Strengthening linear reformulations of pseudo-Boolean optimization problems

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Definitions

Definition: Pseudo-Boolean functions

A pseudo-Boolean function is a mapping $f: \{0,1\}^n \to \mathbb{R}$.

Multilinear representation

Every pseudo-Boolean function f can be represented uniquely by a multilinear polynomial (Hammer, Rosenberg, Rudeanu [4]).

Example:

$$f(x_1, x_2, x_3) = 9x_1x_2x_3 + 8x_1x_2 - 6x_2x_3 + x_1 - 2x_2 + x_3$$

Pseudo-Boolean Optimization

Many problems formulated as optimization of a pseudo-Boolean function

Pseudo-Boolean Optimization

$$\min_{x \in \{0,1\}^n} f(x)$$

- Optimization is \mathcal{NP} -hard, even if f is quadratic (MAX-2-SAT, MAX-CUT modelled by quadratic f).
- Approaches:
 - Linearization: standard approach to solve non-linear optimization.
 - **Quadratization**: Much progress has been done for the quadratic case (exact algorithms, heuristics, polyhedral results...).

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$$\min_{\{0,1\}^n} \sum_{S \in \mathcal{S}} a_S \prod_{k \in S} x_k,$$

$$\mathcal{S} = \{S \subseteq \{1,\dots,n\} \mid a_S \neq 0\} \text{ (non-constant monomials)}$$

1 Substitute monomials

$$\min \sum_{S \in \mathcal{S}} a_S z_S$$
s.t. $z_S = \prod_{k \in S} x_k$, $\forall S \in \mathcal{S}$

$$z_S \in \{0, 1\}, \qquad \forall S \in \mathcal{S}$$

$$x_k \in \{0, 1\}, \qquad \forall k = 1, \dots, n$$

$$\min_{\{0,1\}^n} \sum_{S \in \mathcal{S}} a_S \prod_{k \in S} x_k,$$

$$S = \{S \subseteq \{1, ..., n\} \mid a_S \neq 0\}$$
 (non-constant monomials)

1. Substitute monomials

$\min \sum a_S z_S$

s.t.
$$z_S = \prod x_k$$
,

 $k \in S$

$$\forall S \in S$$

$$z_S \in \{0,1\}, \qquad \forall S \in \mathcal{S}$$

$x_k \in \{0,1\}, \quad \forall k = 1,\ldots,n$

$$\min \sum_{S \in S} a_S z_S$$

$$S \in \mathcal{S}$$

s.t. $z_S \leq x_k$,

s.t.
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, $\forall k \in S, \forall S \in S$
 $z_S \ge \sum x_k - (|S| - 1), \ \forall S \in S$

$$k \in S$$
 $(|S| 1), \forall S \in S$

$$\forall k \in \{0,1\}$$
 $\forall k = 1$

$$x_k \in \{0,1\}, \qquad \forall k = 1,\ldots,n$$

$$\min_{\{0,1\}^n} \sum_{S \in \mathcal{S}} a_S \prod_{k \in S} x_k,$$

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1. Substitute monomials

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 $x_k \in \{0,1\}, \quad \forall k = 1,\ldots,n$

 $z_S \in \{0,1\},$

2. Linearize constraints

$$\begin{aligned} \min \sum_{S \in \mathcal{S}} a_S z_S \\ \text{s.t. } z_S &\leq x_k, & \forall k \in S, \forall S \in \mathcal{S} \\ z_S &\geq \sum_{k \in S} x_k - (|S| - 1), & \forall S \in \mathcal{S} \\ z_S &\in \{0, 1\}, & \forall S \in \mathcal{S} \\ x_k &\in \{0, 1\}, & \forall k = 1, \dots, n \end{aligned}$$

$$\min_{\{0,1\}^n} \sum_{S \in \mathcal{S}} a_S \prod_{k \in S} x_k,$$

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$\min \sum a_S z_S$ s.t. $z_S = \prod x_k$,

 $k \in S$

$$\forall S \in \mathcal{S}$$

$$z_S \in \{0,1\}, \qquad \forall S \in \mathcal{S}$$

$$x_k \in \{0,1\}, \quad \forall k = 1,\ldots,n$$

3. Linear relaxation

$\min \sum a_S z_S$

s.t.
$$z_S \leq x_k$$
, $\forall k \in S, \forall S \in S$

$$z_S \ge \sum_{k \in S} x_k - (|S| - 1), \quad \forall S \in S$$

$$0 \le z_S \le 1, \quad \forall S \in \mathcal{S}$$

$$0 \le x_k \le 1, \quad \forall k = 1, \dots, n$$

Intermediate substitutions (IS) (one monomial)

SL substitution

$$z_S = \prod_{k \in S} x_k$$

SL linearization

$$z_S \le x_k,$$
 $\forall k \in S$ $z_S \ge \sum_{k \in S} x_k - (|S| - 1)$

IS substitution

$$z_{S} = z_{A} \prod_{k \in S \setminus A} x_{k}$$
$$z_{A} = \prod_{k \in A} x_{k}$$

Intermediate substitutions (IS) (one monomial)

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$$z_A = \prod_{k \in A} x_k$$

$$z_S \leq z_A$$
,

$$z_S \ge z_A + \sum_{k \in S \setminus A} x_k - |S \setminus A|,$$

$$=$$
 $\sum_{i=1}^{N} (|A| - 1)$

$$z_A \geq \sum x_k - (|A| - 1).$$

 $\forall k \in S \backslash A$

 $\forall k \in S$

Intermediate substitutions (IS) (one monomial)

SL substitution

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SL linearization

$$z_{S} \leq x_{k},$$

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$$z_{S} \leq x_{k},$$
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 $z_{S} \leq z_{A},$
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 $z_{A} \leq x_{k},$ $\forall k \in A$

 $z_A \geq \sum_{k \in A} x_k - (|A| - 1).$

 $\forall k \in S$

Intermediate Substitutions (IS) (one monomial)

Polytope $P_{SL,1} \subseteq \mathbb{R}^{n+1}$ $\forall k \in S$ $z_S \leq x_k$ $z_S \geq \sum_{k \in S} x_k - (|S| - 1)$ $0 < x_k < 1$. $\forall k = 1, \ldots, n$ $0 < z_S < 1$, $\forall S \in S$

Polytope $P_{IS,1} \subseteq \mathbb{R}^{n+2}$

 $0 < z_5 < 1$.

$$z_{S} \leq x_{k},$$
 $\forall k \in S \setminus A$
 $z_{S} \leq z_{A},$
 $z_{S} \geq z_{A} + \sum_{k \in S \setminus A} x_{k} - |S \setminus A|,$
 $z_{A} \leq x_{k},$ $\forall k \in A$
 $z_{A} \geq \sum_{k \in A} x_{k} - (|A| - 1).$
 $0 \leq x_{k} \leq 1,$ $\forall k = 1, \dots, n$

 $\forall S \in S$

Calculating projections: Fourier-Motzkin Elimination

Notation

 $\mathbb{P}_{n,S}$: projection over the space of variables z_S and $x_k, k = 1, \ldots, n$.

We calculate $\mathbb{P}_{n,S}(P_{IS,1})$ using the Fourier-Motzkin Elimination:

$$z_S \le z_A$$
 $z_A \le x_k$, $\sum_{k \in A} x_k - (|A| - 1) \le z_A$ $z_A \le z_S - \sum_{k \in S \setminus A} x_k + |S \setminus A|$.

We also take into account the inequalities of $P_{IS,1}$ that do not involve z_A

$$z_S \leq x_k, \forall k \in S \backslash A$$

 $\forall k \in A$

Single monomials

Theorem

$$\mathbb{P}_{n,S}(P_{IS,1}) = P_{SL,1}$$

Theorem holds for disjoint several monomials:

$$z_S = \prod_{k \in S} x_k, \ z_T = \prod_{k \in T} x_k, \ \text{take } A \subseteq S, \ B \subseteq T.$$

$$z_S = z_A^S \prod_{k \in S \setminus A} x_k$$

$$z_A^S = \prod_{k \in A} x_k$$

$$z_T = z_B^T \prod_{k \in T \setminus B} x_k$$

$$z_B^T = \prod_{k \in B} x_k$$

Linearize, and apply Fourier-Motzkin as before (constraints never contain at the same time z_A^S and z_B^T).

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Theorem holds for disjoint several monomials:

$$z_S = \prod_{k \in S} x_k$$
, $z_T = \prod_{k \in T} x_k$, take $A \subseteq S$, $B \subseteq T$.

$$z_S = z_A^S \prod_{k \in S \setminus A} x_k$$

$$z_A^S = \prod_{k \in A} x_k$$

$$z_T = z_B^T \prod_{k \in T \setminus B} x_k$$

$$z_B^T = \prod_{k \in B} x_k$$

Linearize, and apply Fourier-Motzkin as before (constraints never contain at the same time z_s^S and z_t^T).

$$z_{S} = z_{A} \prod_{k \in S \setminus A} x_{k}$$

$$z_{T} = z_{A} \prod_{k \in T \setminus A} x_{k}$$

$$z_{A} = \prod_{k \in A} x_{k},$$

$$z_{S} = z_{A} \prod_{k \in S \setminus A} x_{k}$$

$$z_{T} = z_{A} \prod_{k \in T \setminus A} x_{k}$$

$$z_{A} = \prod_{k \in A} x_{k},$$

$$z_{S} \leq x_{k}, \qquad \forall k \in S \backslash A$$

$$z_{S} \leq z_{A}$$

$$z_{S} \geq z_{A} + \sum_{k \in S \backslash A} x_{k} - |S \backslash A|$$

$$z_{T} \leq x_{k}, \qquad \forall k \in T \backslash A$$

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$$z_{A} \leq x_{k}, \qquad \forall k \in A$$

$$z_{A} \geq \sum_{k \in T} x_{k} - (|A| - 1).$$

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$$z_{S} \leq z_{A}$$

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$$z_{T} = z_{A} \prod_{k \in T \backslash A} x_{k} \qquad z_{T} \leq x_{k}, \qquad \forall k \in T \backslash A$$

$$z_{A} = \prod_{k \in A} x_{k}, \qquad z_{T} \geq z_{A} + \sum_{k \in T \backslash A} x_{k} - |T \backslash A|$$

$$z_{A} \leq x_{k}, \qquad \forall k \in A$$

$$z_{A} \geq \sum_{k \in T} x_{k} - (|A| - 1).$$

What happens with *non-disjoint* monomials? $A \subseteq S \cap T$, $(|A| \ge 2)$.

$$z_{S} \leq z_{A}$$

$$z_{S} \geq z_{A} + \sum_{k \in S \setminus A} x_{k} - |S \setminus A|$$

$$z_{T} = z_{A} \prod_{k \in T \setminus A} x_{k}$$

$$z_{T} \leq z_{A}$$

$$z_{A} = \prod_{k \in A} x_{k},$$

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$$z_{A} \leq x_{k},$$

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 $z_S < x_k$

 $\forall k \in S \backslash A$

$$z_{S} = z_{A} \prod_{k \in S \setminus A} x_{k}$$

$$z_{T} = z_{A} \prod_{k \in T \setminus A} x_{k}$$

$$z_{A} = \prod_{k \in A} x_{k},$$

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$$z_{A} \leq x_{k}, \qquad \forall k \in A$$

$$z_{A} \geq \sum_{k \in A} x_{k} - (|A| - 1).$$

Theorem

$$\mathbb{P}_{n,S,T}(P_{IS}) \subset P_{SL}$$

Proof:

Fourier-Motzkin gives:

$$z_{S} \le z_{T} - \sum_{k \in T \setminus A} x_{k} + |T \setminus A|, \tag{1}$$

$$z_T \le z_S - \sum_{k \in S \setminus A} x_k + |S \setminus A|, \tag{2}$$

- ② $\mathbb{P}_{n,S,T}(P_{lS}) = P_{SL} \cap \{(x_k, z_S, z_T) \mid (1), (2) \text{ are satisfied}\}$
- 3 Point $x_k = 1$ for $k \notin A$, $x_k = \frac{1}{2}$ for $k \in A$, $z_S = 0$, $z_T = \frac{1}{2}$, is in P_{SL} but does not satisfy (2).

Consider $B \subset A \subseteq S \cap T$, $|B| \ge 2$.

Take the first cut for both subsets:

$$z_{S} \leq z_{T} - \sum_{k \in T \setminus A} x_{k} + |T \setminus A|,$$

$$z_{S} \leq z_{T} - \sum_{k \in T \setminus B} x_{k} + |T \setminus B|,$$

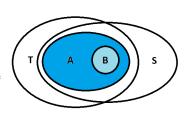
 $k \in T \setminus B$

2

$$z_{S} \leq z_{T} - \sum_{k \in T \setminus A} x_{k} + |T \setminus A| \leq$$

$$\leq z_{T} - \sum_{k \in T \setminus A} x_{k} + |T \setminus A| - \sum_{k \in A \setminus B} x_{k} + |A \setminus B| =$$

$$= z_{T} - \sum_{k \in T \setminus A} x_{k} + |T \setminus B|.$$



Theorem

$$\mathbb{P}_{n,S,T}(P_{IS}^A) \subset \mathbb{P}_{n,S,T}(P_{IS}^B).$$

(Point $x_k=1$ for $k\notin A$, $x_k=\frac{1}{2}$ for $k\in A\backslash B$, $k\in B$, $z_T=0$, $z_S=\frac{1}{2}$ satisfies cut for B but not for A.)

Definition: 2-link inequalities

$$z_S \le z_T - \sum_{k \in T \setminus S} x_k + |T \setminus S|$$

$$z_T \le z_S - \sum_{k \in S \setminus T} x_k + |S \setminus T|$$

Theorem

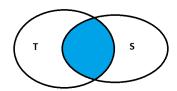
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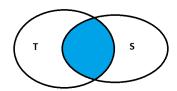
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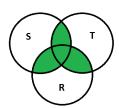
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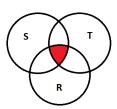
$$z_T \le z_S - \sum_{k \in S \setminus T} x_k + |S \setminus T|$$



Corollary

Consider three monomials R, S, T, with intersections $R \cap S = A$, $S \cap T = B$, $R \cap T = C$, $(|A|, |B|, |C| \ge 2)$. Then it is better to do intermediate substitutions of the two-by-two intersections, than a single intermediate substitution of the common intersection $A \cap B \cap C$.





Improving the SL formulation: 2-links

SL relaxation with 2-links

$$\begin{split} \min \sum_{S \in \mathcal{S}} a_S z_S \\ \text{s.t.} \ \ z_S & \leq x_k, & \forall k \in S, \forall S \in \mathcal{S} \\ z_S & \geq \sum_{k \in S} x_k - (|S| - 1), & \forall S \in \mathcal{S} \\ z_S & \leq z_T - \sum_{k \in T \setminus S} x_k + |T \setminus S| & \forall S, T, |S \cap T| \geq 2 \\ z_T & \leq z_S - \sum_{k \in S \setminus T} x_k + |S \setminus T| & \forall S, T, |S \cap T| \geq 2 \\ 0 & \leq z_S \leq 1, & \forall S \in \mathcal{S} \\ 0 & \leq x_k \leq 1 & \forall k = 1, \dots, n \end{split}$$

How strong are the 2-links?

Standard linearization polytope:

$$\begin{split} P_{SL}^{conv} &= \text{conv}\{(x,y_S) \in \{0,1\}^{n+|\mathcal{S}|} \mid y_S = \prod_{i \in S} x_i, \forall S \in \mathcal{S}\} \\ &= \text{conv}\{(x,y_S) \in \{0,1\}^{n+|\mathcal{S}|} \mid y_S \leq x_i, y_S \geq \sum_{i \in S} x_i - (|S|-1), \forall S \in \mathcal{S}\}, \end{split}$$

with linear relaxation

$$P_{SL} = \{(x, y_S) \in [0, 1]^{n+|S|} \mid y_S \le x_i, y_S \ge \sum_{i \in S} x_i - (|S| - 1), \forall S \in S\}$$

• Question 1: Are the 2-links facet-defining for P_{SI}^{conv} ?

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Facet-defining cuts (2 monomials)

Theorem: 2-term objective function

The 2-links are facet-defining for $P_{SL.2}^{conv}$:

$$z_{S} \leq z_{T} - \sum_{k \in T \setminus S} x_{k} + |T \setminus S|$$

$$z_T \le z_S - \sum_{k \in S \setminus T} x_k + |S \setminus T|$$

Facet-defining cuts (2 monomials)

Special forms of the cuts in some cases:

lacksquare If $S \subseteq T$,

$$z_S \le z_T - \sum_{k \in T \setminus S} x_k + |T \setminus S|$$

 $z_T \le z_S$

② If $T = \emptyset$ (and setting by definition $z_{\emptyset} = 1$),

$$z_{S} \leq 1$$

$$1 \leq z_{S} - \sum_{i \in S} x_{i} + |S|$$

Conjecture on the convex hull (2 monomials)

Conjecture

Consider a pseudo-Boolean function consisting of two terms, its standard linearization polytope $P_{SL,2}^{conv}$ and its linear relaxation $P_{SL,2}$. Then,

$$P_{SL,2}^{conv} = P_{SL,2} \cap \{(x, y_S, y_T) \in [0, 1]^{n+2} \mid 2\text{-links are satisfied}\}.$$

Facet-defining cuts (nested monomials)

Theorem: Nested sequence of terms

Consider a pseudo-Boolean function $f(x) = \sum_{l \in L} a_{S^{(l)}} \prod_{i \in S^{(l)}} x_i$, such that $S^{(1)} \subseteq S^{(2)} \subseteq \cdots \subseteq S^{(|L|)}$, and its standard linearization polytope $P_{SL,nest}^{conv}$. The 2-links

$$z_{S^{(l)}} \le z_{S^{(l+1)}} - \sum_{k \in S^{(l+1)} \setminus S^{(l)}} x_k + |S^{(l+1)} \setminus S^{(l)}|$$

 $z_{S^{(l+1)}} \le z_{S^{(l)}},$

-3(i+1) = -3(i)

are facet-defining for $P_{SL,nest}^{conv}$ for two consecutive monomials in the nest (and cuts are redundant for non-consecutive monomials).

Conjectures for *m* monomials

Conjecture: facet-defining

The 2-links are facet-defining for the case of m monomials.

Convex-hull for the general case

The 2-links and standard linearization inequalities are **not** enough to define the convex hull P_{SL}^{conv} (otherwise we could solve an \mathcal{NP} -hard problem efficiently...).

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• m=3, set of 3 monomials for which there exists an objective function which has a fractional optimal solution on $P_{SI} \cap \{2\text{-links}\}$:

$$\{x_1x_2x_4, x_1x_3x_4, x_1x_2x_3\}$$

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• m=3, set of 3 monomials for which there exists an objective function which has a fractional optimal solution on $P_{SL} \cap \{2\text{-links}\}$:

$$\{x_1x_2x_4, x_1x_3x_4, x_1x_2x_3\}$$



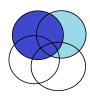








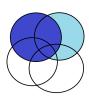










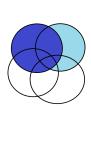




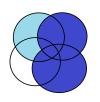








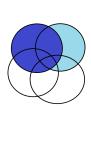




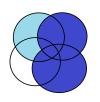




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A short summary and some ideas

- We have obtained interesting cuts for P_{SL} by applying intermediate substitutions for subsets of size ≥ 2 .
- We could apply iteratively these intermediate substitutions, the last substitution step has only quadratic constraints

$$z_{ij} = x_i x_j,$$

$$z_{iJ} = x_i z_J,$$

$$z_{IJ} = z_I z_J,$$

x: original variables, z: variables that are already substitutions of other subsets.

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