Structure of Quadratizations of Pseudo-Boolean Functions

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Joint work with
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Latin America School of Mathematics (ELAM)
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Agenda

- Introduction to pseudo-Boolean functions and optimization
- Present some frontier results on quadratizations of PBFs
- Discuss some open problems and future directions

Quadratizations of Pseudo-Boolean Functions

In a nutshell:

Quadratic reformulations (resorting to binary auxiliary variables) of unconstrained, nonlinear binary optimization problems specified through high-degree multilinear polynomials.

Objective:

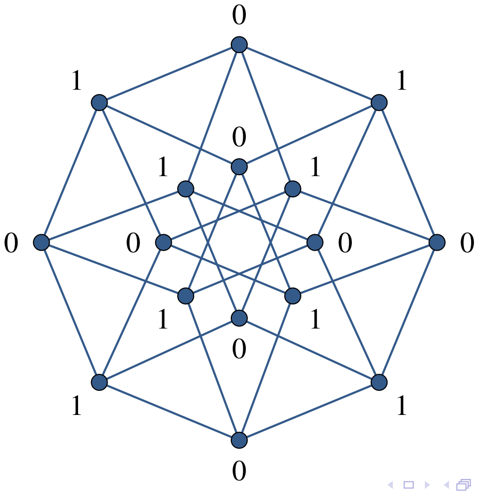
To allow their continuous relaxations to be handled though maximum flow techniques, so that:

- some variables can be fixed to their provably optimal values (*persistences*),
- and allow NP-hard problems to be decomposed into smaller, disjoint subproblems.

Boolean Functions

Binary-valued mappings of binary vectors:

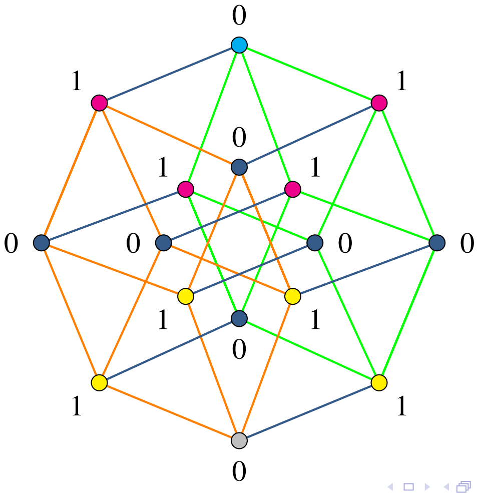
$$\mathscr{B}^n = \{0,1\}^{\{0,1\}^n} := \{\, h : \{0,1\}^n \to \{0,1\} \}$$



Boolean Functions

Parity function:

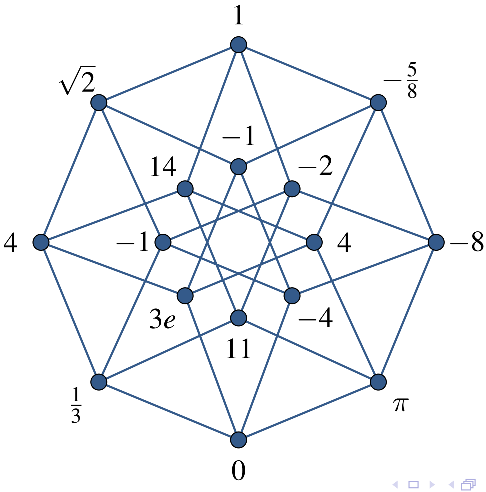
$$\bigoplus_4(x_1, x_2, x_3, x_4) = (x_1 + x_2 + x_3 + x_4) \pmod 2$$



Pseudo-Boolean Functions

Real-valued mappings of binary vectors:

$$\mathscr{P}^n = \mathbb{R}^{\{0,1\}^n} := \left\{ f : \{0,1\}^n \to \mathbb{R} \right\}$$



Pseudo-Boolean Functions

Theorem (Hammer and Rudeanu '68):

Each PBF $f : \{0,1\}^n \to \mathbb{R}$ can be uniquely represented as a *multilinear polynomial* in the binary variables $x_1, x_2, \ldots, x_n$:

$$f(x_1, x_2, \ldots, x_n) = \sum_{S \subseteq [n]} c_S \prod_{j \in S} x_j,$$

where $c_S \in \mathbb{R}$ for all $S \subseteq [n] := \{1, 2, \ldots, n\}$.

Example

$$f(x_1, x_2, x_3) = 3 + x_1 - 4x_2 + x_3 - 5x_1x_2 + 9x_1x_3 + 2x_2x_3 - 6x_1x_2x_3$$

Pseudo-Boolean Functions

Proof:

Existence by interpolation: for each $\mathbf{a} \in \{0,1\}^n$,

$$\chi_{\mathbf{a}}(\mathbf{x}) := \prod_{i:a_i=1} x_i \cdot \prod_{j:a_j=0} (1-x_j).$$

As $\chi_{\mathbf{a}}(\mathbf{x}) = 1 \iff \mathbf{x} = \mathbf{a}$,

$$f(\mathbf{x}) = P_f(\mathbf{x}) := \sum_{\mathbf{a}\in\{0,1\}^n} f(\mathbf{a})\chi_{\mathbf{a}}(\mathbf{x}) = \sum_{S\subseteq[n]} c_S \prod_{i\in S} x_i.$$

Uniqueness: $\{\chi_{\mathbf{a}} : \mathbf{a} \in \{0,1\}^n\}$ is a basis for $\mathscr{P}^n$. □

Degree of $f : \{0,1\} \to \mathbb{R}$:

$$\deg(f) = \deg(P_f) := \max\{|S| : S \subseteq [n], c_S \neq 0\}.$$

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Pseudo-Boolean Optimization

Unrestricted problem:

Determine

$$f(\mathbf{x}^*) = \min\{f(\mathbf{x}) : \mathbf{x} \in \{0,1\}^n\}$$

for a PBF $f : \{0,1\}^n \to \mathbb{R}$ in multilinear polynomial form.

Applications in many fields:

- Artificial Intelligence / Machine Learning.
- Combinatorics / Graph Theory / Coding Theory.
- Computational Complexity / Quantum Computing.
- Computer Vision / Integer Programming / VLSI Design.
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Pseudo-Boolean Optimization

Complexity:

- Polytime(n) solution if f is:

  submodular, *unimodular*, *signed balanced*.

- NP-hard in general, even when f is quadratic:

  encompasses MAX-SAT, MAX-CUT, MAX-STABLESET.

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  where $\mathbf{x} \odot \mathbf{y} = (x_1 \odot y_1, \ldots, x_n \odot y_n)$, with $\odot \in \{\wedge, \vee\}$.

- In other words, f has the *diminishing returns* property.
- $\min f(\mathbf{x})$ available in strongly polytime:
  - Grötschel, Lováz, Schrijver '81: $O(n^8 + \gamma n^7)$,
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Quadratic Pseudo-Boolean Optimization

Submodularity:

- Quadratic PBF f is submodular if and only if all quadratic coefficients are nonpositive.
- Similar, albeit slightly more involved, result if f is cubic.
- co-NP-hard to decide if f is submodular when $\deg(f) \geq 4$.

Theorem (Hammer '65)): submodular QPBO $\in$ P

1-to-1 correspondence between values of f and (s,t)-cut values of a network G_f, whenever f is a submodular QPBF.

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Network Model for Submodular QPBO

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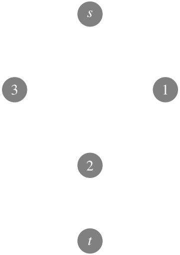

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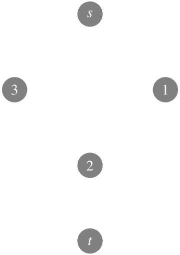

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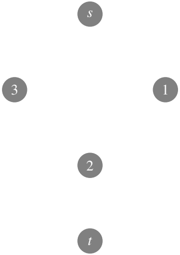

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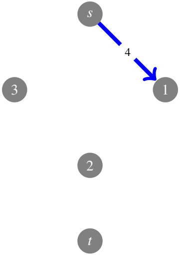

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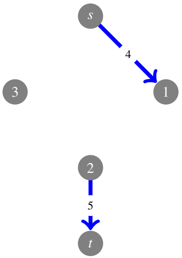

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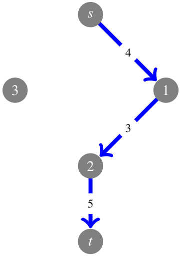

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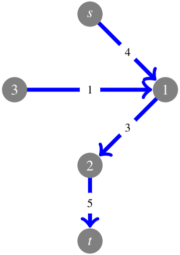

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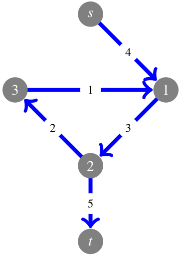

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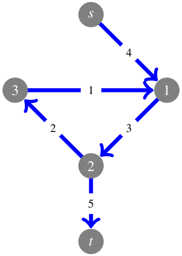

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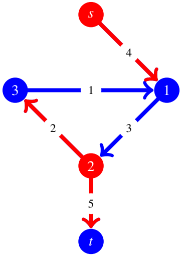

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$$\mathbf{f(0,1,0) \;=\; \partial(\{s,2\},\{1,3,t\}) \;=\; 11}$$

Network Model for Non-submodular QPBO

When f is non-submodular:

- Implication Networks: Boros and Hammer '89, Boros, Hammer, Sun '91, Boros, Hammer, Sun, Tavares '06, '08.
- Associates a different network H_f to a QPBF f.
  - Binary vectors $\mathbf{x}$ correspond to cuts in H_f with value $= f(\mathbf{x})$.
  - Max-Flow provides lower bounds for f: *roof duality*.
  - Residual network provides optimal values for some of the variables (*persistencies*) and a decomposition of the residual problem.
- Strongly polynomial preprocessing fixes $60 - 90\%$ of the variables in many applications (especially in computer vision).
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Pseudo-Boolean Optimization

For higher degree PBFs:

No combinatorial algorithms for degree larger than 3, and no persistence results for degree larger than 2.

Quadratizations of Pseudo-Boolean Functions

Quadratizations:

PBF $g : \{0,1\}^{n+m} \to \mathbb{R}$ is an *m-quadratization* of $f : \{0,1\}^n \to \mathbb{R}$ if g is **quadratic** and

$$f(x) = \min\{g(x,y) : y \in \{0,1\}^m\} \quad \text{for all} \quad \mathbf{x} \in \{0,1\}^n;$$

g is *y-linear* if there are no monomials of the form

$$y_i y_j \quad \text{for} \quad i,j \in [m],\ i \neq j.$$

The y-variables are called *auxiliary* variables.

Example

$$-x_1x_2x_3 = \min_{y_1}\{2y_1 - x_1y_1 - x_2y_1 - x_3y_1\}$$

$$= \min_{y_1,y_2}\{x_3 + 2y_2 - x_1x_3 + x_1y_1 - x_1y_2 - x_2y_2 - x_3y_1 - y_1y_2\}$$

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Goals:

- Keep m small!
- Have g "as submodular as possible!"
- With no large coefficients!

- Rosenberg '75: All PBFs have quadratizations.

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Rosenberg's Penalty Function Method '75

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

$$\begin{aligned} f(x_1, x_2, x_3, x_4, x_5) &:= 5x_1x_2 - 7x_1x_2x_3x_4 + 2x_1x_2x_3x_5 \\ &= 45y_1 + 45y_2 + 20x_1x_2 - 30x_1x_6 - 30x_2x_6 \\ &+ 15x_3y_1 - 30x_3y_2 - 7x_4y_2 + 2x_5y_2 - 30y_1y_2 \\ &=: g(x_1, x_2, x_3, x_4, x_5, y_1, y_2) \end{aligned}$$

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Possible drawbacks:

- Many positive quadratic terms with large coefficients, even if the input f is submodular!
- Does not generalize for the substition of 3 or more variables at once.
- Introduces many auxiliary variables in the worst case: $O(n^n)$.
- Can we find better estimates? $O(n^n)$ seems ludicrous!
- NP-hard to find a quadratization with a minimum number of auxiliary variables (reduction from MAX-STABLESET).

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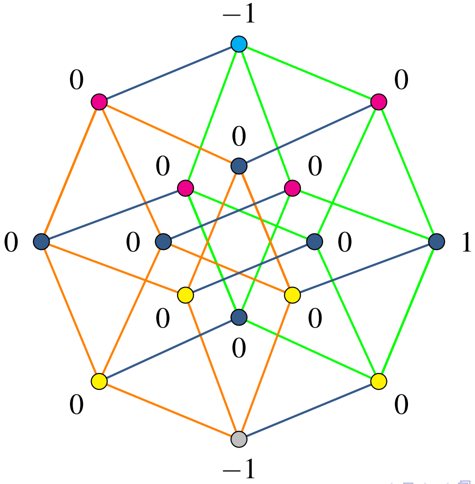
Živný, Cohen, Jeavons '09

Not all submodular PBFs have submodular quadratizations!
Quasi-indecomposable function $\theta_t(w, x, y, z)$ for $t = (1, 1, 0, 0)$.



Higher-Degree Substitution for Negative Terms

Kolmogorov and Zabih '04, Fredman and Drineas '05:

Only one auxiliary variable, no positive quadratic term, no large coefficient:

$$N(\mathbf{x}) := -\prod_{i=1}^{n} x_i = \min_{y\in\{0,1\}} y\left(n-1-\sum_{i=1}^{n} x_i\right).$$

Proof:

It holds that

$$-x_1x_2\cdots x_n \leq 0 \quad \text{and} \quad -x_1x_2\cdots x_n \leq (n-1)-\sum_{j=1}^{n} x_j.$$

RHS correspond to $y=0$ and $y=1$ above, respectively, and so $y=\prod_{j=1}^{d} x_j$ at a minimum. □

Higher-Degree Substitution for Negative Terms

Negating variables:

For binary variables $x_1, x_2, \ldots, x_n$ and y, it holds that

$$-\bar{x}_1\bar{x}_2\cdots\bar{x}_n = \min_{y\in\{0,1\}} y\left((n-1) - \sum_{j=1}^{n}\bar{x}_j\right)$$

$$= -1 + \sum_{j=1}^{n} x_j + \min_{\bar{y}\in\{0,1\}} \bar{y}\left(1 - \sum_{j=1}^{n} x_j\right).$$

Rother, Kohli, Feng and Jia '09:

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

Two auxiliary variables, $|N|$ positive quadratic terms, no large coefficients.

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Characterizing Negative Terms

Theorem: 1-Quadratizations of negative monomials

Up to a permutation of the $\mathbf{x}$-variables and to a switch of the y-variable,

$$s_n = \left(n - 1 - \sum_{i=1}^{n} x_i\right) y$$

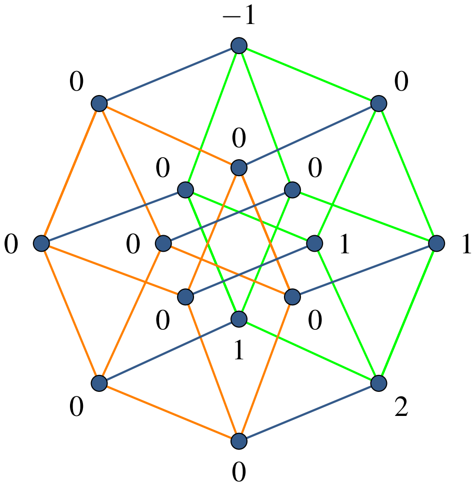
$$s_n^+ = (n-2)x_n y - \sum_{i=1}^{n-1} x_i(y - \bar{x}_n)$$

are the only *prime* 1-quadratizations of $N_n := -\prod_{i=1}^{n} x_i$.

Proof. Long and technical… □

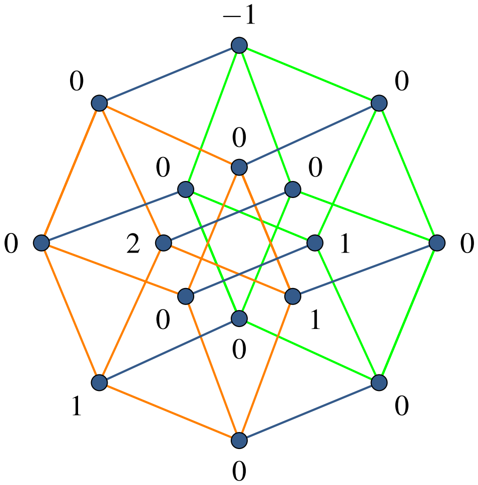
Characterizing Negative Terms

$$s_3(w; x, y, z) = 2w - xw - yw - zw$$



Characterizing Negative Terms

$$s_3^+(w; x, y, z) = x + y - xz - yz - xw - yw + zw$$



What About Positive Terms, $P_n(\mathbf{x}) := \prod_{i=1}^n x_i$?

- Can be written as $P_n(\mathbf{x}) = -x_1 \cdots x_{n-1}\bar{x}_n + P_{n-1}(\mathbf{x})$.
- So P_n can be quadratized using $n-2$ additional variables.

Ishikawa '09, '11:

$k = \left\lfloor \frac{n-1}{2} \right\rfloor$ auxiliary variables suffice:

$$P_n(\mathbf{x}) = \sum_{1 \le i < j \le n} x_i x_j + \min_{y \in \{0,1\}^k} \sum_{j=1}^{k} y_j \left(c_{j,n} \left(-\sum_{i=1}^{n} x_i + 2j \right) - 1 \right),$$

where $c_{j,n} = 1$ if $n = j$ is odd, and $c_{j,n} = 2$ otherwise.

No large coefficients, $\binom{n}{2}$ positive quadratic terms.

Every PBF has a quadratization with at most $O(n2^n)$ auxiliary variables. No characterization for P_n is known!

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Multiple Split of Terms

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

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

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

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

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

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

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

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

Splitting Off Common Parts

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

$$g(x) = \sum_{H \in \mathcal{H}} \alpha_H \prod_{j \in C \cup H} x_j, \quad \text{with} \quad \alpha_H \geq 0.$$

Theorem (Set of Positive Terms)

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

Theorem (Set of Negative Terms)

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

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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
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. (Fix, Gruber, Boros, Zabih '11, '15))

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Symmetric Pseudo-Boolean Functions

A PBF $f : \{0,1\}^n \to \mathbb{R}$ is *symmetric* if for all permutations $\sigma \in \mathfrak{S}_n$

$$f(x_1, x_2, \ldots, x_n) = f\left(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(n)}\right).$$

Example

- Positive and Negative Monomials
- Majority:

  $\mathrm{Maj}_3(x_1, x_2, x_3) = x_1x_2 + x_1x_3 + x_2x_3 - 2x_1x_2x_3$
- Parity:

  $\bigoplus_3(x_1, x_2, x_3) = x_1 + x_2 + x_3 - 2x_1x_2 - 2x_1x_3 - 2x_2x_3 + 4x_1x_2x_3$

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Quadratization of Symmetric PBFs

How many auxiliary variables suffice?

- Negative Monomials: 1 (Freedman and Drineas ’05).
- Positive Monomials: $\left\lfloor \frac{n-1}{2} \right\rfloor$ (Ishikawa ’09, ’11).
- $n-1$ auxiliary variables suffice (Fix ’11, ad hoc argument).

- We show that $n-2$ auxiliary variables suffice to y-linear quadratize SPBF.

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Representation Theorem:

For all $0 < \epsilon_i \leq 1$, $i = 0, \dots n$, every SPBF $f : \{0,1\}^n \to \mathbb{R}$ can be uniquely represented in the form

$$f(x) = \sum_{i=0}^{n} \alpha_i \left[i - \epsilon_i - \sum_{j=1}^{n} x_j \right]^{-},$$

where $[a]^{-} := \min(a, 0)$ for any real value a.

- Idea: $\left[i - \epsilon_i - \sum_{j=1}^{n} x_j \right]^{-}$ reflects whether $\sum_{j=1}^{n} x_j$ is larger than i.
- Lower triangular system of linear equations: $\alpha_0, \dots, \alpha_n$ can be efficiently computed.

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So, for a symmetric pseudo-Boolean function f:

$$f(x) = \sum_{i=0}^{n} \alpha_i \left[i - \epsilon_i - \sum_{j=1}^{n} x_j \right]^-$$

$$\stackrel{?}{=} \min_{y \in \{0,1\}} \sum_{i=0}^{n} \alpha_i \left(i - \epsilon_i - \sum_{j=1}^{n} x_j \right) y_i.$$

Well, not quite: $-[a]^- = -\min(a,0) \neq \min_{y \in \{0,1\}}(-ay)$.

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Quadratization of Zeros

- $E(l) = l(l-1) + 2\sum_{i=1}^{n-1} [i-l]^-$,
- $E'(l) = \frac{l(l-1)}{2} + 2\sum_{i=2\,:\,i \text{ even}}^{n} \left[i - \frac{1}{2} - l\right]^-$,
- $E''(l) = \frac{l(l+1)}{2} + 2\sum_{i=1\,:\,i \text{ odd}}^{n} \left[i - \frac{1}{2} - l\right]^-$.

Lemma:

For all $l = 0, \ldots, n$, $E(l) = E'(l) = E''(l) = 0$.

Modify first the representation of f by adding one of $E(\sum x_j)$, $E'(\sum x_j)$, or $E''(\sum x_j)$ so as to cancel negative coefficients.

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Upper Bounds for Symmetric PBFs

Theorem: Positive monomials

The positive monomial P_n has a $\lfloor \frac{n-1}{2} \rfloor$-quadratization ($y$-linear).

Theorem: k-out-of-n and exact-k functions

The k-out-of-n function has a $\lceil \frac{n}{2} \rceil$-quadratization ($y$-linear), and the exact-$k$ function has a $\lfloor \frac{n}{2} \rfloor$-quadratization ($y$-linear).

Theorem: Parity function

The parity function has a $\lfloor \frac{n}{2} \rfloor$-quadratization ($y$-linear), and its complement has a $\lfloor \frac{n-1}{2} \rfloor$-quadratization ($y$-linear).

Theorem: General symmetric pseudo-Boolean functions

Every symmetric pseudo-Boolean function has a y-linear quadratization involving at most $(n-2)$ auxiliary variables.

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Polyhedral Cone of Quadratizations

For

- $f : \{0,1\}^n \to \mathbb{R}$ a PBF in n variables,
- m : an upper bound on the number of auxiliary variables of (some of) the quadratizations $g : \{0,1\}^{n+m} \to \mathbb{R}$ of f,
- $\delta(n,m) = 1 + n + m + \binom{n+m}{2}$,

$$\mathscr{P}_f(n,m) := \Big\{ g(\mathbf{x},\mathbf{y}) \in \mathbb{R}^{\delta(n,m)} \ : \ g(\mathbf{x},\mathbf{y}) \text{ is quadratic and } f(\mathbf{x}) \le g(\mathbf{x},\mathbf{y}) \text{ for all } \mathbf{x} \in \{0,1\}^n, \mathbf{y} \in \{0,1\}^m \Big\},$$

is the *polyhedral cone of quadratizations of* f.

Polyhedral Cone of Quadratizations

of quadratizations for pos e neg terms:

n	m	# vert (+)	# rays (+)	# vert (-)	# rays (-)
2	1	1	16	1	16
2	2	1	56	1	56
3	1	12	109	12	148
3	2	292	2109	292	3808
4	1	328	4807	353	6024
4	2	100824	1677491	74107	1484561
5	1	95954	1448766	52902	1187510

Polyhedral Cone of Quadratizations

$f(x)$	# quadr	$(2,1)$	$(2,2)$	$(3,1)$	$(3,2)$	$(4,1)$	$(4,2)$	$(5,1)$
pos	total:	1	1	8	288	2	5048	0
mono	up to $\simeq$:	1	1	2	28	1	138	0
neg	total:	1	1	8	288	10	3504	12
mono	up to $\simeq$:	1	1	2	28	2	91	2

Theorem

Every m-quadratization of a PBF $f : \{0,1\}^n \to \mathbb{R}$ is on the boundary of $\mathscr{P}_f(n,m)$. Moreover, every prime m-quadratization of $f : \{0,1\}^n \to \mathbb{R}$ is a vertex of $\mathscr{P}_f(n,m)$.

A Change of Perspective

Freedman and Drineas '05 + Ishikawa '09:

Every PBF in n variables can be quadratized with at most $O(n\,2^n)$ auxiliary variables.

Is it possible to do better? How?

Functions, not variables:

All new variables $y_1, \ldots, y_m$, when minimized, are Boolean functions of the original variables $x_1, \ldots, x_n$:

$$y^*(\mathbf{x}) \;=\; \operatorname{argmin}_{\mathbf{y}}\, g(\mathbf{x}, \mathbf{y}).$$

Then x_i, $x_i y_j^*(\mathbf{x})$ and $y_i^*(\mathbf{x}) y_j^*(\mathbf{x})$ are also Boolean functions, all viewed as vectors in $\{0,1\}^{2^n}$.

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Non-Termwise Quadratizations

Universal Sets

A set of BFs $\mathscr{U}$ is *universal* for a set of PBFs $\mathscr{F}$, both in n variables, if

- for every $f \in \mathcal{F}$, there is a m-quadratization $g(\mathbf{x}, \mathbf{y})$ with $m \leq |\mathscr{U}|$,
- there is $\{y_1^*, y_2^*, \ldots, y_m^*\} \subseteq \mathcal{U}$ such that

$$y^*(\mathbf{x}) = \left(y_1^*(\mathbf{x}), \ldots, y_m^*(\mathbf{x})\right)$$

is a minimizer of $g(\mathbf{x}, \mathbf{y})$ for all $\mathbf{x} \in \{0, 1\}^n$.

Non-Termwise Quadratizations

Universal Sets

- When $\mathscr{U}$ is a universal set, then all minimizers $(y_1^*(\mathbf{x}), \ldots, y_m^*(\mathbf{x}))$ can be chosen in $\mathscr{U}$, for $f \in \mathscr{F}$.
- Clearly, we can take $\mathscr{U}$ as $\mathscr{B}^n$, the set of all 2^{2^n} BFs in n-variables.
- For $\mathscr{F}$ as the set of submodular PBFs, there is no $\mathscr{U}$ comprized solely of submodular QPBFs.
- Surprisingly, rather small universal sets can be exhibited through combinatorial constructions.

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Universal Sets for PBFs

- Given a hypergraph $\mathscr{H}$ we call another hypergraph $\mathscr{C}$ a pairwise cover of $\mathscr{H}$, if for all $H \in \mathscr{H} \cup \mathscr{C}$, $\exists A, B \in \mathscr{C}$:
  - $A, B \subsetneq H$
  - $H = A \cup B$.
- If $\mathscr{H} = 2^V$, then assuming $V = E \cup O$, we have that

$$\mathscr{C} = 2^E \cup 2^O$$

  is a pairwise cover.
- For $\mathscr{H} = \{S \subseteq V : |S| \leq d\}$, we have

$$\mathscr{C} = \bigcup_{\substack{j \geq 1, \\ k = \left\lceil \frac{d}{2^j} \right\rceil \geq 2}}^{d} \binom{V}{k}$$

  as a pairwise cover of $\mathscr{H}$.
- Pairwise covers are related to *2-covers* (Erdős '62).

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- For $\mathscr{H} = \{S \subseteq V : |S| \leq d\}$, we have

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Universal Sets for PBFs

- Given a hypergraph $\mathscr{H}$ we call another hypergraph $\mathscr{C}$ a pairwise cover of $\mathscr{H}$, if for all $H \in \mathscr{H} \cup \mathscr{C}$, $\exists A, B \in \mathscr{C}$:
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Upper Bounds on the Number of Auxiliary Variables

Theorem:

Every PBF $f : \{0,1\}^n \to \mathbb{R}$ has a quadratization involving at most $O(2^{n/2})$ auxiliary variables.

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For a given hypergraph $\mathscr{H}$ what is the smallest pairwise cover? How easy/hard is to find a "small" pairwise cover of $\mathscr{H}$?

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Theorem:

Every PBF $f : \{0,1\}^n \to \mathbb{R}$ has a y-linear quadratization involving at most

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Proof:

- Different slicing of the Boolean hypercube: attractive partitions.
- Somewhat related to Turán's set systems.
- Recursive construction to bound each level of the hypercube.
- Afar from the regular construction; highly technical!

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Lower Bounds on the Number of Auxiliary Variables

Recall that:

All new variables, when minimized, are Boolean functions of the original variables $x_1, \ldots, x_n$

$$\mathbf{h}(\mathbf{x}) \;=\; \mathrm{argmin}_{\mathbf{y}}\, g(\mathbf{x}, \mathbf{y}).$$

Then x_i, $x_i h_j(\mathbf{x})$ and $h_j(\mathbf{x}) h_i(\mathbf{x})$ are also Boolean functions, all viewed as vectors in $\{0, 1\}^{2^n}$.

Lower Bounds on the Number of Auxiliary Variables

- A quadratization $g \in \mathbb{R}^{2^n}$ (viewed as a vector of values) in $n + m$ variables is a linear combination of

$$N = 1 + n + m + \binom{n+m}{2}$$

vectors, out of 2^{2^n} vectors in $\mathbb{R}^{2^n}$.

- Finitely many subspaces of dimension $< 2^n$ cannot cover $\mathbb{R}^{2^n}$. Thus, we must have $N \geq 2^n$.

Theorem:

Almost all PBFs in n variables require at least $\Omega(2^{n/2})$ auxiliary variables in any quadratization.

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Lower and Upper Bounds in a Nutshell

For $f : \{0,1\}^n \to \mathbb{R}$ a PBF in n variables:

$f(x)$	$g(x,y)$	lower bound	upper bound
any	regular	$\Omega(2^{n/2})$	$O(2^{n/2})$
degree-d	regular	$\Omega(n^{d/2})$	$O(n^{d/2})$
any	y-linear	$\Omega\left(\frac{2^n}{n}\right)$	$O\left(\frac{2^n}{n}\log n\right)$

Lower Bounds for Symmetric PBFs

Theorem

There exist SPBFs on n variables for which any quadratization must involve at least $\Omega(\sqrt{n})$ auxiliary variables.

Theorem

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Lower Bounds for Symmetric PBFs

Proof idea:

- inspired by Siu, Roychowdhury, Kailath '95 work on representation of Boolean functions by *threshold circuits*;
- relates quadratizations of arbitrary functions to the quadratization of symmetric functions on a larger number of variables;
- given $f(\mathbf{x})$ on n variables, let $F(\mathbf{z})$ on $2^n - 1$ variables be such that $F(\mathbf{z}) = f(\mathbf{x})$ if $\mathbf{x}$ is the binary representation of the Hamming weight of $\mathbf{z}$;
- if F has an m-quadratization, then so does f;
- use lower bounds $\Omega(2^{n/2})$ and $\Omega(2^n/n)$ on the number of auxiliary variables for f. □

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Lower Bounds for Symmetric PBFs

Theorem (parity functions)

Every y-linear quadratization of the parity function on n variables must involve at least $\Omega(\sqrt{n})$ auxiliary variables.

Proof idea: y-linear quadratization implies no quadratic term $y_i y_j$, i.e.,

$$g(\mathbf{x}, \mathbf{y}) = q(\mathbf{x}) + \sum_{i=1}^{m} y_i(\ell_i(x) - b_i),$$

where $q(\mathbf{x})$ is quadratic, and $\ell_1(\mathbf{x}), \ldots, \ell_m(\mathbf{x})$ are linear functions of $\mathbf{x}$.

- link with threshold circuit representations of parity and slicing of hypercubes by hyperplanes (Impagliazzo, Paturi, Saks '97);
- regions obtained by fixing y to all possible 2^m values;
- if m is too small, some region contains the parity function on 3 variables.

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Conclusions

- Tight lower and upper bounds on the number of auxiliary variables required for arbitrary and for fixed-degree functions.
- Generic constructions for quadratization of symmetric functions.
- Structure and properties of quadratizations are still poorly understood.
- Many intriguing questions and conjectures, much computational and theoretical work to be done.

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