0$, $Q$ is nonnegative and the quadratic function is supermodular. The parameter $\Omega$ is chosen to ensure that quadratic and linear terms are well-balanced to avoid trivial solutions.

In Table 1 we report the integrality gap at the root node, solution time, and the number of nodes explored with and without adding cuts. Each row shows the average for five instances with $n = 50$. We observe in Table 1 that the integrality gap of the convex relaxations increases with $\lambda$, achieving the highest value for the submodular case ($\lambda = 1$). The inequalities from the outer relaxations are particularly effective for these cases with high integrality gap. Indeed, for the submodular case, the gap is closed completely at the root node and the problems are solved without branching. For all values of $\lambda$ we observe a substantial reduction in the integrality gaps, leading to reduction in the number of nodes as well as the solution times.

The second set of experiments are done on the 0–1 knapsack problem with a mean-risk objective involving higher moments:

$$\min -\Omega \mu'x + \lambda \left( \sum \sigma_i^2 x_i^2 \right)^{1/2} - (1 - \lambda) \left( \sum \gamma_i^3 x_i^3 \right)^{1/3} + \lambda \left( \sum \kappa_i^4 x_i^4 \right)^{1/4}$$

$$s.t. \; a'x \leq b, \; x \in \{0, 1\}^n.$$ 

The data is generated following Bergman and Cire [5]. The parameters $\mu_i$ and $a_i$ are drawn from Uniform[0,100], $\sigma_i$, $\gamma_i$, $\kappa_i$ are drawn from Uniform[0, $\mu_i$]. The knapsack capacity is set to $0.5 \sum a_i$. As before, the parameter $\lambda$ controls the distance of the objective function from submodularity. For $\lambda = 1$ the objective is submodular; for $\lambda = 0$ it is supermodular. $\Omega$ is chosen to ensure that positive and negative terms in the objective are well-balanced to avoid trivial solutions.

The results for this experiment are summarized in Table 2. Each row shows the average for five instances with $n = 100$. For this problem the integrality gap is highest for $\lambda = 0.4$. 19 instances out of 30 could not be solved to optimality within the one hour time limit without cuts. 14 of those 19 are solved to optimality within time limit with the cuts. Utilizing the cuts reduced the root gaps substantially and, consequently, led to smaller search trees, faster solution times and better solutions.
Table 2. Optimization with higher moments.

| λ  | 0.0 | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
|----|-----|-----|-----|-----|-----|-----|
| gap (%) | 0.1 | 6.3 | 51.8 | 29.1 | 19.2 | 10.1 |
| cgap (%) | 0.1 | 0.1 | 14.3 | 0.2 | 0.2 | 0.2 |
| time (sec.) | 0.1 | 3,600.0 | 3,600.0 | 3,600.0 | 2,906.9 | 39.5 |
| ctime (sec.) | 0.1 | 1,371.1 | 2,998.8 | 1,474.3 | 325.9 | 0.4 |
| #nodes | 151.1 | 46,451.2 | 43,324.0 | 54,864.9 | 49,823.2 | 9,108.3 |
| # cnodes | 151.1 | 1,068.3 | 1,616.7 | 1,096.2 | 928.2 | 226.5 |
| # cuts | 0.0 | 124.4 | 537.1 | 379.3 | 180.1 | 43.0 |

These preliminary computational experiments demonstrate that, when used as cutting planes, the valid inequalities from a submodular-supermodular decomposition of general set functions can be effective to improve the branch-and-bound algorithms.

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