# Quadratizations of pseudo-Boolean functions 

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Partially supported by Belspo - IAP Project COMEX

4th December 2014
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combinatorial optimization:
metaheuristics \& exact methods

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## Definitions

## Definition: Pseudo-Boolean functions

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

## Multilinear representation

Every pseudo-Boolean function $f$ can be represented uniquely by a multilinear polynomial (Hammer, Rosenberg, Rudeanu [7]).

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Example:

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f\left(x_{1}, x_{2}, x_{3}\right)=9 x_{1} x_{2} x_{3}+8 x_{1} x_{2}-6 x_{2} x_{3}+x_{1}-2 x_{2}+x_{3}
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## Applications: MAX-SAT

## MAX-SAT problem

- INPUT: a set of Boolean clauses $C_{k}=\left(\vee_{i \in A_{k}} \bar{x}_{i}\right) \vee\left(\vee_{j \in B_{k}} x_{j}\right)$, for $k=1, \ldots, m$, where $x_{i} \in\{0,1\}$, and $\bar{x}_{i}=1-x_{i}$.
- OBJECTIVE: find an assignment of the variables, $x^{*} \in\{0,1\}^{n}$ that maximizes the number of satisfied clauses.


## Pseudo-Boolean formulation


$C_{k}$ takes value 1 iff the term $\prod_{i \in A_{k}} x_{i} \prod_{j \in B_{k}} \bar{x}_{j}$ takes value 0 .

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\min \sum_{k=1}^{m}\left(\prod_{i \in A_{k}} x_{i}\right)\left(\prod_{j \in B_{k}} \bar{x}_{j}\right)
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## Applications: Computer Vision

Image restoration problems modelled as energy minimization

$$
E(I)=\sum_{p \in \mathcal{P}} D_{p}\left(I_{p}\right)+\sum_{S \subseteq \mathcal{P},|S| \geq 2} \sum_{p_{1}, \ldots, p_{s} \in S} V_{p_{1}, \ldots, p_{s}}\left(l_{p_{1}}, \ldots, l_{p_{s}}\right),
$$

where $I_{p} \in\{0,1\} \quad \forall p \in \mathcal{P}$.


## Applications

- Constraint Satisfaction Problem
- Data mining, classification, learning theory...
- Graph theory
- Operations research
- Production management
- ...


## Pseudo-Boolean Optimization

Many problems formulated as optimization of a pseudo-Boolean function

## Pseudo-Boolean Optimization

$$
\min _{x \in\{0,1\}^{n}} f(x)
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- Optimization is $\mathcal{N} \mathcal{P}$-hard, even if $f$ is quadratic (MAX-2-SAT, MAX-CUT modelled by quadratic $f$ ).


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## Quadratizations

## Definition: Quadratization

Given a pseudo-Boolean function $f(x)$ on $\{0,1\}^{n}$, we say that $g(x, y)$ is a quadratization of $f$ if $g(x, y)$ is a quadratic polynomial depending on $x$ and on $m$ auxiliary variables $y_{1}, \ldots, y_{m}$, such that

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f(x)=\min \left\{g(x, y): y \in\{0,1\}^{m}\right\} \quad \forall x \in\{0,1\}^{n}
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Then, $\min \left\{f(x): x \in\{0,1\}^{n}\right\}=\min \left\{g(x, y): x \in\{0,1\}^{n}, y \in\{0,1\}^{m}\right\}$.
Which quadratizations are "good"?

- Small number of auxiliary variables.
- Good optimization properties: submodularity.


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- Algorithms based on MAX-CUT (which reduces to a polynomial MIN-CUT problem when $f$ is submodular).


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## Rosenberg

## Rosenberg (1975) [11]: first quadratization method.

(1) Take a product $x_{i} x_{j}$ from a highest-degree monomial of $f$ and substitute it by a new variable $y_{i j}$.
(2) Add a penalty term $M\left(x_{i} x_{j}-2 x_{i} y_{i j}-2 x_{j} y_{i j}+3 y_{i j}\right)$ ( $M$ large enough) to the objective function to force $y_{i j}=x_{i} x_{j}$ at all optimal solutions.
(3) Iterate until obtaining a quadratic function.

- Advantages:
- Can be applied to any pseudo-Boolean function $f$.
- The transformation is polynomial in the size of the input.


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## Termwise quadratizations

## Multilinear expression of a pseudo-Boolean function:

$$
f(x)=\sum_{S \in 2^{[n]}} a_{S} \prod_{i \in S} x_{i}
$$

Idea: quadratize monomial by monomial, using different sets of auxiliary variables for each monomial.

## Termwise quadratizations: negative monomials

## Kolmogorov and Zabih [10], Freedman and Drineas [6].

$$
a \prod_{i=1}^{n} x_{i}=\min _{y \in\{0,1\}} a y\left(\sum_{i=1}^{n} x_{i}-(n-1)\right), a<0 .
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- Advantages: one single auxiliary variable, submodular quadratization.


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## Termwise quadratizations: positive monomials

## Ishikawa [9]

$$
a \prod_{i=1}^{d} x_{i}=a \min _{y_{1}, \ldots y_{n_{d}} \in\{0,1\}} \sum_{i=1}^{n_{d}} y_{i}\left(c_{i, d}\left(-S_{1}+2 i\right)-1\right)+a S_{2},
$$

$S_{1}, S_{2}$ : elementary linear and quadratic symmetric polynomials in $d$ variables, $\mathbf{n}_{\mathbf{d}}=\left\lfloor\frac{\mathbf{d}-\mathbf{1}}{2}\right\rfloor$ and $c_{i, d}=\left\{\begin{array}{l}1, \text { if } d \text { is odd and } i=n_{d}, \\ 2, \text { otherwise. }\end{array}\right.$

- Number of variables: best known bound for positive monomials.
- Submodularity: $\binom{d}{2}$ positive quadratic terms, but very good computational results.


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## Number of variables

Using termwise quadratizations:

- One variable per negative monomial and \} \lfloor \frac { d - 1 } { 2 } \rfloor per positive monomial ( $d$ : degree of the monomial).
- Best known upper bounds: $O\left(n^{d}\right)$ variables for a polynomial of fixed degree $d, O\left(n 2^{n}\right)$ for an arbitrary function.


## Can we do better?

Tight upper and lower bounds independent of the quadratization procedure by Anthony, Boros, Crama and Gruber [1]

- $\Theta\left(2^{\frac{n}{2}}\right)$ for a general pseudo-Boolean function.
- $\Theta\left(n^{\frac{d}{2}}\right)$ for a fixed polynomial of degree $d$.


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Specific quadratization procedures, experimental evaluations...

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Systematic study of quadratizations, understand properties and structure.

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## Polynomial pseudo-Boolean optimization



## Standard linearization

## Original polynomial problem

$$
\min _{x \in\{0,1\}^{n}} f(x)=\sum_{S \in \mathcal{S}} a_{S} \prod_{i \in S} x_{i}
$$

$\mathcal{S}$ : set of non-constant monomials.

## 1. Substitute monomials



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## 1. Substitute monomials

## 2. Linearize constraints

$$
\begin{aligned}
& \min _{z s} \sum_{S \in \mathcal{S}} a_{s} z_{S} \\
& \text { s.t. } z_{S}=\prod_{i \in S} z_{i}, \forall S \in \mathcal{S} \\
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z_{S} \in\{0,1\}, \forall S \in \mathcal{S} & z_{S} \geq \sum_{i \in S} z_{i}-|S|+1, \forall S \in \mathcal{S} \\
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## 1. Define quadratization for $f$

$$
\min _{x \in\{0,1\}^{n+m}} \sum_{Q \in \mathcal{Q}} b_{Q} \prod_{i \in Q} x_{i}
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where $\mathcal{Q}$ is the set of non-constant monomials in the original $\left\{x_{1}, \ldots, x_{n}\right\}$ and the auxiliary $\left\{x_{n+1}, \ldots, x_{n+m}\right\}$ variables and all $Q \in \mathcal{Q}$ have degree at most 2.

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## 3. Linearize constraints



## Linearization of a quadratization

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\min _{w_{Q}} & \sum_{Q \in \mathcal{Q}} b_{Q} w_{Q} \\
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## Comparing relaxations of linearizations

Relaxation of standard linearization (A)

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## Relaxation of linearized quadratization (B)

$$
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## Comparing polytopes at substitution step

## Standard linearization (A)

## Quadratization (B)

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## Comparing polytopes at substitution step

## Questions:

- Do we have a better knowledge of one of the convex hull of feasible solutions of one of these problems? (i.e., polyhedral description, good separation algorithms...).


## Buchheim and Rinaldi's approach

## Polynomial Optimization Problem

LP-relaxation (standard lin.), polytope $P$


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## Buchheim and Rinaldi's approach: Polytope $P^{*}$ ?

Presented in [2], [3].

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$\mathcal{S}$ : set of non-constant monomials

- Assumption: every $S \in \mathcal{S}$ can be written as the union of two other monomials $S_{l}, S_{r} \in \mathcal{S}$.


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Presented in [2], [3].

## Original polynomial problem

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\min _{x \in\{0,1\}^{n}} f(x)=\sum_{S \in \mathcal{S}} a_{S} \prod_{i \in S} x_{i}
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$\mathcal{S}$ : set of non-constant monomials

- Assumption: every $S \in \mathcal{S}$ can be written as the union of two other monomials $S_{l}, S_{r} \in \mathcal{S}$.
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Buchheim and Rinaldi's formulation over a quadric polytope
Consider the set $\mathcal{S}^{*}=\{\{S, T\} \mid S, T \in \mathcal{S}$ and $S \cup T \in \mathcal{S}\}$.

$$
\begin{aligned}
\min _{\{S\}} & \sum_{S \in \mathcal{S}} a_{S} y_{\{S\}} \\
\text { s.t. } & y_{\{S, T\}}=y_{\{S\}} y_{\{T\}}, \forall\{S, T\} \in \mathcal{S}^{*} \\
& y_{\{S, T\}} \in\{0,1\}, \forall\{S, T\} \in \mathcal{S}^{*}
\end{aligned}
$$

$P^{*}$ : convex hull of feasible solutions of problem (C)
Observation: $P^{*}$ is a boolean quadric polytope.

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## Buchheim and Rinaldi's formulation and Rosenberg's quadratization

## Theorem

Buchheim and Rinaldi's formulation over a quadric polytope can be obtained (up to elimination of redundant constraints) by linearizing a variant of Rosenberg's quadratization where:

- the order of substituting variables is induced by the decomposition $S_{l}, S_{r}$ of each monomial $S$, and
- when substituting a product by a variable, we do not impose $y_{i j}=x_{i} x_{j}$ with a penalty, but with a constraint.

Assumption: every $S \in \mathcal{S}$ can be written as the union of two other monomials $S_{l}, S_{r} \in \mathcal{S}$.


## Conclusions

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