

A Strongly Polynomial Preprocessing for QUBO

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Joint work with P.L. Hammer¹ and G. Tavares

¹(1936-2006)

Outline

- 1 Quadratic Unconstrained Binary Optimization
 - Quadratic Pseudo-Boolean Functions
- 2 Quadratic Posiforms
 - Representations and Bounds
 - Origin of Graph Cut Models
 - Network Model for General QUBO
- 3 Polynomial Time Preprocessing
 - Components of the Algorithm
 - Computational Results

Quadratic Unconstrained Binary Optimization (QUBO)

Variables and Literals

- **Variables:** $x_1, x_2, \dots, x_n \in \{0, 1\}$.
- **Negations:** $\bar{x}_i = 1 - x_i \in \{0, 1\}$ for $i = 1, \dots, n$
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Quadratic Pseudo-Boolean Function (QPBF): $f : \{0, 1\}^n \rightarrow \mathbb{R}$

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

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$$\min_{(x_1, \dots, x_n) \in \{0, 1\}^n} f(x_1, \dots, x_n)$$

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Roof Dual Bound: $C_2(f) \leq f$ (Hammer, Hansen and Simeone, 1984)

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

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$$C_2(f) \leq C_3(f) \leq \dots \leq C_n(f) = \min f$$

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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
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- 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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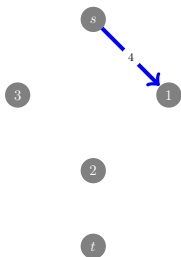
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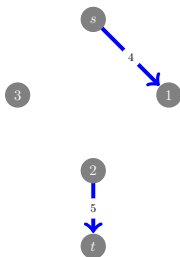


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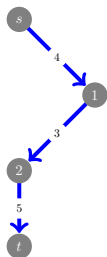
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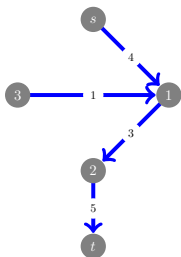


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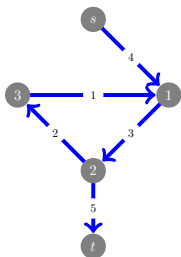


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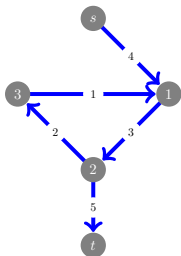


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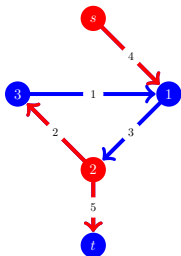


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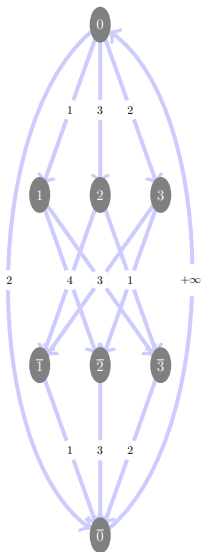
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$$f(\mathbf{0}, \mathbf{1}, \mathbf{0}) = C(\{\mathbf{s}, \mathbf{2}\}, \{\mathbf{1}, \mathbf{3}, \mathbf{t}\}) = 11$$

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



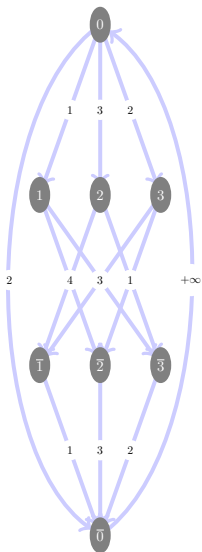
To a quadratic posiform

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

we associate a directed network N_ϕ on vertex set

$$V(N_\phi) = \{x_0, \bar{x}_0, x_1, \bar{x}_1, \dots, x_n, \bar{x}_n\} \quad (x_0 \equiv 1)$$

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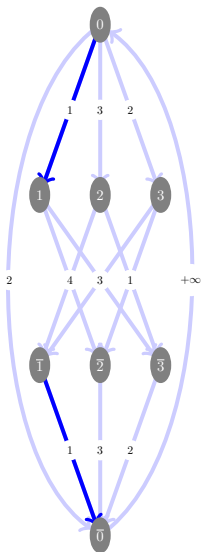
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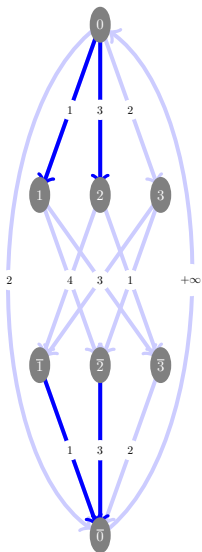
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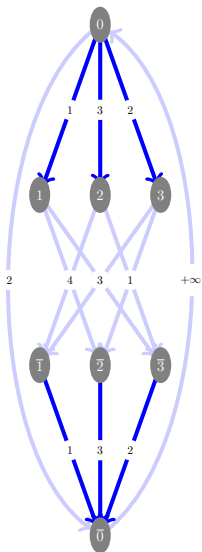
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we associate a directed network N_ϕ on vertex set

$$V(N_\phi) = \{x_0, \bar{x}_0, x_1, \bar{x}_1, \dots, x_n, \bar{x}_n\} \quad (x_0 \equiv 1)$$

- Homogenize it by x_0 .
- Associate to each term αuv ($u \neq v$) two arcs (u, \bar{v}) and (v, \bar{u}) with capacities $c(u, \bar{v}) = c(v, \bar{u}) = \alpha/2$.
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Implication Networks (Boros, Hammer, Sun, 1989, 1992)



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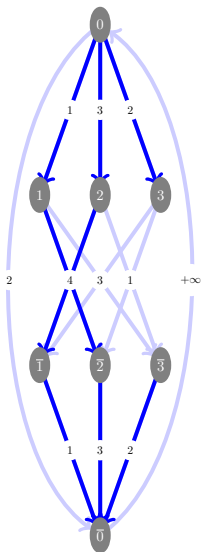
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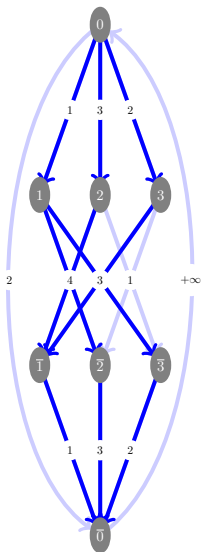
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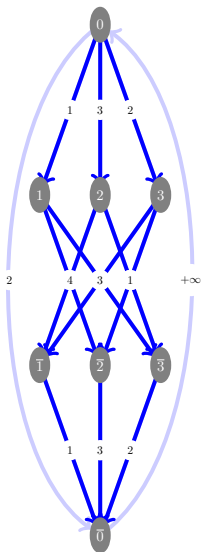
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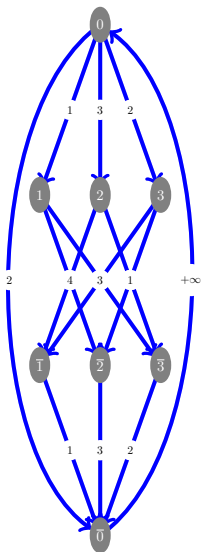
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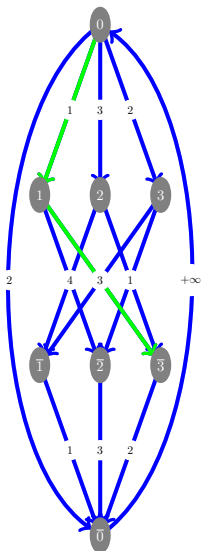
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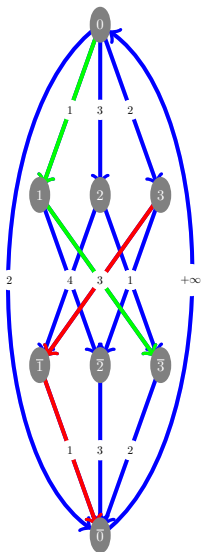
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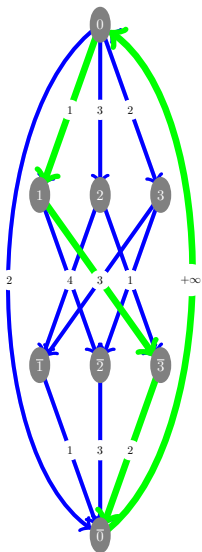
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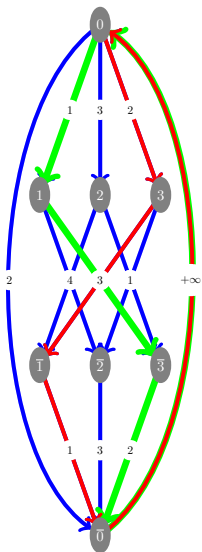


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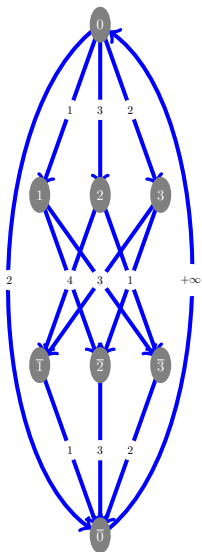
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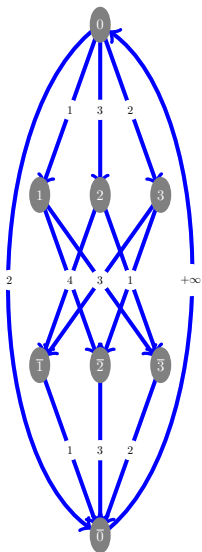
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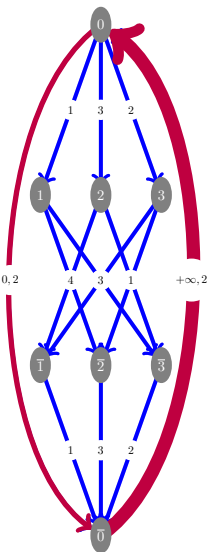
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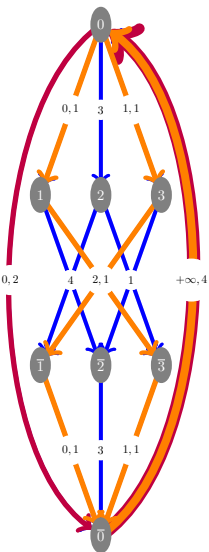
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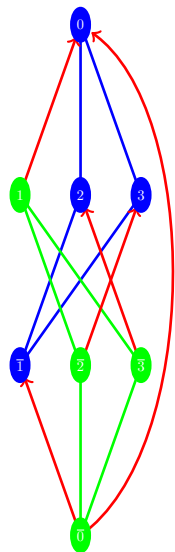
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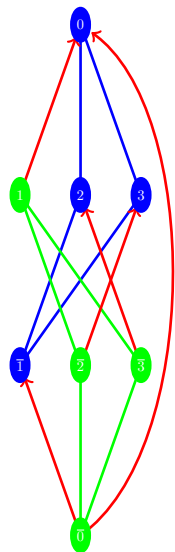
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Outline

- 1 Quadratic Unconstrained Binary Optimization
 - Quadratic Pseudo-Boolean Functions
- 2 Quadratic Posiforms
 - Representations and Bounds
 - Origin of Graph Cut Models
 - Network Model for General QUBO
- 3 Polynomial Time Preprocessing
 - Components of the Algorithm
 - Computational Results

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.

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Via Minimization in VLSI Design

Problem ²	n	Percentage of Variables Fixed by				ALL TOOLS	Time (sec)
		Roof Duality		Probing			
		(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

²S. 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. ³	QUBO ⁴	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

³Alber, 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

⁴Pentium 4, 2.8 GHz, Windows XP, 512 MB

Jumbo Vertex Cover in Planar Graphs

Vertices	Computing Times (min) ⁵		
	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

⁵Averages 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 ⁶	Biq Maq ⁵	QUBO ⁷
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

⁶F. Rendl, G. Rinaldi, A. Wiegele. (2007). Solving max-cut to optimality by intersecting semidefinite and polyhedral relaxations.

⁷ALL problems were solved by QUBO.

Larger One Dimensional Ising Models

σ	n	Average of 3 Problems	
		Variables not fixed	QUBO Time (s) ⁸
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

⁸Pentium M, 1.6 GHz 760 MB RAM