Compact quadratizations for pseudo-Boolean functions

Elisabeth Rodríguez-Heck joint work with Endre Boros (Rutgers University), and Yves Crama (University of Liège)

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Pseudo-Boolean optimization

General problem: pseudo-Boolean optimization Given a pseudo-Boolean function $f : \{0,1\}^n \to \mathbb{R}$ $\min_{x \in \{0,1\}^n} f(x).$



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Given f, finding its unique multilinear representation can be costly! (Size of the input: O(2ⁿ))



Multilinear 0–1 optimization

Assumption: f given as a multilinear polynomial Set of monomials $S \subseteq 2^{[n]}$, $a_S \neq 0$ for $S \in S$.

$$\min \sum_{S \in S} \sum_{i \in S} x_i$$
s. t. $x_i \in \{0, 1\}$, for $i = 1, ..., n$

Example:

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



Definition (Anthony, Boros, Crama, & Gruber, 2017)

Given a pseudo-Boolean function f(x) where $x \in \{0,1\}^n$, a *quadratization* g(x, y) is a function satisfying

- ▶ g is quadratic
- ▶ g(x, y) depends on the original variables x and on m auxiliary variables y
- satisfies

$$f(x) = \min\{g(x, y) : y \in \{0, 1\}^m\} \ \forall x \in \{0, 1\}^n.$$



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Which quadratizations are "good"?

- Small number of auxiliary variables (*compact*).
- Small number of positive quadratic terms (x_ix_j, x_iy_j...) (empirical measure of submodularity).



Application in computer vision: image restoration



Image from the Corel database.



Persistencies

Weak Persistency Theorem (Hammer, Hansen, & Simeone, 1984)

Let (QP) be a quadratic optimization problem on $x \in \{0, 1\}^n$, and let (\tilde{x}, \tilde{y}) be an optimal solution of the *continuous standard linearization of* (QP)

$$\begin{array}{ll} \min & c_0 + \sum_{j=1}^n c_j x_j + \sum_{1 \le i < j \le n} c_{ij} y_{ij} \\ \text{s. t. } y_{ij} \ge x_i + x_j - 1 & i, j = 1, \dots, n, i < j \\ & y_{ij} \le x_i & i, j = 1, \dots, n, i < j \\ & y_{ij} \le x_j & i, j = 1, \dots, n, i < j \\ & 0 \le y_{ij} \le 1 & i, j = 1, \dots, n, i < j \\ & 0 \le x_i \le 1 & i = 1, \dots, n \end{array}$$

such that $\tilde{x}_j = 1$ for $j \in O$ and $\tilde{x}_j = 0$ for $j \in Z$. Then, for any minimizing vector x^* of (QP) switching $x_j^* = 1$ for $j \in O$ and $x_j^* = 0$ for $j \in Z$ will also yield a minimum of f.



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- There are ways to compute, in polynomial time, a maximal set of variables to fix, based on a network flow algorithm (Boros et al., 2008).
- In computer vision, image restoration and related problems of up to *millions* of variables are efficiently solved, thanks to the use of persistencies.



Main idea

Quadratize monomial by monomial using disjoint sets of auxiliary variables.

 $f(x) = -35x_1x_2x_3x_4x_5 + 50x_1x_2x_3x_4 - 10x_1x_2x_4x_5 + 5x_2x_3x_4 + 5x_4x_5 - 20x_1$



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Negative monomial

(Kolmogorov & Zabih, 2004; Freedman & Drineas, 2005)

$$-\prod_{i=1}^{n} x_{i} = \min_{y \in \{0,1\}} -y(\sum_{i=1}^{n} x_{i} - (n-1))$$

- One variable is sufficient.
- No positive quadratic terms.



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If $x_i = 1 \ \forall i$, then $min_y - y$, minimum value of -1 reached for y = 1.



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- If x_i = 1 ∀i, then min_y y, minimum value of -1 reached for y = 1.
- If ∃i such that x_i = 0, then min_y - Cy, where C ≤ 0, minimum value of 0 reached for y = 0.



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Positive monomial

(Ishikawa, 2011)

$$\begin{split} \prod_{i=1}^n x_i &= \min_{y \in \{0,1\}^k} \sum_{i=1}^k y_i (c_{i,n}(-|x|+2i)-1) \\ &+ \frac{|x|(|x|-1)}{2}, \end{split}$$

- Number of variables: $k = \lfloor \frac{n-1}{2} \rfloor$.
- $\binom{n}{2}$ positive quadratic terms.



Theorem 3 (simplified version)

Assume that $n = 2^{\ell}$ and let $|x| = \sum_{i=1}^{n} x_i$ be the Hamming weight of $x \in \{0,1\}^n$. Then,

$$g(x,y) = rac{1}{2}(|x| - \sum_{i=1}^{\ell-1} 2^i y_i)(|x| - \sum_{i=1}^{\ell-1} 2^i y_i - 1)$$

is a quadratization of the positive monomial $P_n(x) = \prod_{i=1}^n x_i$ using $\lfloor \log(n) \rfloor - 1$ auxiliary variables.



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Proof idea: Check that, for every $x \in \{0,1\}^n$, $min_y g(x,y) = \prod_{i=1}^n x_i$.

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- For |x| ≤ n − 1, one factor to reach the minimum value of zero for odd |x| and the other factor for even |x|.



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- Use y variables to express which powers of 2 are in the sum.
- For |x| ≤ n − 1, one factor to reach the minimum value of zero for odd |x| and the other factor for even |x|.
- Case 2 (|x| = n): Similarly, we can show $min_yg(x, y) = 1$.

Theorem 3

If g(x, y) is a quadratization of the positive monomial $P_n(x) = \prod_{i=1}^n x_i$ using m variables, then

 $m \geq \lceil \log(n) \rceil - 1$



Results for more general functions

Function	Lower Bound	Upper Bound
Zero until <i>k</i>	$\Omega(2^{rac{n}{2}})$ for some function ¹ $\lceil \log(k) ceil - 1$ for all functions	$O(2^{\frac{n}{2}})^{-1}$
Symmetric	$\Omega(\sqrt{n})$ for some function ²	$O(\sqrt{n}) = 2\lceil \sqrt{n+1} \rceil$
Exact k-out-of-n	$\max(\lceil \log(k) \rceil, \lceil \log(n-k) \rceil) - 1$	$\max(\lceil \log(k) \rceil, \lceil \log(n-k) \rceil)$
At least <i>k</i> -out-of- <i>n</i>	$\lceil \log(k) ceil - 1$	$\max(\lceil \log(k) \rceil, \lceil \log(n-k) \rceil)$
Positive monomial	$\lceil \log(n) \rceil - 1$	$\lceil \log(n) \rceil - 1$
Parity	$\lceil \log(n) ceil - 1$	$\lceil \log(n) \rceil - 1$



¹see (Anthony et al., 2017)

²see (Anthony, Boros, Crama, & Gruber, 2016)



Ongoing computational work

Which quadratizations work better in practice?



Anthony, Boros, Crama and Gruber (2017)

Substituting common sets of variables

 $f(x) = -35x_1x_2x_3x_4x_5 + 50x_1x_2x_3x_4 - 10x_1x_2x_4x_5 + 5x_2x_3x_4 + 5x_4x_5 - 20x_1$ could be replaced by $f(x) = -35y_{12}y_{345} + 50y_{12}y_{34} - 10y_{12}y_{45} + 5x_2y_{34} + 5x_4x_5 - 20x_1 + P(x, y)$ where P(x, y) imposes $y_{12} = x_1x_2$, $y_{345} = y_{34}x_5$...



Heuristics for small Pairwise Covers

Three heuristics:

- PC1: Separate first two variables from the rest.
- PC2: Most "popular" intersections first.
- PC3: Most "popular" pairs of variables first.

Main idea: identifying *subterms* that appear as subsets of one or more monomials in the input monomial set S.



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- ... but we already obtain some interesting observations.
- We compare the results with the resolution of linearized instances (SL) using CPLEX 12.7.



Instances: Vision



Up to n = 900 variables and m = 6788 terms



p.15

Vision: all methods 15×15 (n = 225, m = 1598)





Vision: best methods 15×15 (n = 225, m = 1598)



Instances



Random polynomials: all methods



Random polynomials: best methods





Quadratization properties

Vision	Pairwise covers	Termwise
Number of <i>y</i> variables Number of positive quadratic terms	less less	more more
Random	Pairwise covers	Termwise
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Conclusions

Summary

- New compact quadratizations for the positive monomial.
- Proof of the lower bound on the number of auxiliary variables.
- First experiments: small number of auxiliary variables might not be the best criterion to define good quadratizations.



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Perspectives

- Experiments will be re-tested using persistencies and other solvers.
- Other properties:
 - Small number of positive quadratic terms.
 - Graph underlying quadratic terms with special structure (e. g. sparse...).



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