Nonconvex Quadratic Programming: 
Return of the Boolean Quadric Polytope

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We consider a nonconvex quadratic programming problem of the form:

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\text{QP : } \min c^T x + x^T Q x \\
\text{s.t. } x \in B \cap C.
\]

- \( B = \{x \mid 0 \leq x_i \leq 1, \ i = 1, \ldots, n\}. \)
- \( C \) is given by additional linear or quadratic constraints.
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- \( C \) is given by additional linear or quadratic constraints.
- For \( C = \mathbb{R}^n \) get the Box-Constrained Quadratic Program

\[ \text{QPB} : \min \ c^T x + x^T Q x \]
\[ \text{s.t. } x \in B. \]
QPB is already NP-hard. In particular, by adding an objective term $\gamma \sum_{i=1}^{n} (x_i - x_i^2)$ can represent the Boolean Quadratic Program

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$$\text{s.t. } x_i \in \{0, 1\}, i = 1, \ldots, n.$$
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BQP is a well-studied problem in the discrete optimization literature. Polyhedral approach to BQP, introduced by Padberg (1989), is based on studying the Boolean Quadric Polytope

$$BQP_n = \text{conv}\{x_i, y_{ij} \mid y_{ij} = x_i x_j, 1 \leq i < j \leq n,\}$$

$$x_i \in \{0, 1\}, i = 1, \ldots, n \}.$$
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$$x_i \in \{0, 1\}, i = 1, \ldots, n\}.$$ 

- BQP is a linear problem over $BQP_n$.
- No terms of the form $y_{ii}$ appear in $BQP_n$ since $x_i = x_i^2$ for $x_i \in \{0, 1\}.$
Relaxations for QPB

To obtain a convex representation of QPB it is natural to follow a similar approach to that used for BQP. In particular, note that

\[ c^T x + x^T Q x = \begin{pmatrix} 1 \\ x \end{pmatrix}^T \begin{pmatrix} 0 & c^T/2 \\ c/2 & Q \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix} = \tilde{Q} \cdot \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T, \]

so can consider

\[ QPB_n = \text{conv} \left\{ \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T \mid 0 \leq x \leq e \right\}. \]
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Can then write QPB in the form

\[ \text{QPB} : \quad \min \ \tilde{Q} \cdot \tilde{Y} \]

s.t. \[ \tilde{Y} = \begin{pmatrix} 1 \\ x^T \\ Y \end{pmatrix} \in QPB_n. \]
• **Good**: exact convex representation with linear objective.
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• **Bad:** *must* be difficult to fully characterize $QPB_n$. 
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• **Bad:** *must* be difficult to fully characterize $QPB_n$.

Full characterization of $QPB_n$ may be impossible, but sensible thing to do is to look for **valid constraints**.
Reformulation-Linearization Technique

If two quantities (such as $x_i$ and $(1 - x_j)$) are nonnegative, then their product is also nonnegative. Forming all products based on the bound constraints $0 \leq x \leq e$ and making the identifications $y_{ij} = x_i x_j$ results in the RLT constraints

\[
\begin{align*}
y_{ij} & \leq x_i, \\
y_{ij} & \leq x_j, \\
y_{ij} & \geq 0, \\
y_{ij} & \geq x_i + x_j - 1.
\end{align*}
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Semidefinite Programming

SDP relaxations are based on the observation that $\tilde{Y} \succeq 0$ (PSD).
Comparison between PSD and RLT

To compare the PSD and RLT conditions it is useful to consider principal submatrix of \( \tilde{Y} \) corresponding to two variables \( x_i \) and \( x_j \). Taking \( i = 1 \) and \( j = 2 \), let

\[
\tilde{Y}^{12} = \begin{pmatrix}
1 & x_1 & x_2 \\
x_1 & y_{11} & y_{12} \\
x_2 & y_{12} & y_{22}
\end{pmatrix}.
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x_2 & y_{12} & y_{22}
\end{pmatrix}.
\]

It is then straightforward to show that the PSD condition \( \tilde{Y}^{12} \succeq 0 \) is equivalent to the constraints

\[
\begin{align*}
    y_{ii} &\geq x_i^2, \quad i = 1, 2, \\
y_{12} &\leq x_1 x_2 + \sqrt{(y_{11} - x_1^2)(y_{22} - x_2^2)}, \\
y_{12} &\geq x_1 x_2 - \sqrt{(y_{11} - x_1^2)(y_{22} - x_2^2)}.
\end{align*}
\]
Easy to see that:

- PSD implies no **upper bounds** on \( y_{ii}, i = 1, 2 \) compared to the RLT upper bounds

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- The PSD lower bounds $y_{ii} \geq x_i^2$, $i = 1, 2$ dominate the RLT lower bounds
  \[ y_{ii} \geq 0, \quad y_{ii} \geq 2x_i - 1. \]
Easy to see that:

- PSD implies no upper bounds on $y_{ii}$, $i = 1, 2$ compared to the RLT upper bounds
  
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- The PSD lower bounds $y_{ii} \geq x_i^2$, $i = 1, 2$ dominate the RLT lower bounds
  
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- The PSD bounds on $y_{12}$ dominate the RLT bounds on $y_{12}$ if $y_{11} - x_1^2$ and $y_{22} - x_2^2$ are sufficiently small.
In fact for $x_1 = x_2 = 1/2$, the PSD bounds on $y_{12}$ dominate the RLT bounds for all $y_{ii}$ that satisfy the RLT upper bounds and PSD lower bounds. In this case can compute that the 3–dimensional volume of the intersection of the PSD and RLT constraints on $y_{11}, y_{22}, y_{12}$ is $1/72$, compared to $1/8$ for RLT constraints alone. So for these “midpoint” values of $x_i$, adding PSD decreases volume by a factor of 9.
Figure 1: RLT versus PSD ∩ RLT regions, $0 \leq x \leq e$, $x_1 = x_2 = 0.5$. 
Computing the 3–dimensional volume of the intersection of the PSD and RLT constraints for general case is a tedious exercise. By interchanging/complemeting variables can assume $x_1 \leq x_2 \leq .5$.

**Theorem 1 (A. 2009)** Suppose that $0 < x_1 \leq x_2 \leq 1/2$. Then the 3-dimensional volume corresponding to the RLT constraints on $y_{11}, y_{22}, y_{12}$ is $x_1^2 x_2$, and the volume corresponding to the PSD and RLT constraints together is

\[
x_1^2 x_2 (1 - x_2) - \frac{1}{9} x_1^3 (6x_2^2 - 6x_2 + 5)
+ \frac{1}{3} x_1^3 ((1 - x_2)^3 - x_2^3)) \ln \left( \frac{1 - x_2}{x_2} \right)
- \frac{1}{3} x_1^3 ((1 - x_2)^3 + x_2^3)) \ln \left( \frac{1 - x_1}{x_1} \right).
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$$x_1^2 x_2 (1 - x_2) - \frac{1}{9}x_1^3 (6x_2^2 - 6x_2 + 5) + \frac{1}{3}x_1^3 ((1 - x_2)^3 - x_2^3) \ln \left( \frac{1 - x_2}{x_2} \right) - \frac{1}{3}x_1^3 ((1 - x_2)^3 + x_2^3) \ln \left( \frac{1 - x_1}{x_1} \right).$$

Implies that maximum factor reduction in volume occurs for $x_1 = x_2 = .5$, and reduction approaches zero for $x_2 \to 0, x_1/x_2 \to 0$. 
Figure 2: RLT versus PSD ∩ RLT regions, $0 \leq x \leq e$, $x_1 = .01$, $x_2 = .1$. 
Can also use Theorem 1 to prove result for five-dimensional volumes of the corresponding feasible regions based on the original bounds $0 \leq x_i \leq 1$, $i = 1, 2$. 

**Theorem 2 (A. 2009)** Suppose that $0 \leq x_i \leq 1$, $i = 1, 2$. Then the volume of $\{(x_1, x_2, y_{11}, y_{22}, y_{12})\}$ feasible for the RLT constraints is $1/60$, and the volume of $\{(x_1, x_2, y_{11}, y_{22}, y_{12})\}$ feasible for the RLT and PSD constraints is $1/240$. 
Can also use Theorem 1 to prove result for five-dimensional volumes of the corresponding feasible regions based on the original bounds $0 \leq x_i \leq 1, \ i = 1, 2$.

**Theorem 2 (A. 2009)** Suppose that $0 \leq x_i \leq 1, \ i = 1, 2$. Then the volume of $\{(x_1, x_2, y_{11}, y_{22}, y_{12})\}$ feasible for the RLT constraints is $1/60$, and the volume of $\{(x_1, x_2, y_{11}, y_{22}, y_{12})\}$ feasible for the RLT and PSD constraints is $1/240$.

So adding PSD to the RLT relaxation removes exactly 75% of the feasible region corresponding to two of the original variables. In fact no further improvement is possible:

**Theorem 3 (A. and Burer 2007)** For $n = 2$, the set of $\tilde{Y} \succeq 0$ such that $(x, Y)$ are feasible for the RLT constraints is equal to $QP B_2$. 
For \( n \geq 3 \) know that PSD and RLT together do not provide full characterization of \( QPB_n \). What additional inequalities are needed?
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- Yajima and Fujie (1998) show that many known inequalities for $BQP_n$ are also valid for $QPB_n$. Obtain good computational results for QPB using RLT, cuts based on $\tilde{Y} \succeq 0$, and inequalities from $BQP_n$. 
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- A. and Burer (2007) found 4 valid inequalities for $QPB_3$ that give deep cuts for certain values of $x_i, y_{ii}$.
Figure 3: Effect of added constraints for $x_i = y_{ii} = .5$, $i = 1, 2, 3$. 
When written out “longhand,” inequalities from A. and Burer (2007) are:

\[
\begin{align*}
y_{11} + y_{22} + y_{33} & \leq y_{12} + y_{13} + y_{23} + 1, \\
y_{11} + y_{22} + y_{33} + y_{12} + y_{13} & \leq 2x_1 + x_2 + x_3 + y_{23}, \\
y_{11} + y_{22} + y_{33} + y_{12} + y_{23} & \leq x_1 + 2x_2 + x_3 + y_{13}, \\
y_{11} + y_{22} + y_{33} + y_{13} + y_{23} & \leq x_1 + x_2 + 2x_3 + y_{12}.
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y_{11} + y_{22} + y_{33} + y_{13} + y_{23} \leq x_1 + x_2 + 2x_3 + y_{12}.
\]

If \(y_{ii} = x_i\), as in \(BQP_3\), then inequalities become:

\[
x_1 + x_2 + x_3 \leq y_{12} + y_{13} + y_{23} + 1,
\]

\[
y_{12} + y_{13} \leq x_1 + y_{23},
\]

\[
y_{12} + y_{23} \leq x_2 + y_{13},
\]

\[
y_{13} + y_{23} \leq x_3 + y_{12}.
\]

These are the well-known triangle inequalities for \(BQP_3\).
It is obvious that $BQP_n \subset \text{proj}(QP\!B_n)$, where $\text{proj}(\tilde{Y})$ returns the elements above the diagonal in $\tilde{Y}$. Also easy to see that $BQP_n = \text{proj}(QP\!B_n \cap \{\tilde{Y} \mid y_{ii} = x_i, \ i = 1, \ldots, n\})$. 
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**Theorem 4 (Burer and Letchford 2008)** For all $n \geq 2$, $\text{proj}(QPB_n) = BQP_n$.

Theorem 4 goes a long way to explain the results of Yajima and Fujie (1998), as well as the inequalities found by A. and Burer (2007). Note the since $BQP_3$ is given exactly by RLT and TRI inequalities, and TRI inequalities dominate those found by A. and Burer (2007), it is reasonable to think that PSD, RLT and TRI might fully characterize $QPB_3$. 
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This turns out to be FALSE.
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- RLT constraints for off-diagonal terms are facets of $QPB_n$.
- TRI inequalities are facets of $QPB_n$.
- Suppose that $v_i \in \{-1, 0, 1\}$, $i = 1, \ldots, n$ and $s$ is an integer scalar. Then $(v^T x + s)(v^T x + s - 1) \geq 0$ for binary $x$. If resulting inequality is a facet of $BQP_n$ then it is also a facet of $QPB_n$. 
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Note that $QPB_n$ is not polyhedral!
Figure 4: RLT versus PSD ∩ RLT regions, $0 \leq x \leq e$, $x_1 = .1$, $x_2 = .5$. 


Computational Results

Consider 54 QPB maximization problems with $n = 20, 30, 40, 50, 60$ from Dieter Vandenbussche. Density of $(c, Q)$ varies from 30% to 100%. Compare bounds using PSD (with upper bound on diagonal components), PSD+RLT and PSD+RLT+TRI. When using TRI inequalities, generate RLT and TRI inequalities in several rounds, with decreasing infeasibility tolerance.
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Exact solution of 50/51 of these problems accomplished using Branch and Cut by Vandenbussche and Nemhauser (2003), using up to $\approx 28,000$ LPs and a total of $\approx 500,000$ cuts.
Table 1: Comparison of bounds for indefinite QPB

<table>
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Table 2: Comparison of bounds for indefinite QPB (cont)

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Average: 5.969% 0.499%
Range Reduction/Fixing Variables

If branching on continuous variables is necessary, range reduction can provide very significant benefits (BARON). Logic for range reduction can be based on a diagonal constraint

\[ y_{ii} \leq x_i \iff x_i - y_{ii} \geq 0. \]

Assume tight, with Lagrange multiplier (dual slack variable) \( \lambda_i > 0 \). Let \( \Delta \) be gap between current bound and known objective value for feasible solution. Then \( \text{optimal } Y = xx^T \) must have

\[ \lambda_i(x_i - x_i^2) \leq \Delta. \]
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\[ \lambda_i(x_i - x_i^2) \leq \Delta. \]

If \( \lambda_i > 4\Delta \), conclude that

\[ x_i \notin (.5 - \delta_i, .5 + \delta_i) \text{ where } \delta_i = \frac{1}{2}\sqrt{\frac{\lambda_i - 4\Delta}{\lambda_i}}. \]

Note that for QPB, can set \( \delta_i = .5 \) for any \( i \) such that \( q_{ii} \leq 0 \). Indicate such \( i \) in tabular output using \textbf{boldface} for \( \delta_i \).
**Example:** Consider problem 30-060-3 with PSD and RLT constraints, using $\Delta$ based on optimal value. Gap to optimality is 0.37%.
Table 3: Solution output for 30-060-3 using PSD and RLT

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<th>$z_u$</th>
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Would also like to be able to do range reduction \textit{without} branching. Requires Lagrange multipliers for tight bound constraints.
Would also like to be able to do range reduction *without* branching. Requires Lagrange multipliers for tight bound constraints.

- Bounds $0 \leq x_i \leq 1$ are redundant with PSD or RLT constraints added. Even if explicitly included, multipliers are zero until gap is nearly zero.
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- Bounds $0 \leq x_i \leq 1$ are redundant with PSD or RLT constraints added. Even if explicitly included, multipliers are zero until gap is nearly zero.

- Could use RLT constraints based on $l_i \leq x_i \leq u_i$ with $l_i > 0$ or $u_i < 1$, but get changes in both variable coefficients and right-hand-side values.
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- With PSD, tight constraints correspond to vectors in $\mathcal{N}(\tilde{Y})$. For BQP, fixing logic based on max-cut formulation developed by Helmberg (2000). Logic can be extended to QPB but results are not encouraging.
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What to do?
**Dumb idea:** Add explicit bounds $\epsilon \leq x_i \leq 1 - \epsilon$, $\epsilon > 0$.

Figure 5: Tightened bound constraints using $\epsilon = .05$. 
• Using $\epsilon > 0$ is *restriction* of original problem, but if constraints are tight can recover rigorous bound using Lagrange multipliers.
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• Tight constraint with multiplier $\lambda_i > 0$ implies $x_i \geq \Delta/\lambda_i$ or $x_i \leq 1 - \Delta/\lambda_i$. 
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• Tight constraint with multiplier $\lambda_i > 0$ implies $x_i \geq \Delta/\lambda_i$ or $x_i \leq 1 - \Delta/\lambda_i$.

• Logic can be combined with excluded range based on $\delta_i$. For variables with $\delta_i = .5$ allows for fixing at 0/1 values.
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• Logic can be combined with excluded range based on $\delta _i$. For variables with $\delta _i = .5$ allows for fixing at 0/1 values.

Consider 30-060-3 with PSD and RLT constraints and $\epsilon = .02$. Gap increases from 0.37% to 0.57%, but using $\Delta$ based on optimal value can fix 7 variables at 0/1 values and reduce the range of 2 more.
Table 4: Solution output for 30-060-3 using PSD and RLT, $\epsilon = .02$

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- Maybe this is not such a dumb idea after all!
What next?

- Would be very nice to obtain explicit characterization of $QPB_3$ without additional variables. (A. and Burer (2007) obtain complete disjunctive representation for $QPB_3$ using triangulation of the cube.)
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- Application to problems with constraints. Expect good effect of cuts from $BQP_n$ on problems where multiple bound constraints are tight.
References


