Linearization and quadratization approaches for non-linear 0-1 optimization

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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

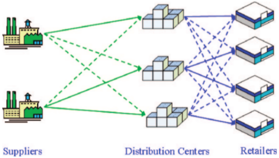
Every pseudo-Boolean function f can be represented uniquely by a multilinear polynomial (Hammer, Rosenberg, Rudeanu [4]).

Example:

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

Applications

Computer vision: image restoration



Supply Chain Design with Stochastic Inventory Management (joint model of F. You, I. E. Grossman) [6]

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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Linearizations:
reductions to the linear case

Standard linearization (SL)

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

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

1. Substitute monomials

$$\begin{aligned}
\min \sum_{S \in \mathcal{S}} a_S z_S & \\
\text{s.t. } z_S = \prod_{k \in S} x_k, & \quad \forall S \in \mathcal{S} \\
z_S \in \{0,1\}, & \quad \forall S \in \mathcal{S} \\
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2. Linearize constraints

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

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3. Linear relaxation

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

Intermediate substitutions (IS) (one monomial)

SL substitution

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

SL linearization

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

IS substitution

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

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IS linearization

$$\begin{aligned} z_S &\le x_k, & \forall k \in S \setminus A \\ z_S &\le z_A, & \\ z_S &\ge z_A + \sum_{k \in S \setminus A} x_k - |S \setminus A|, & \\ z_A &\le x_k, & \forall k \in A \\ z_A &\ge \sum_{k \in A} x_k - (|A| - 1). & \end{aligned}$$

Intermediate Substitutions (IS) (one monomial)

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

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

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

$$
\begin{aligned}
& z_S \leq x_k, && \forall k \in S \setminus A \\
& z_S \leq z_A, && \\
& z_S \geq z_A + \sum_{k \in S \setminus A} x_k - |S \setminus A|, && \\
& z_A \leq x_k, && \forall k \in A \\
& z_A \geq \sum_{k \in A} x_k - (|A| - 1). && \\
& 0 \leq x_k \leq 1, && \forall k = 1, \dots, n \\
& 0 \leq z_S \leq 1, && \forall S \in \mathcal{S}
\end{aligned}
$$

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**:

$$
\begin{aligned}
z_S &\leq z_A & z_A &\leq x_k, & \forall k \in A \\
\sum_{k \in A} x_k - (|A| - 1) &\leq z_A & z_A &\leq z_S - \sum_{k \in S \setminus A} x_k + |S \setminus A|.
\end{aligned}
$$

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

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

Single monomials

Theorem

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

Theorem holds for *disjoint* several monomials:
$z_S = \prod_{k \in S} x_k$, $z_T = \prod_{k \in T} x_k$, take $A \subseteq S$, $B \subseteq T$.

$$z_S = z_A^S \prod_{k \in S \setminus A} x_k \qquad z_T = z_B^T \prod_{k \in T \setminus B} x_k$$

$$z_A^S = \prod_{k \in A} x_k \qquad z_B^T = \prod_{k \in B} x_k$$

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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Several monomials with common intersection

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

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

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

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Several monomials with common intersection

Theorem

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

Proof:

1. Fourier-Motzkin gives:

$$\mathbf{z_S} \le \mathbf{z_T} - \sum_{\mathbf{k} \in \mathbf{T} \setminus \mathbf{A}} \mathbf{x_k} + |\mathbf{T} \setminus \mathbf{A}|, \tag{1}$$

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

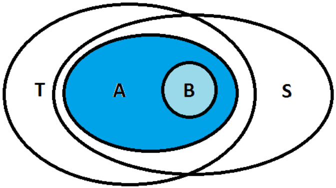
2. $\mathbb{P}_{n,S,T}(P_{IS}) = P_{SL} \cap \{(x_k, z_S, z_T) \mid (1), (2) \text{ are satisfied}\}$
3. Point $x_k = 1$ for $k \notin A$, $x_k = \frac{1}{2}$ for $k \in A$, $z_S = 0$, $z_T = \frac{1}{2}$, is in P_{SL} but does not satisfy (2).

Larger subset substitutions are better

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

1. Take the first cut for both subsets:
   $z_S \leq z_T - \sum_{k \in T \setminus A} x_k + |T \setminus A|$,
   $z_S \leq z_T - \sum_{k \in T \setminus B} x_k + |T \setminus B|$,
2.

$$
\begin{aligned}
z_S \leq z_T - \sum_{k \in T \setminus A} x_k + |T \setminus A| \leq \\
\leq z_T - \sum_{k \in T \setminus A} x_k + |T \setminus A| - \sum_{k \in A \setminus B} x_k + |A \setminus B| = \\
= z_T - \sum_{k \in T \setminus B} x_k + |T \setminus B|.
\end{aligned}
$$



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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.)

Corollary

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

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Improving the SL formulation: 2-intersection-cuts

SL relaxation with 2-intersection-cuts

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

$$\text{s.t. } z_S \leq x_k, \qquad \forall k \in S, \forall S \in \mathcal{S}$$

$$z_S \geq \sum_{k \in S} x_k - (|S| - 1), \qquad \forall S \in \mathcal{S}$$

$$\mathbf{z_S} \leq \mathbf{z_T} - \sum_{\mathbf{k} \in \mathbf{T} \setminus \mathbf{S}} \mathbf{x_k} + |\mathbf{T} \setminus \mathbf{S}| \qquad \forall \mathbf{S}, \mathbf{T}, |\mathbf{S} \cap \mathbf{T}| \geq \mathbf{2}$$

$$\mathbf{z_T} \leq \mathbf{z_S} - \sum_{\mathbf{k} \in \mathbf{S} \setminus \mathbf{T}} \mathbf{x_k} + |\mathbf{S} \setminus \mathbf{T}| \qquad \forall \mathbf{S}, \mathbf{T}, |\mathbf{S} \cap \mathbf{T}| \geq \mathbf{2}$$

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

$$0 \leq x_k \leq 1 \qquad \forall k = 1, \ldots, n$$

How strong are the 2-intersection-cuts?

Consider the *standard linearization polytope*:

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

and its linear relaxation

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

- **Question 1**: Are the 2-intersection-cuts *facet-defining* for P_{SL}^{conv}?

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- **Question 1**: Are the 2-intersection-cuts *facet-defining* for P_{SL}^{conv}?
- **Question 2**: Is there some case for which we obtain the *convex hull* P_{SL}^{conv} when adding the 2-intersection-cuts to P_{SL}?

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Facet-defining cuts (2 monomials)

Theorem: 2-term objective function

The 2-intersection-cuts are facet-defining for $P^{conv}_{SL,2}$:

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

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

Facet-defining cuts (2 monomials)

Special forms of the cuts in some cases:

1. If $S \subseteq T$,

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

$$z_T \leq z_S$$

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,

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

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 $P^{conv}_{SL,nest}$. The 2-intersection-cuts

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

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

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

Conjectures for m monomials

Conjecture: facet-defining

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

Convex-hull for the general case

The 2-intersection-cuts 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...).

Conjectures for m monomials

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Convex-hull for the general case

The 2-intersection-cuts 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...).

- $m = 3$, set of 3 monomials for which there exists an objective function which has a fractional optimal solution on $P_{SL} \cap \{$2-intersection-cuts$\}$: $\{x_1x_2x_4, x_1x_3x_4, x_1x_2x_3\}$

Conjectures for m monomials

Conjecture: facet-defining

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A (vague) idea of the convex hull for the general case

Idea of the convex hull

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

s.t. SL-constraints: linking a term with its variables

2-intersection inequalities: linking terms 2 by 2

3-intersection inequalities: linking terms 3 by 3

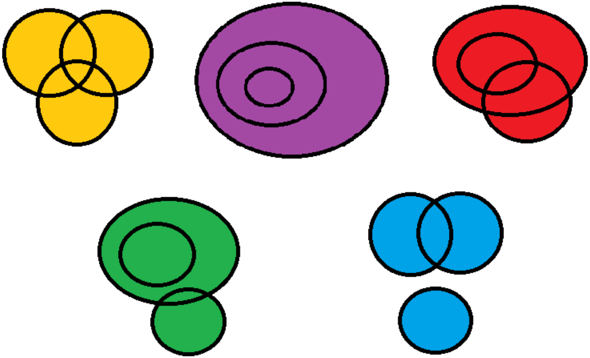
$\dots$

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

$$0 \leq x_k \leq 1 \qquad \forall k = 1, \dots, n$$

One way of viewing the difficulty of the convex hull

For 3 monomials we already have many different possible ways for them to intersect:



A short summary of the linearizations part 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

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Quadratizations:
reductions to the quadratic case

Linearizations vs. quadratizations

Initial objective function (polynomial and binary):

$$f(x) = \sum_{S \in \mathcal{S}} a_S \prod_{i \in S} x_i$$

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Introduce **new variables** to obtain an equivalent **linear** problem.

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$$\min_{x \in \{0,1\}^4} 3x_1x_2x_3x_4 + 2x_1x_2x_5 - 5x_1x_2 + 6x_3x_4 - x_1 + x_2 - x_3 + x_4$$

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Rosenberg (1975) [5]: first quadratization method.

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Quadratization methods: Rosenberg with constraints

Rosenberg (1975) [5]: first quadratization method (Variant).

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Rosenberg and intermediate substitutions

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Linearization of Rosenberg

$$\begin{aligned} \min_{x\in\{0,1\}^4, y_{12}, y_{34}, y_{1234}, y_{125}\in\{0,1\}} \quad & 3y_{1234} + 2y_{125} - 5y_{12} + 6y_{34} - x_1 + x_2 - x_3 + x_4 \\ \text{s.t.} \quad & y_{12} = x_1x_2 \\ & y_{34} = x_3x_4 \\ & y_{1234} = y_{12}y_{34} \\ & y_{125} = y_{12}x_5 \end{aligned}$$

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Linearization of quadratic vs. polynomial functions

Buchheim and Rinaldi's result [2]:

Consider linearization of a polynomial function:

$$P_{SL}^{conv} = \text{conv}\{(x, y_S) \in \{0,1\}^{n+|\mathcal{S}|} \mid y_S = \prod_{i \in S} x_i, \forall S \in \mathcal{S}\}$$

Define an extended quadratic formulation and linearize it:

$$P^* = \text{conv}\{y_{\{S,T\}} \in \{0,1\} \mid y_{\{S,T\}} = y_S y_T, \forall \{S, T\} \text{ where } S, T, S \cup T \in \mathcal{S}\}$$

If we know P^* then we can construct P_{SL}^{conv}.

Questions: If instead of having P^*, we have a relaxation,

- what do we know about P_{SL}^{conv}?
- for the standard linearization, 2-intersection, 3-intersection (up to m-intersection) cuts help to obtain information about P_{SL}^{conv}, what about other relaxations?

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