Quadratic reformulations for the optimization of pseudo-boolean functions

ISAIM 2022

Sourour Elloumi, ENSTA Paris, France Yves Crama, HEC Management School of the University of Liège, Belgium Amélie Lambert, Cnam Paris, France Elisabeth Rodríguez-Heck, Aachen University, Germany

Pseudo-boolean functions and polynomial optimization with binary variables

We consider the Unconstrained Binary Polynomial Programming problem

$$\begin{cases} \min \quad f(x) = \sum_{M \in \mathcal{M}} a_M \prod_{i \in M} x_i \\ \text{s. t.} \quad x_i \in \{0, 1\} \qquad \forall i \in [n] \end{cases}$$

If degree of f = 2: the quadratic case of qpb functions We suppose all monomials have degree 3 or more We focus on solution approaches in two phases:

- 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

 $\mathbf{O}\textsc{ur}$ work: unify Phase 1 and study the links between Phase 1 and Phase 2

- Quadratic reformulation of the pseudoboolean function into a quadratic problem
- 2 The unifying notion of quadratization scheme
- Ossible reformulations from the quadratization scheme
- 4 Solving the reformulated quadratic problem
- 5 Building quadratization schemes
- 6 A few computational results

Quadratic reformulation of the pseudoboolean function into a quadratic problem

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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 $|M| \ge 3$, is a directed acyclic graph $G_M = (V_M, A_M)$ 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 $(E, I_M(E)) \in A_M$ and $(E, r_M(E)) \in A_M$, 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: $0 < |I_M(E)| < |E|$, $0 < |r_M(E)| < |E|$, and $E = I_M(E) \cup r_M(E)$.

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



non-disjoint quadratization scheme

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 $\{G_M = (V_M, A_M) : M \in \mathcal{M}\}$, where each G_M is a quadratization scheme for the corresponding monomial $M \in \mathcal{M}$.



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Straightforward reformulation as a QCQP

- Rename the initial variables $x_1 \dots x_n$ into $z_1 \dots z_n$
- Add a new variable z_E per new monomial E ∈ E in the quadratization scheme → get a total of N binary variables

$$(QCQP) \begin{cases} \min_{z \in \{0,1\}^N} g(z) = \sum_{M \in \mathcal{M}} a_M z_{I_M(M)} z_{r_M(M)} \\ \text{s.t.} \\ z_E = z_{I_M(E)} z_{r_M(E)} \quad \forall E \in \mathcal{E}, \forall M \in \mathcal{M} : E \in \mathcal{E}_M \end{cases}$$



• Proof of equivalence: Iteratively check $z_{I_{M}(M)}z_{r_{M}(M)} = \prod_{i \in M} z_{i} = \prod_{i \in M} x_{i}$

Example- Straightforward reformulation for $f = a_1x_1x_2x_3x_4x_5 + a_2x_1x_2x_3x_4$

$$\begin{array}{c|c} \hline \{1,2,3,4,5\} & [1,2,3,4] \\ \hline \{1,2,3,4\} z_{1234} & \{1,2,3\} z_{123} \\ \hline \{1,2\} z_{12} & \{3,4\} z_{34} & \{1,2\} z_{12} \\ \hline \\ \{1,2\} z_{12} & \{3,4\} z_{34} & \{1,2\} z_{12} \\ \hline \\ \{1\} z_{1} \{2\} z_{2} & \{3\} z_{3} \{4\} z_{4} & \{5\} z_{5} & \{1\} z_{1} \{2\} z_{2} \{3\} z_{3} \{4\} z_{4} \end{array}$$

$$\begin{cases} \min_{z \in \{0,1\}^{10}} a_1 z_{1234} z_5 + a_2 z_{123} z_4 \\ \text{s.t.} \\ z_{1234} = z_{12} z_{34} \quad z_{12} = z_1 z_2 \\ z_{123} = z_{12} z_3 \quad z_{12} = z_1 z_2 \end{cases}$$

• Linearly constrained binary quadratic problem (use Fortet inequalities)

$$LCBQ \begin{cases} \min_{z \in \{0,1\}^N} \sum_{M \in \mathcal{M}} a_M z_{l_M}(M) z_{r_M}(M) \\ z_E \le z_{l_M}(E), z_E \le z_{r_M}(E), z_E \ge z_{l_M}(E) + z_{r_M}(E) - 1, z_E \ge 0 \qquad \forall E \in \mathcal{E}, \forall M \in \mathcal{M} : E \in \mathcal{E}_M \end{cases}$$

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 LCBQ ?

- Icinearize again: add a new variable and Fortet's inequalities per quadratic term → get a MILP
- O Use Quadratic Convex Reformulation methods \rightarrow get an MIQP with a convex continuous relaxation
 - The Smallest Eigenvalue method
 - 2 "basic" QCR
 - QCR improved by the valid quadratic equalities: PQCR

Quadratic Convex Reformulation methods

Smallest Eigenvalue Method

$$(\mathsf{BQP}) \begin{cases} \min q(x) = x^T Q x \\ \text{s. t.} \\ A_x \le b \\ x \in \{0,1\}^n \end{cases} \iff \begin{cases} \min x^T Q x + |\lambda_1(Q)| \sum_{i=1}^n (x_i^2 - x_i) \\ \text{s. t.} \\ Ax \le b \\ x \in \{0,1\}^n \text{ convex continuous relaxation} \end{cases}$$

basic Quadratic Convex Reformulation QCR (Billionnet and E. 2007)

$$\min x^T Q x + \sum_{i=1}^n u_i (x_i^2 - x_i)$$
s. t.
$$Ax \le b$$

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

$$(SDP) \begin{cases} \min < Q, X > \\ \text{s. t.} \\ X_{ij} = x_j \\ Ax \le b \\ \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succeq 0 \end{cases}$$

Quadratic Convex Reformulation methods

• QCR works in 2 steps:

- solve (*SDP*) and deduce optimal coefficients u_i^*
- solve the "convex" MIQP

$$\begin{cases} \min x^T Q x + \sum_{i=1}^n u_i^* (x_i^2 - x_i) \\ \text{s. t.} \\ Ax \le b \\ x \in \{0, 1\}^n \end{cases}$$

• 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

•
$$z_E = z_{I_M(E)} z_{r_M(E)} \ \forall E \in \mathcal{E}, \forall M \in \mathcal{M} : E \in \mathcal{E}_M$$

•
$$z_E z_F = z_E \ \forall E, F \in \mathcal{E} : F \subset E$$

• $z_E z_{E'} = z_F z_{F'} \ \forall E, E', F, F' \in \mathcal{E} : E \cup E' = F \cup F'$

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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- 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 $M \setminus \{i, j\}$. (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 $M = \{1, ..., d\}$ with $d \ge 2$ into $I_M(M) = \{1, ..., d-1\}$ and $r_M(M) = \{d\}$
- QD Recursively split any monomial $M = \{1, \ldots, d\}$ with $d \ge 2$ 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 .





• In our test instances, we got in average N = 217, 234, 656, and 885 by QA, QB, QC, and QD resp.

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- 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

- 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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