## Quadratic reformulations for the optimization of pseudo-boolean functions

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## Pseudo-boolean functions and polynomial optimization with binary variables

We consider the Unconstrained Binary Polynomial Programming problem

$$
\left\{\begin{array}{ll}
\min & f(x)=\sum_{M \in \mathcal{M}} a_{M} \prod_{i \in M} x_{i} \\
\text { s. t. } & x_{i} \in\{0,1\}
\end{array} \quad \forall i \in[n]\right.
$$

If degree of $f=2$ : the quadratic case of qpb functions We suppose all monomials have degree 3 or more

## Resolution through quadratic reformulation

We focus on solution approaches in two phases:
(1) Rewrite into a binary quadratic problem (Quadratic reformulation)

- we know this is possible from (Rosenberg 75)
- but many other ways exist
(2) Solve the obtained binary quadratic problem

Our work: unify Phase 1 and study the links between Phase 1 and Phase 2

## Outline

(1) Quadratic reformulation of the pseudoboolean function into a quadratic problem
(2) The unifying notion of quadratization scheme
(3) Possible reformulations from the quadratization scheme

4 Solving the reformulated quadratic problem
(5) Building quadratization schemes
(6) A few computational results

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## Rewrite into a binary quadratic problem (Quadratic reformulation)

- (Rosenberg 75) Iteratively, substitute the product of two variables by a new one until degree 2 is reached for all monomials. Enforce the equivalence by a penality function.
- (Buchheim \& Rinaldi 2007) Add enough submonomials to make your instance reducible i.e. each monomial is the union of two others.
Build a linear reformulation together with a family of valid inequalities.
- (Anthony et al. 2017) Represent $f$ by a hypergraph and find a pairwise cover. Enforce the equivalence by a penality function.
- (Lazare 2020) Iteratively partition each monomial (degree $>2$ ) into two (new)submonomials. Write an equivalent binary quadratic problem with linear constraints.

We show: These methods rely on a commun decomposition principle and use different reformulations into quadratic or linear problems

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## Definition (Quadratization scheme of a monomial)

A quadratization scheme for a monomial $M$, with $|M| \geq 3$, is a directed acyclic graph $G_{M}=\left(V_{M}, A_{M}\right)$ with the following properties:
i) each vertex in $V_{M}$ is a subset of $M, M \in V_{M}$, and $\{i\} \in V_{M}$ for all $i \in M$;
ii) vertex $M$ is the root of $G_{M}$ : it has indegree 0 , and every other vertex has nonzero indegree;
iii) the singletons $\{i\}, i \in M$, are the leaves of $G_{M}$ : they have outdegree $0 ;$
iv) when a vertex $E \in V$ is not a leaf, its outdegree is 2; the arcs leaving $E$ are denoted as $\left(E, I_{M}(E)\right) \in A_{M}$ and $\left(E, r_{M}(E)\right) \in A_{M}$, respectively; $I_{M}(E)$ and $r_{M}(E)$ are the children of $E$;
v) when $E$ is not a leaf, $I_{M}(E)$ and $r_{M}(E)$ define a nontrivial decomposition of $E$ into two subsets: $0<\left|I_{M}(E)\right|<|E|$, $0<\left|r_{M}(E)\right|<|E|$, and $E=I_{M}(E) \cup r_{M}(E)$.

## Example- Quadratization scheme for $M=\{1,2,3,4,5\}$



## Definition (Quadratization scheme for a set of monomials)

A quadratization scheme for a polynomial $\mathcal{M} \subseteq 2^{[n]}$ is a collection of quadratization schemes $\left\{G_{M}=\left(V_{M}, A_{M}\right): M \in \mathcal{M}\right\}$, where each $G_{M}$ is a quadratization scheme for the corresponding monomial $M \in \mathcal{M}$.

Example: $f=a_{1} x_{1} x_{2} x_{3} x_{4} x_{5}+a_{2} x_{1} x_{2} x_{3} x_{4}$


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## Straightforward reformulation as a QCQP

- Rename the initial variables $x_{1} \ldots x_{n}$ into $z_{1} \ldots z_{n}$
- Add a new variable $z_{E}$ per new monomial $E \in \mathcal{E}$ in the quadratization scheme $\rightarrow$ get a total of $N$ binary variables

$$
(Q C Q P)\left\{\begin{array}{l}
\min _{z \in\{0,1\}^{N}} g(z)=\sum_{M \in \mathcal{M}} a_{M} z_{I_{M}(M)} z_{r_{M}(M)} \\
\text { s.t. } \\
z_{E}=z_{l_{M}(E)} z_{r_{M}(E)} \quad \forall E \in \mathcal{E}, \forall M \in \mathcal{M}: E \in \mathcal{E}_{M}
\end{array}\right.
$$



- Proof of equivalence: Iteratively check

$$
z_{l_{M}(M)} z_{r_{M}(M)}=\prod_{i \in M} z_{i}=\prod_{i \in M} x_{i}
$$

## Example- Straightforward reformulation for

 $f=a_{1} x_{1} x_{2} x_{3} x_{4} x_{5}+a_{2} x_{1} x_{2} x_{3} x_{4}$$$
\begin{aligned}
& \{1,2,3,4,5\} \\
& \{1,2,3,4\} z_{1234} \\
& \{1,2\} z_{12} \\
& \text { < } \\
& \{3,4\} z_{34} \\
& \text { \& } \downarrow \\
& \{1\} z_{\{ }\{2\} z_{2} \quad\{3\} z_{\{ }\{4\} z_{4} \quad\{5\} z_{5} \quad\{1\} z_{\mathfrak{Z}}\{2\} z_{2}\{3\} z_{3}\{4\} z_{4} \\
& \left\{\begin{array}{l}
\min _{z \in\{0,1\}^{10}} \quad a_{1} z_{1234} z_{5}+a_{2} z_{123} z_{4} \\
\text { s.t. } \\
z_{1234}=z_{12} z_{34} \quad z_{12}=z_{1} z_{2} \quad z_{34}=z_{3} z_{4} \\
z_{123}=z_{12} z_{3} \quad z_{12}=z_{1} z_{2}
\end{array}\right.
\end{aligned}
$$

## A more pratical quadratic reformulation

- Linearly constrained binary quadratic problem (use Fortet inequalities)

$$
L C B Q\left\{\begin{array}{l}
\min _{z \in\{0,1\}^{N}} \sum_{M \in \mathcal{M}} a_{M} z_{M}(M)^{z_{r}}{ }_{M}(M) \\
z_{E} \leq z_{I_{M}(E)}, z_{E} \leq z_{r_{M}(E)}, z_{E} \geq z_{l_{M}(E)}+z_{r_{M}(E)}-1, z_{E} \geq 0 \quad \forall E \in \mathcal{E}, \forall M \in \mathcal{M}: E \in \mathcal{E}_{M}
\end{array}\right.
$$

Enforce $z_{E}=z_{I_{M}(E)} z_{r_{M}(E)}$ in any feasible solution

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## Phase 2- Solution of the obtained binary quadratic problems

How to solve $L C B Q$ ?
(1) Linearize again: add a new variable and Fortet's inequalities per quadratic term $\rightarrow$ get a MILP
(2) Use Quadratic Convex Reformulation methods $\rightarrow$ get an MIQP with a convex continuous relaxation
(1) The Smallest Eigenvalue method
(2) "basic" QCR
(3) QCR improved by the valid quadratic equalities: PQCR

## Quadratic Convex Reformulation methods

## Smallest Eigenvalue Method

(BQP) $\left\{\begin{array}{l}\min q(x)=x^{T} Q x \\ \text { s. t. } \\ A x \leq b \\ x \in\{0,1\}^{n}\end{array} \Longleftrightarrow\left\{\begin{array}{l}\min x^{T} Q x+\left|\lambda_{1}(Q)\right| \sum_{i=1}^{n}\left(x_{i}^{2}-x_{i}\right) \\ \text { s. t. } \\ A x \leq b \\ x \in\{0,1\}^{n} \text { convex continuous relaxation }\end{array}\right.\right.$
basic Quadratic Convex Reformulation QCR (Billionnet and E. 2007)

- Q. How to find coefficients $u_{i}$ s.th. the continuous relaxation bound is the tightest?
- A. Solve a semidefinite programming problem
s. t .

$$
A x \leq b
$$

$x \in\{0,1\}^{n}$ convex continuous relaxation for some correct choices of $u_{i}$

$$
(S D P)\left\{\begin{array}{l}
\min <Q, X> \\
\text { s. t. } \\
X_{i i}=x_{i} \\
A x \leq b \\
\left(\begin{array}{cc}
1 & x^{T} \\
x & x
\end{array}\right) \succeq 0
\end{array}\right.
$$

## Quadratic Convex Reformulation methods

- QCR works in 2 steps:
(1) solve (SDP) and deduce optimal coefficients $u_{i}^{*}$
(2) solve the "convex" MIQP

$$
\left\{\begin{array}{l}
\min x^{T} Q x+\sum_{i=1}^{n} u_{i}^{*}\left(x_{i}^{2}-x_{i}\right) \\
\text { s. t. } \\
\quad A x \leq b \\
x \in\{0,1\}^{n}
\end{array}\right.
$$

- PQCR (Lazare 2020; E. et al. 2021) uses the Valid Quadratic Equalities associated to the quadratization scheme in order to build more parametrized reformulations, based on a stronger SDP
- $z_{E}=z_{I_{M}(E)} z_{r_{M}(E)} \forall E \in \mathcal{E}, \forall M \in \mathcal{M}: E \in \mathcal{E}_{M}$
- $z_{E} Z_{F}=z_{E} \forall E, F \in \mathcal{E}: F \subset E$
- $z_{E} z_{E^{\prime}}=z_{F} z_{F^{\prime}} \forall E, E^{\prime}, F, F^{\prime} \in \mathcal{E}: E \cup E^{\prime}=F \cup F^{\prime}$


## Summary

For a given a quadratization scheme, we can derive 3 solution methods

|  | LCBQ |
| :---: | :---: |
| Lin | $($ LCBQ + Lin $)$ |
| QCR | $($ LCBQ + QCR $)$ |
| PQCR | (LCBQ + QCR + Valid Quadratic Equalities) |

## Questions:

- how to build quadratization schemes?
- how does the quadratization scheme impact the performance of the solution methods? that is, how does Phase 1 interact with Phase 2?


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## Our four quadratization algorithms

- QA (Lazare 2020) Sort the monomial set in lexicographical order. In this order, iteratively (i) Select the first product of variables $x_{i} x_{j}$ that appears in a monomial of degree at least 3. (ii) For any monomial $M$ containing $i$ and $j$, set $I_{M}(M)$ to $\{i, j\}$ and $r_{M}(M)$ to $M \backslash\{i, j\}$. (iii) Add $I_{M}(M)$ and $r_{M}(M)$ to the sorted monomial set
- QB (Rodriguez-Heck 2018) is similar to QA. The product $x_{i} x_{j}$ that appears the most frequently is selected
- QC Recursively split any monomial $M=\{1, \ldots, d\}$ with $d \geq 2$ into $I_{M}(M)=\{1, \ldots, d-1\}$ and $r_{M}(M)=\{d\}$
- QD Recursively split any monomial $M=\{1, \ldots, d\}$ with $d \geq 2$ into $I_{M}(M)=\{1, \ldots, d-1\}$ and $r_{M}(M)=\{2, \ldots, d\}$. This is our only quadratization scheme with non-disjoint subsets $I_{M}$ and $r_{M}$.



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## Settings

- We use 8 instances of the Low Autocorrelation Binary Sequence problem (polynomials of degree 4, up to 35 variables)
- We use Gurobi to solve MILPs or convex MIQPs


## MILP reformulation


gap: QA, QC, and QD are the best time: QA and QC are the best

## QCR reformulation


gap: QA is the best
time: QA is the best

## PQCR



- In PQCR, QA (followed by QB) performs much better than QC and QD
- PQCR is the best method. When coupled to QA, the 8 instances are solved within 3 minutes in av.
- Over the 4 quadratizations, QA is globally the best and QD is the worst. Recall $N=$ 217, 234, 656, and 885 variables by QA, QB, QC, and QD
gap: QA is the best time: QA is the best


## Conclusions

- We provide a unifying notion of "quadratization scheme"
- We show that several reformulations and solution methods can be deduced from a given quadratization scheme
- We present some computational results suggesting that quadratization schemes with fewer variables have best performances
- Similar results are obtained with the unconstrained penalized quadratic reformulations of (Rosenberg 75) and (Anthony et al. 2017)
- Similar results with other instances

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