Quadratization of Pseudo-Boolean Functions

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[1] Joint work with A. Fix, A. Gruber, G. Tavares and R. Zabih

Outline

Quadratic Unconstrained Binary Optimization (QUBO)

Variables and Literals

- **Variables**: $x_1, x_2, \ldots, x_n \quad \in \{0,1\}$.
- **Negations**: $\overline{x}_i = 1 - x_i \quad \in \{0,1\}$ for $i = 1, \ldots, n$
- **Literals**: $x_1, \overline{x}_1, \ldots, x_n, \overline{x}_n$

Quadratic Pseudo-Boolean Function (QPBF): $f : \{0,1\}^n \to \mathbb{R}$

$$f(x_1, \ldots, x_n) = c_0 + \sum_{j=1}^{n} c_j x_j + \sum_{1 \le i < j \le n} c_{ij} x_i x_j$$

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Posiforms: Nonnegative (except maybe the constant terms) multi-linear polynomials in $2n$ literals x_1, $\overline{x}_1$, ..., x_n, $\overline{x}_n$

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$$\begin{aligned} f &= -2 - x_1 - x_2 - x_3 + x_1x_2 + x_1x_3 + x_2x_3 && \text{QPBF} \\ &= -5 + \overline{x}_1 + \overline{x}_2 + \overline{x}_3 + x_1x_2 + x_1x_3 + x_2x_3 && \text{quadratic posiform} \end{aligned}$$

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$\mathbf{C_2}(f)$ = largest C s.t. $f = C + \phi$ for some **quadratic posiform** ϕ.

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$$\mathbf{C_2}(f) \leq \mathbf{C_3}(f) \leq \cdots \leq \mathbf{C_n}(f) = \min f$$

Outline

Network Model for Submodular QUBO (Hammer, 1965)

- A QPBF is submodular IFF all quadratic coefficients are nonpositive. (*Doit Yourself, anytime*)
- To a submodular QPBF f associate a network G_f as follows

$$=$$

- There is a one-to-one correspondence between values of f and $s-t$ cut values of G_f. (*Hammer, 1965*)

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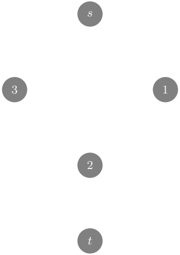

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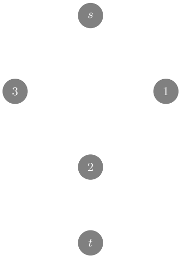

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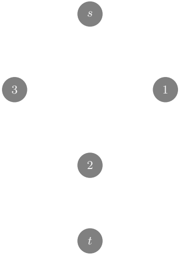

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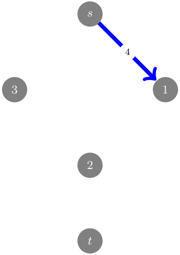

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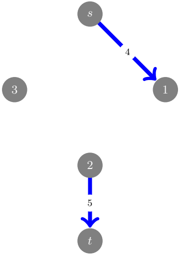

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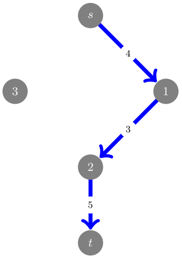

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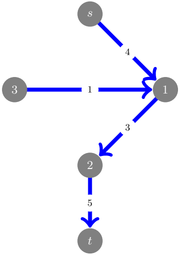

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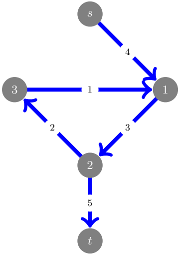

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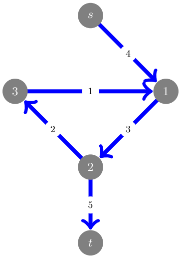

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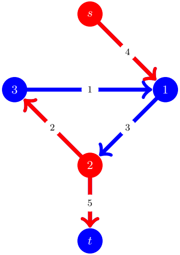

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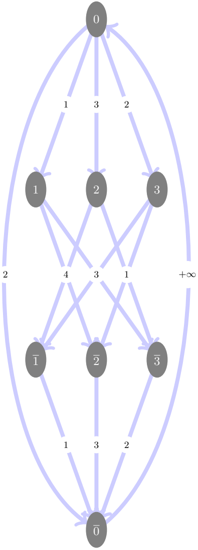
$$\mathbf{f}(0,1,0) = \mathbf{C}(\{s,2\},\{1,3,t\}) = 11$$

Outline

Implication Networks (Boros, Hammer, Sun, 1989, 1992)



To a quadratic posiform

$$\phi = \mathbf{2}x_0x_0 + \mathbf{2\overline{x}_1}x_0 + \mathbf{6\overline{x}_2}x_0 + \mathbf{4\overline{x}_3}x_0 + \mathbf{8x_1x_2} + \mathbf{6x_1x_3} + \mathbf{2x_2x_3}$$

we associate a directed network N_ϕ on vertex set

$$V(N_\phi) = \{x_0, \overline{x}_0, x_1, \overline{x}_1, \ldots, x_n, \overline{x}_n\} \qquad (x_0 \equiv 1)$$

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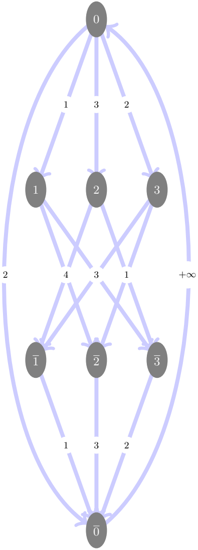

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- Associate to each term $\alpha\, uv$ $(u \neq v)$ two arcs $(u, \overline{v})$ and $(v, \overline{u})$ with capacities $c(u, \overline{v}) = c(v, \overline{u}) = \alpha/2$.
- Associate to $\gamma\, x_0x_0$ one arc $(x_0, \overline{x}_0)$ with capacity $c(x_0, \overline{x}_0) = \gamma$ and add arc $(\overline{x}_0, x_0)$ with capacity $c(\overline{x}_0, x_0) = +\infty$.

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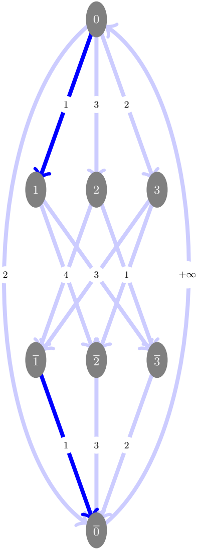

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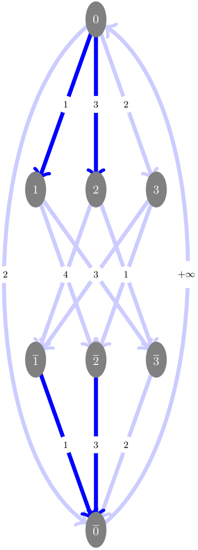

To a quadratic posiform

$$\phi = 2x_0x_0 + 2\overline{x}_1x_0 + 6\overline{x}_2x_0 + 4\overline{x}_3x_0 + 8x_1x_2 + 6x_1x_3 + 2x_2x_3$$

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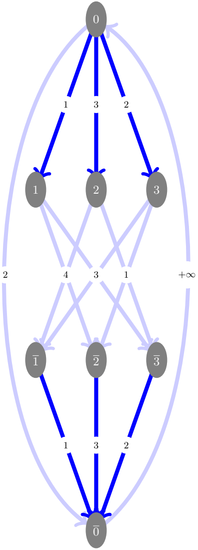

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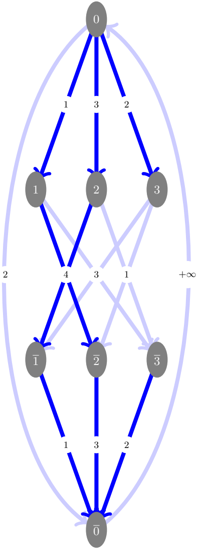

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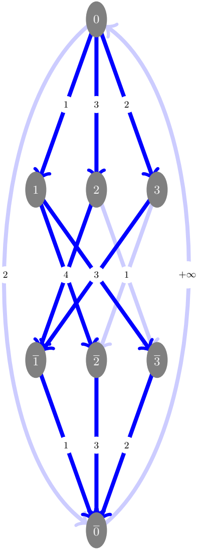

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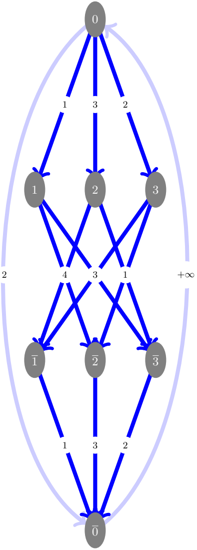

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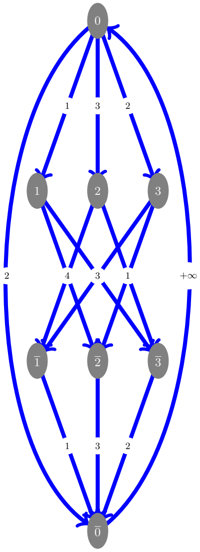

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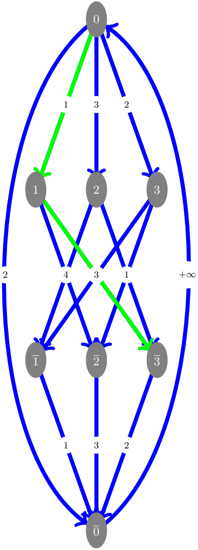

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N_ϕ is a symmetric network: twin pair of paths, cycles and flows

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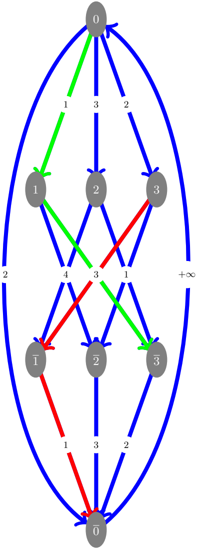

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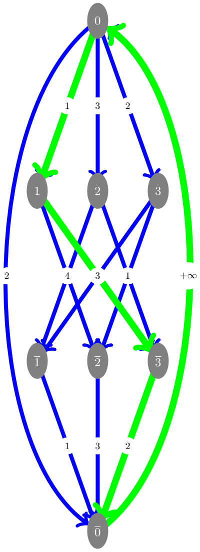

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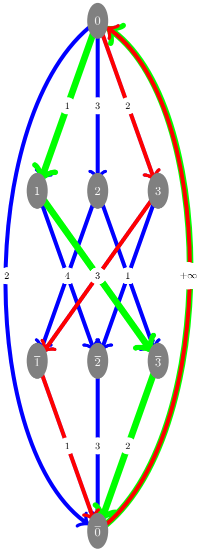

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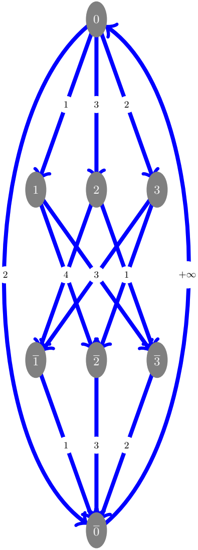

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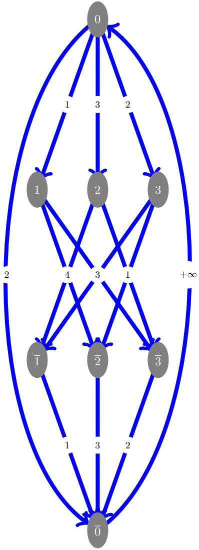

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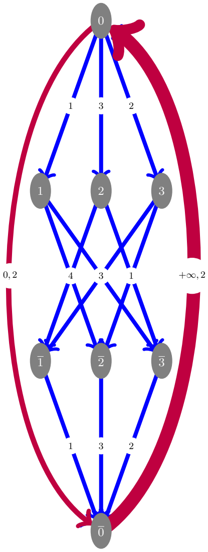

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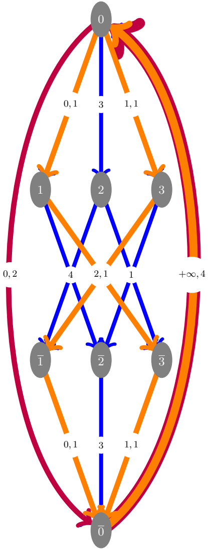

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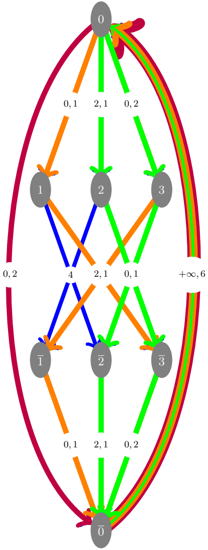

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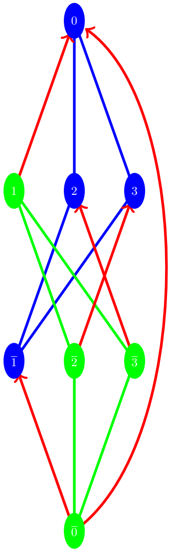

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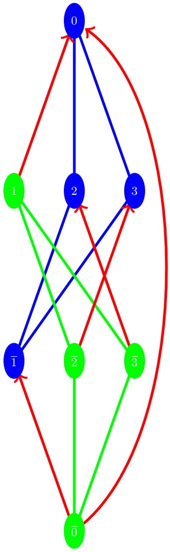

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Outline

Components of the Algorithm

The **purpose** of the preprocessing algorithm is to **fix** some of the variables at their optimum values and **decompose** the remaining problem into several smaller problems which do not share variables.

- Build implication network
- Compute maximum flow; **fix variables by persistency** (increase capacities of some arcs)
- Probe remaining variables and repeat all of the above as long as there is some change.
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If the input QPBF is submodular, then the above procedure will fix all the variables at their optimal values in the first round, without any probing.

Outline

Via Minimization in VLSI Design

		Percentage of Variables Fixed by					
Problem[1]	n	Roof Duality		Probing		ALL TOOLS	Time (sec)
		(strong)	(weak)	(forcing)	(equalities)		
via.c1y	829	93.6%	6.4%	0%	0%	**100%**	**0.03**
via.c2y	981	94.7%	5.3%	0%	0%	**100%**	**0.06**
via.c3y	1328	94.6%	5.4%	0%	0%	**100%**	**0.09**
via.c4y	1367	96.4%	3.6%	0%	0%	**100%**	**0.09**
via.c5y	1203	93.1%	6.9%	0%	0%	**100%**	**0.08**
via.c1n	828	57.4%	9.6%	32.4%	0.6%	**100%**	**0.49**
via.c2n	980	12.4%	4.4%	83.1%	0.1%	**100%**	**7.14**
via.c3n	1327	6.8%	5.7%	87.3%	0.2%	**100%**	**18.17**
via.c4n	1366	11.1%	1.3%	87.6%	0%	**100%**	**23.08**
via.c5n	1202	3.4%	1.4%	95.0%	0.2%	**100%**	**17.13**

[1] S. Homer and M. Peinado. Design and performance of parallel and distributed approximation algorithms for maxcut. *Journal of Parallel and Distributed Computing* **46** (1997) 48-61.

Vertex Cover in Planar Graphs

	Averages for 100 graphs in each of the 4 groups			
	Variables Fixed (%)		Time (sec)	
n	A. D. N.[2]	**QUBO**[3]	A. D. N.[2]	**QUBO**[3]
1000	68.4	**100**	4.06	**0.05**
2000	67.4	**100**	12.24	**0.16**
3000	65.5	**100**	30.90	**0.27**
4000	62.7	**100**	60.45	**0.53**

[2] Alber, Dorn, Niedermeier. Experimental evaluation of a tree decomposition based algorithm for vertex cover on planar graphs. Discrete Applied Mathematics 145 (2005) 219-231; 750 GHz, Linux PC, 720 MB

[3] Pentium 4, 2.8 GHz, Windows XP, 512 MB

Jumbo Vertex Cover in Planar Graphs

Vertices	Computing Times (min)[4]		
	Planar Density		
	10%	50%	90%
50,000	0.7	2.3	0.9
100,000	2.9	10.2	3.9
250,000	19.5	69.8	26.3
500,000	79.3	277.3	106.9

[4] Averages over 3 experiments on a Xeon 3.06 GHz, XP, 3.5 GB RAM; ALL problems had 100% of their variables fixed.

One Dimensional Ising Models

σ	Number of Spins	Average Computing Time (s)		
		Branch, Cut & Price[5]	Biq Maq[5]	**QUBO**[6]
2.5	100	699	68	**1**
	150	92 079	388	**3**
	200	N/A	993	**9**
	250	N/A	6 567	**14**
	300	N/A	34 572	**21**
3.0	100	256	59	**1**
	150	13 491	293	**2**
	200	61 271	1 034	**3**
	250	55 795	3 594	**4**
	300	55 528	8 496	**5**

[5] F. Rendl, G. Rinaldi, A. Wiegele. (2007). Solving max-cut to optimality by intersecting semidefinite and polyhedral relaxations.

[6] ALL problems were solved by QUBO.

Larger One Dimensional Ising Models

		Average of 3 Problems	
σ	n	**Variables not fixed**	**QUBO Time (s)**[7]
2.5	500	**5**	**13**
	750	**22**	**30**
	1000	**24**	**53**
	1250	**20**	**81**
	1500	**32**	**124**
3.0	500	**0**	**4**
	750	**0**	**12**
	1000	**0**	**23**
	1250	**0**	**37**
	1500	**0**	**59**

[7] Pentium M, 1.6 GHz 760 MB RAM

Outline

Quadratization of PBFs

- Given $f : \{0,1\}^n \rightarrow \mathbb{R}$ **find** **quadratic** $g : \{0,1\}^{n+m} \rightarrow \mathbb{R}$ such that

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

- ♣ Keep m **small**!
- ♢ Have g as **submodular** as possible!
- ♡ Do not introduce **large** coefficients!
- ♠ Have it **ALL**!

Rosenberg, 1975: **All** PBFs have **polynomial sized** quadratizations.

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Outline

Submodular PBFs

- A PBF $f : \{0,1\}^n \to \mathbb{R}$ is **submodular** if

$$f(\mathbf{x} \wedge \mathbf{y}) + f(\mathbf{x} \vee \mathbf{y}) \;\leq\; f(\mathbf{x}) + f(\mathbf{y}) \qquad \forall \;\; \mathbf{x}, \mathbf{y} \in \{0,1\}^n.$$

- **Polynomial recognition if** $\deg(f) \leq 3$.
  (Billionnet and Minoux, 1985)
- **Recognition is NP-hard if** $\deg(f) \geq 4$.
  (Gallo and Simeone, 1989; Crama 1989)
- **A QPBF is submodular iff it has no positive quadratic terms.**
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- **A submodular QPBO is solved by the network based preprocessing.**
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- **Which PBFs have submodular quadratization?**
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Rosenberg's Penalty Functions Method (1975)

$$p(x,y,w) \;=\; xy - 2xw - 2yw + 3w \;=\; \begin{cases} = 0 \text{ if } w = xy, \\ \geq 1 \text{ if } w \neq xy \end{cases}$$

$$f(x,y,\ldots) \;=\; xyA + B \;=\; \min_{w\in\{0,1\}} wA + B + Mp(x,y,w)$$

if M is large enough.

- **Many positive quadratic terms with large coefficients (recursion!), even if the input is subodular.**
- **NP-hard** to find a quadratization in this way with the **minimum number of new variables.**
- **Not possible** to substitute the product of 3 or more variables with a single new variable.

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Negative Terms

- *Kolmogorov and Zabih (2004), Fredman and Drineas (2005)*:

$$-x_1 x_2 \cdots x_d \;=\; \min_{w \in \{0,1\}} w(d - 1 - x_1 - x_2 \cdots - x_d)$$

- *Rother, Kohli, Feng and Jia (2009)*:

$$-\prod_{j \in N} \overline{x}_j \prod_{j \in P} x_j \;=\; \min_{u,v \in \{0,1\}} -uv + u \sum_{j \in N} x_j + v \sum_{j \in P} \overline{x}_j$$

- **Only one or two new variables per term; at most one positive quadratic term; no large coefficients.**

Theorem (vs. Billionet and Minoux (1985))

Cubic submodular functions have submodular quadratization of polynomial size with no ***large*** *coefficients.*

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Positive Terms

- *Ishikawa (2009, 2011)*:

$$\prod_{j=1}^{d} x_j = S_2(\mathbf{x}) + \min_{\mathbf{w}\in\{0,1\}^k} B(\mathbf{w}) - 2A(\mathbf{w})S_1(\mathbf{x}) + \rho\left[S_1(\mathbf{x}) - d + 1\right]$$

where $d = 2k + 2 - \rho, \;\; \rho \in \{0,1\}$, and

$$S_1(\mathbf{x}) = \sum_{j=1}^{d} x_j \qquad S_2(\mathbf{x}) = \sum_{1\le i<j\le d} x_i x_j$$

$$A(\mathbf{w}) = \sum_{j=1}^{k} w_j \qquad B(\mathbf{w}) = \sum_{j=1}^{k} (4j-1) w_j$$

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Multiple Splits

Assume that $\phi_i(\mathbf{w}) \in \{0,1\}$ for $i \in [q]$, $\mathbf{w} \in \{0,1\}^p$ such that

$$\min_{\mathbf{w}\in\{0,1\}^p} \sum_{i=1}^{q} \phi_i(\mathbf{w}) \;=\; 1, \qquad \text{and}$$

$$\forall I \subsetneq [q] \quad \exists \mathbf{w}^* \in \{0,1\}^p \quad \text{s.t.} \quad \sum_{i\in I} \phi_i(\mathbf{w}^*) = 0.$$

For instance $\phi_1 = w_1$, $\phi_2 = w_2$, and $\phi_3 = \overline{w}_1\overline{w}_2$ is such a system.

Theorem

If P_i, $i \in [q]$ are subsets of indices covering $[d]$, then we have

$$\prod_{j=1}^{d} x_j \;=\; \min_{\mathbf{w}\in\{0,1\}^p} \sum_{i=1}^{q} \phi_i(\mathbf{w}) \prod_{j\in P_i} x_j .$$

With $p = \lceil \log q \rceil$ new variables we can split a degree $d = kq$ term into q terms of degree $k + p$.

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With $p = \lceil \log q \rceil$ new variables we can split a degree $d = kq$ term into q terms of degree $k + p$.

Multiple Splits

Assume that $\phi_i(\mathbf{w}) \in \{0,1\}$ for $i \in [q]$, $\mathbf{w} \in \{0,1\}^p$ such that

$$\min_{\mathbf{w}\in\{0,1\}^p} \sum_{i=1}^{q} \phi_i(\mathbf{w}) \;=\; 1, \qquad \text{and}$$

$$\forall I \subsetneq [q] \quad \exists \mathbf{w}^* \in \{0,1\}^p \quad \text{s.t.} \quad \sum_{i\in I} \phi_i(\mathbf{w}^*) = 0.$$

For instance $\phi_1 = w_1$, $\phi_2 = w_2$, and $\phi_3 = \overline{w}_1\overline{w}_2$ is such a system.

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Outline

Let $C \subseteq [n]$, $\mathcal{H} \subseteq 2^{[n]\setminus C}$, and consider the following fragment of a pseudo-Boolean function:

$$g(\mathbf{x}) = \sum_{H \in \mathcal{H}} \alpha_H \prod_{j \in C \cup H} x_j,$$

where $\alpha_H \geq 0$ for all $H \in \mathcal{H}$.

Theorem (Set of Positive Terms)

$$g(\mathbf{x}) = \min_{w \in \{0,1\}} \left(\sum_{H \in \mathcal{H}} \alpha_H \right) w \prod_{j \in C} x_j + \sum_{H \in \mathcal{H}} \alpha_H \overline{w} \prod_{j \in H} x_j.$$

Theorem (Set of Negative Terms)

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Outline

Corollary

A PBF in n variables, with t terms of degree d has a quadratization with $\approx n + k\binom{n}{k} + \frac{td}{k}$ new variables and with at most $n-1$ positive quadratic terms, for any $k \geq 1$.

Ishikawa's method provides a quadratization with $\approx n + \frac{td}{2}$ new variables and $\max\{\binom{n}{2}, t\binom{d}{2}\}$ positive quadratic terms.

	New variables	# positive terms	# terms	% fixed by QPBO
Ishikawa	224,346	421,897	1,133,811	80.4%
Our method	236,806	38,343	677,183	96.1%
Δ	+6%	−90%	−40%	+20%

Figure : Performance comparison of reductions, on Ishikawa's benchmarks. Relative performance of our method is shown as Δ. (Joint work with Alexander Fix and Ramin Zabih (Cornell University).)

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