Of (hyper)graphs and functions of binary variables: Old and recent results

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Grenoble, September 2019

Outline

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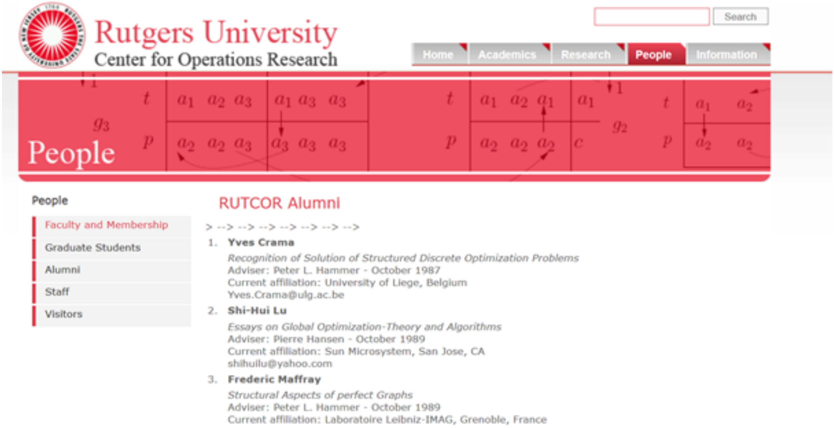
1. Joint work with Frédéric
2. Nonlinear 0-1 optimization
3. Standard linearization
4. Quadratization
   - Upper bounds
   - Lower bounds
5. Conclusions

At Rutgers University

- Both at Rutgers University, RUTCOR
- Frédéric's PhD degree: 1989

At Rutgers University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People

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- Staff
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RUTCOR Alumni

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1. **Yves Crama**
   Recognition of Solution of Structured Discrete Optimization Problems
   Adviser: Peter L. Hammer - October 1987
   Current affiliation: University of Liege, Belgium
   Yves.Crama@ulg.ac.be
2. **Shi-Hui Lu**
   Essays on Global Optimization-Theory and Algorithms
   Adviser: Pierre Hansen - October 1989
   Current affiliation: Sun Microsystem, San Jose, CA
   shihuilu@yahoo.com
3. **Frederic Maffray**
   Structural Aspects of perfect Graphs
   Adviser: Peter L. Hammer - October 1989
   Current affiliation: Laboratoire Leibniz-IMAG, Grenoble, France

At Rutgers University

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- Frédéric's PhD degree: 1989
- Advisor: Peter L. Hammer
- Interest in combinatorial structures and functions of 0-1 variables:

P.L. Hammer, F. Maffray. Completely separable graphs. *Discrete Applied Mathematics* 27 (1990), 85-99.

P.L. Hammer, F. Maffray, M. Queyranne. Cut-threshold graphs. *Discrete Applied Mathematics* 30 (1991), 163-179.

C. Benzaken, Y. Crama, P. Duchet, P.L. Hammer, F. Maffray. More characterizations of triangulated and cotriangulated graphs. *Journal of Graph Theory* 14 (1990), 413-422.

Graph-parameter functions

- $G = (V, E)$ is *perfect* if, for all $S \subseteq V$: $\alpha(G[S]) = \theta(G[S])$ (stability number of $G[S]$ = clique cover number of $G[S]$).

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$$\alpha_G(x_1, \ldots, x_n) = \alpha(G[S]), \quad S \text{ is indexed by } (x_1, \ldots, x_n).$$

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- What does this polynomial look like??

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Some examples:

- If $G = K_n$, then $\alpha_G = \theta_G = 1 - (1 - x_1)(1 - x_2) \ldots (1 - x_n)$

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Theorem (BCDHM 1990)

The polynomial expression of the stability function of G has all its coefficients equal to 0, - 1, or + 1 if and only if G is triangulated. Moreover, when this is the case, the coefficients alternate in sign between odd and even degree terms.

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- Generalization: the hypergraph $H = \{123, 124, 34\}$ has $\alpha_H = x_1 + x_2 + x_3 + x_4 - x_3x_4 - x_1x_2x_3 - x_1x_2x_4 + x_1x_2x_3x_4$.

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- Anything special about it? What hypergraphs have all coefficients equal to 0, - 1, or + 1 ?

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Definitions

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Every pseudo-Boolean function can be represented – in a unique way – as a *multilinear polynomial* in its variables, of the form

$$f(x_1, \ldots, x_n) = \sum_{S \in \mathcal{S}} a_S \prod_{k \in S} x_k + \sum_{i=1}^{n} a_i x_i$$

where $\mathcal{S} = \{S \in 2^{[n]} \mid a_S \neq 0, |S| \geq 2\}$.

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Example:

$f = 4 - 9x_1 - 5x_2 - 2x_3 + 13x_1x_2 + 13x_1x_3 + 6x_2x_3x_4 - 13x_1x_2x_3x_4$

Co-occurrence hypergraph

Co-occurrence hypergraph

When

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Multilinear optimization in binary variables

We are frequently interested in:

$$\text{(MOB)} \quad \min_{x \in \{0,1\}^n} \sum_{S \in \mathcal{S}} a_S \prod_{k \in S} x_k + \sum_{i=1}^{n} a_i x_i$$

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  - Direct resolution methods
  - *Linearization*: extensive literature in integer programming.
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\min \quad & \sum_{S \in \mathcal{S}} a_S y_S + \sum_{i=1}^{n} a_i x_i \\
\text{s.t.} \quad & y_S = \prod_{k \in S} x_k, && \forall S \in \mathcal{S} \\
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2. Linearize constraints

$$\begin{aligned} \min & \sum_{S\in\mathcal{S}} a_S y_S + \sum_{i=1}^{n} a_i x_i \\ \text{s.t. } & y_S \le x_k, && \forall k\in S, \forall S\in\mathcal{S} \\ & y_S \ge \sum_{k\in S} x_k - (|S|-1), && \forall S\in\mathcal{S} \\ & y_S \in \{0,1\}, && \forall S\in\mathcal{S} \\ & x_k \in \{0,1\} && \forall k=1,\dots,n \end{aligned}$$

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& y_S \geq \sum_{k \in S} x_k - (|S| - 1), & \forall S \in \mathcal{S} \\
& 0 \leq y_S \leq 1, & \forall S \in \mathcal{S} \\
& 0 \leq x_k \leq 1 & \forall k = 1, \dots, n
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Linear relaxation

A natural question: does the **standard linearization polytope**

$$P_{SL} = \{(x, y) \in [0, 1]^{n+|\mathcal{S}|} \mid y_S \leq x_k \;\; \forall k \in S, y_S \geq \sum_{k \in S} x_k - (|S| - 1) \;\; \forall S \in \mathcal{S}\}$$

have fractional vertices?

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- So, when is P_{SL} integral?

Co-occurrence hypergraph

Recall: co-occurrence hypergraph

When

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Definition: Berge cycles

For a hypergraph $H = (V, \mathcal{S})$, a **Berge cycle** of length p is a sequence

$$(i_1, S_1, i_2, S_2, \ldots, i_p, S_p, i_1),$$

where

1. $i_1, i_2, \ldots, i_p$ are pairwise distinct vertices of V,
2. $S_1, S_2, \ldots, S_p$ are pairwise distinct edges of $\mathcal{S}$,
3. $i_j, i_{j+1} \in S_j$ for $j = 1, \ldots p-1$, and $i_1, i_p \in S_p$.

Perfect standard linearization

(E. Rodríguez-Heck, Ch. Buchheim, Y. Crama, 2016)

P_{SL} is integral if and only if H_f has no Berge cycles.

Proof:

- $\Leftarrow$ If H_f is Berge-acyclic then the constraint matrix of P_{SL} is balanced, a property that guarantees integrality.
- $\Rightarrow$ If H_f has a cycle, then construct an objective function that reaches its optimum at a fractional vertex of P_{SL}.

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- Generalizes a result of Padberg (1989) for quadratic functions.
- Closely related to a result of Crama (1988,1993) for an "irredundant" relaxation of P_{SL}.
- Independently obtained by Del Pia and Khajavirad (2016).

Multilinear optimization in binary variables

$$(\text{MOB}) \quad \min_{x \in \{0,1\}^n} \sum_{S \in \mathcal{S}} a_S \prod_{k \in S} x_k + \sum_{i=1}^{n} a_i x_i$$

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  - Yes, in many ways!

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Quadratization

Observations

- Say $g(x, y)$, $(x, y) \in \{0, 1\}^{n+m}$, is a quadratic function.

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- Conversely...

Quadratization

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The quadratic function $g(x, y)$, $(x, y) \in \{0, 1\}^{n+m}$ is an *m-quadratization* of the pseudo-Boolean function $f(x)$, $x \in \{0, 1\}^n$, if

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The y-variables are called *auxiliary* variables.

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- $\min\{f(x) \,|\, x \in \{0, 1\}^n\} = \min\{g(x, y) \,|\, (x, y) \in \{0, 1\}^{n+m}\}$.
- Does every function f have a quadratization?

Existence

Existence of quadratizations (Rosenberg 1975)

Given the multilinear expression of a pseudo-Boolean function $f(x), x \in \{0,1\}^n$, one can find in polynomial time a quadratization $g(x,y)$ of $f(x)$.

- Idea: in each term $\prod_{i \in A} x_i$ of f, with $\{1,2\} \subseteq A$, replace the product $x_1 x_2$ by a new variable y;
- Introduce a penalty term to force $y = x_1 x_2$ in every minimizer of the transformed expression;
- $t(x,y) = \left(\prod_{i \in A \setminus \{1,2\}} x_i\right) y \, + \, M(x_1 x_2 - 2x_1 y - 2x_2 y + 3y).$
- Potential drawbacks: introduces many auxiliary variables, big M.

Questions arising...

- Many quadratization procedures proposed in recent years. Which ones are “best”? Small number of variables, of positive terms, good properties with respect to persistencies, submodularity?
- Easier question: What if f is a single monomial?
- How many variables are needed in a quadratization?
- etc.

Refs: Boros and Gruber (2011); Buchheim and Rinaldi (2007); Fix, Gruber, Boros and Zabih (2011): Freedman and Drineas (2005); Ishikawa (2011); Kolmogorov and Zabih (2004); Ramalingam et al. (2011); Rosenberg (1975); Rother et al. (2009); Živný, Cohen and Jeavons (2009); etc.

Outline

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- lower and upper bounds on size of quadratizations

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M. Anthony, E. Boros, Y. Crama and M. Gruber, Quadratization of symmetric pseudo-Boolean functions, *Discrete Applied Mathematics* 203 (2016) 1–12.

M. Anthony, E. Boros, Y. Crama and M. Gruber, Quadratic reformulations of nonlinear binary optimization problems *Mathematical Programming* 162 (2017) 115-144.

E. Boros, Y. Crama and E. Rodrìguez-Heck, Compact quadratizations for pseudo-Boolean functions, Working paper, 2018.

Outline

General question

- How many auxiliary variables are needed in general?

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Every term of the form $a\prod_{i=1}^{n} x_i$ can be quadratized using $n-2$ auxiliary variables (Rosenberg 1975), and even $\lfloor \frac{n-1}{2} \rfloor$ auxiliary variables (Ishikawa 2011).

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Ishikawa (2011)

For every n-variable pBf, one can find in polynomial time a quadratization involving $\left\lfloor \frac{n-1}{2} \right\rfloor 2^n$ auxiliary variables.

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- Best known bound, until recently.

Upper bound

- Upper bound based on termwise quadratizations:

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For every n-variable pBf, one can find in polynomial time a quadratization involving at most $\left\lfloor \frac{n-1}{2} \right\rfloor 2^n$ auxiliary variables.

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- We prove:

Theorem: upper bound (*Math. Prog.* (2017))

For every n-variable pBf, one can find in polynomial time a quadratization involving at most $O(2^{n/2})$ auxiliary variables.

Pairwise cover

Based on a construction using small *pairwise covers:*

Pairwise cover

A hypergraph $\mathcal{H}$ is a *pairwise cover* of $\{1, \ldots, n\}$ if, for every $S \subseteq \{1, \ldots, n\}$ with $|S| \geq 3$, there are sets $A, B \in \mathcal{H}$ such that $|A| < |S|$, $|B| < |S|$ and $A \cup B = S$.

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Theorem: From pairwise cover to quadratization

If there exists a pairwise cover of $\{1, \ldots, n\}$ of size m, then every pseudo-Boolean function has an m-quadratization.

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- Idea of the proof: write $\prod_{i \in S} x_i = (\prod_{j \in A} x_j)(\prod_{k \in B} x_k)$; substitute y_A for $\prod_{j \in A} x_j$ and y_B for $\prod_{k \in B} x_k$;
- Introduce a penalty term to force the correct values of y_A and y_B in every minimizer of the transformed expression.

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- Pairwise covers are (almost) identical to so-called 2-*bases* investigated by Erdös, Füredi and Katona (2006), Frein, Lévêque and Sebö (2008), Ellis and Sudakov (2011).
- $\mathcal{P}(even)$ = all subsets of even integers in $\{1, \dots, n\}$.
- $\mathcal{P}(odd)$ = all subsets of odd integers in $\{1, \dots, n\}$.
- $\mathcal{H} = \mathcal{P}(even) \cup \mathcal{P}(odd)$ is a “small” pairwise cover with size $O(2^{n/2})$.

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Theorem: lower bound (*Math. Prog.* (2017))

There are pseudo-Boolean functions of n variables for which every quadratization must involve at least $\Omega(2^{n/2})$ auxiliary variables.

- This lower bound matches the $O(2^{n/2})$ upper bound.
- Non constructive proof based on dimensionality argument: if too few auxiliary variables, then we cannot generate the whole vector space of pseudo-Boolean functions.

Outline

Conclusions

- Many fruitful connections between functions of Boolean variables, graphs and hypergraphs.
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- See also

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