Nonconvex Quadratic Programming: Return of the Boolean Quadric Polytope

Kurt M. Anstreicher
Dept. of Management Sciences
University of Iowa

Integer Programming at CORE, May 2009

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- Say nice things about Laurence.

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In this talk I will not:

- Talk about our joint research.

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- C is given by additional linear or quadratic constraints.
- For $C = \Re^n$ get the *Box–Constrained Quadratic Program*

$$\begin{aligned} \text{QPB}: \quad & \min \ c^T x + x^T Q x \\ & \text{s.t.} \ \ x \in B. \end{aligned}$$

QPB is already NP-hard. In particular, by adding an objective term $\gamma \Sigma_{i=1}^{n}(x_i - x_i^2)$ can represent the Boolean Quadratic Program

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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*

$$\begin{aligned} BQP_n = \text{conv}\{x_i, y_{ij} \mid \; & y_{ij} = x_i x_j, 1 \le i < j \le n, \\ & x_i \in \{0, 1\}, i = 1, \ldots, n\}. \end{aligned}$$

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- 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

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

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Can then write QPB in the form

$$\begin{aligned} \mathrm{QPB}: \quad & \min \ \tilde{Q} \bullet \tilde{Y} \\ & \text{s.t.} \ \tilde{Y} = \begin{pmatrix} 1 & x^T \\ x & Y \end{pmatrix} \in QPB_n. \end{aligned}$$

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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 $0 \le x \le e$ and making the identifications $y_{ij} = x_i x_j$ results in the RLT constraints

$$
\begin{aligned}
y_{ij} &\le x_i, \\
y_{ij} &\le x_j, \\
y_{ij} &\ge 0, \\
y_{ij} &\ge x_i + x_j - 1.
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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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It is then straightforward to show that the PSD condition $\tilde{Y}^{12} \succeq 0$ is equivalent to the constraints

$$\begin{aligned} y_{ii} &\geq x_i^2, \quad i = 1, 2, \\ y_{12} &\leq x_1 x_2 + \sqrt{(y_{11} - x_1^2)(y_{22} - x_2^2)}, \\ y_{12} &\geq x_1 x_2 - \sqrt{(y_{11} - x_1^2)(y_{22} - x_2^2)}. \end{aligned}$$

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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.

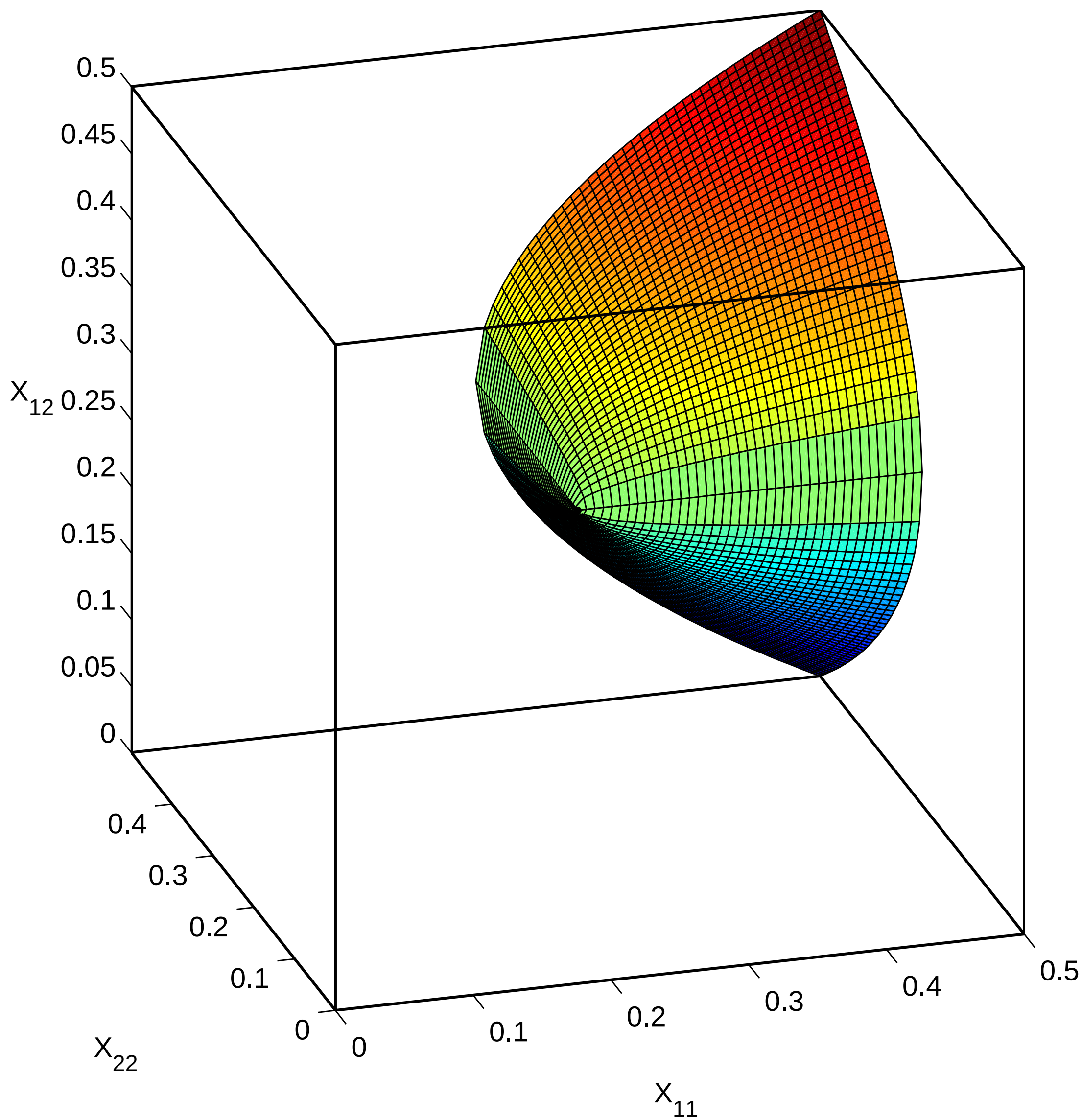

Figure 1: RLT versus PSD$\cap$RLT regions, $0 \le x \le e$, $x_1 = x_2 = .5$.

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*

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

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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 $x_2 \to 0$, $x_1/x_2 \to 0$.

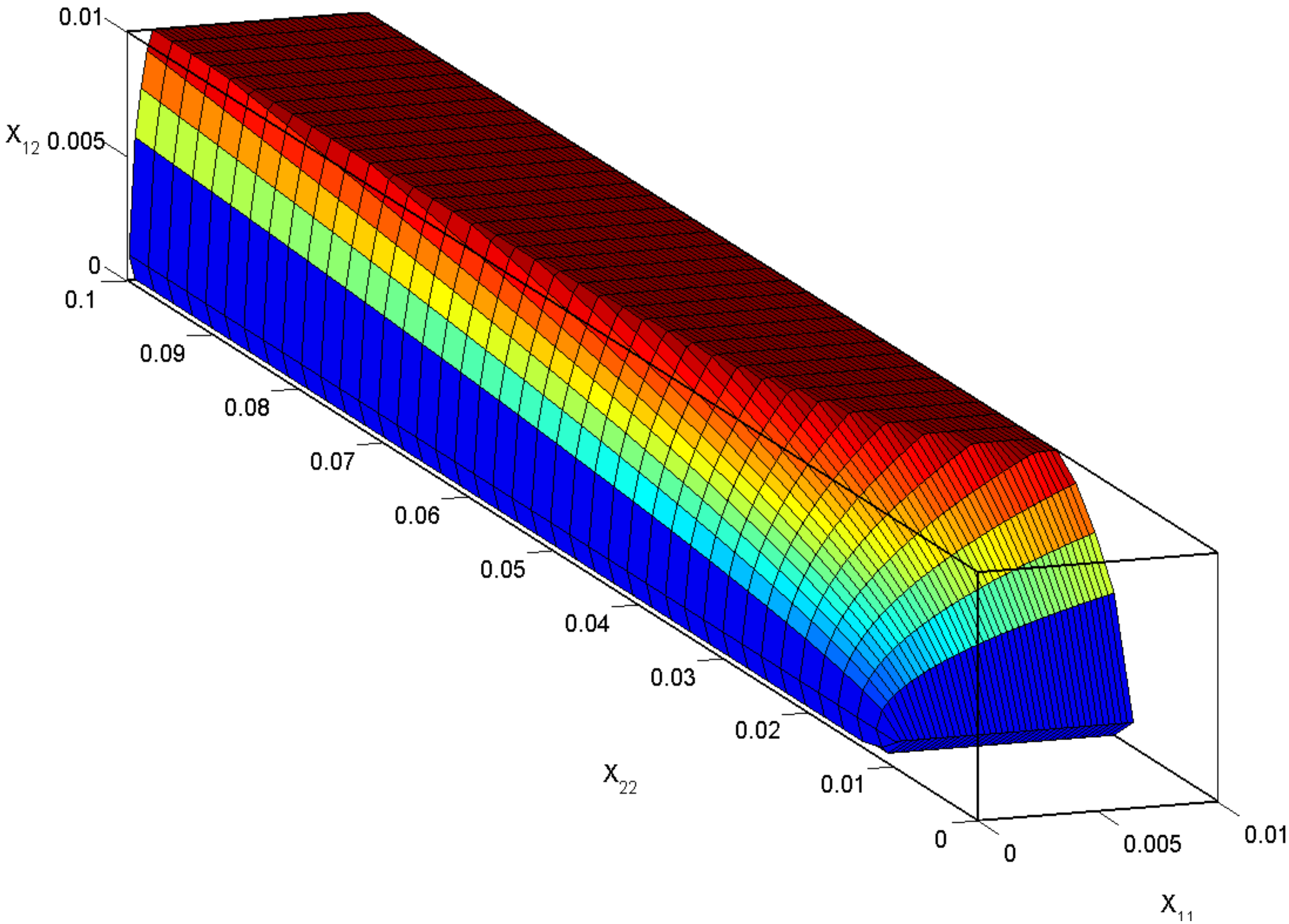

Figure 2: RLT versus PSD$\cap$RLT regions, $0 \leq x \leq e$, $x_1 = .01$, $x_2 = .1$.

Can also use Theorem 1 to prove result for five-dimensional volumes of the corresponding feasible regions based on the original bounds $0 \le x_i \le 1$, $i = 1, 2$.

Theorem 2 (A. 2009) *Suppose that* $0 \le x_i \le 1$*,* $i = 1, 2$*. 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* $1/240$*.*

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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* QPB_2.

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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}.

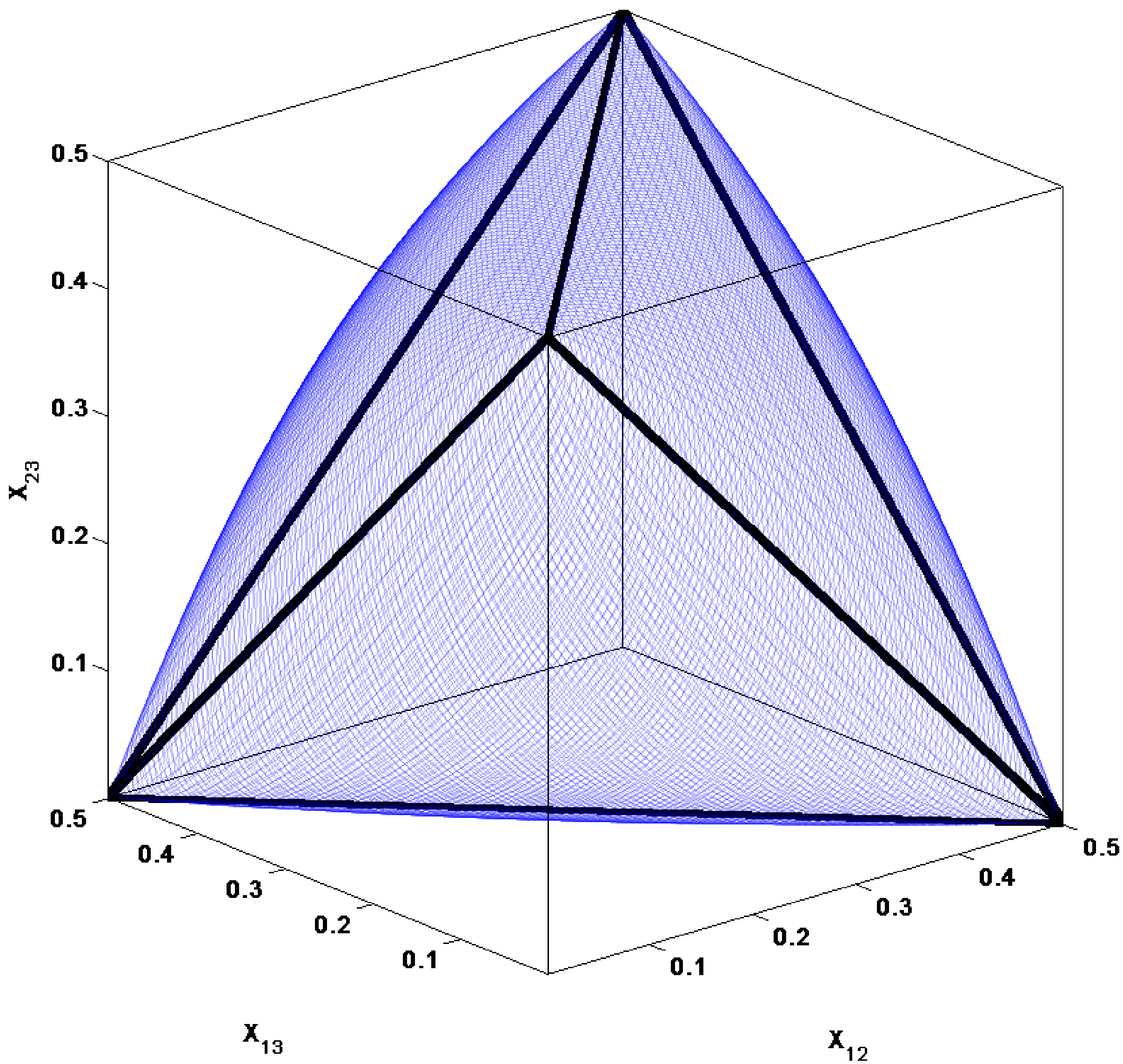

Figure 3: Effect of added constraints for $x_i = y_{ii} = .5$, $i = 1, 2, 3$.

When written out "longhand," inequalities from A. and Burer (2007) are:

$$\begin{aligned}
y_{11} + y_{22} + y_{33} &\le y_{12} + y_{13} + y_{23} + 1, \\
y_{11} + y_{22} + y_{33} + y_{12} + y_{13} &\le 2x_1 + x_2 + x_3 + y_{23}, \\
y_{11} + y_{22} + y_{33} + y_{12} + y_{23} &\le x_1 + 2x_2 + x_3 + y_{13}, \\
y_{11} + y_{22} + y_{33} + y_{13} + y_{23} &\le x_1 + x_2 + 2x_3 + y_{12}.
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If $y_{ii} = x_i$, as in BQP_3, then inequalities become:

$$\begin{aligned} x_1 + x_2 + x_3 &\leq y_{12} + y_{13} + y_{23} + 1, \\ y_{12} + y_{13} &\leq x_1 + y_{23}, \\ y_{12} + y_{23} &\leq x_2 + y_{13}, \\ y_{13} + y_{23} &\leq x_3 + y_{12}. \end{aligned}$$

These are the well-known triangle inequalities for BQP_3.

It is obvious that $BQP_n \subset \text{proj}(QPB_n)$, where $\text{proj}(\tilde{Y})$ returns the elements above the diagonal in $\tilde{Y}$. Also easy to see that $BQP_n = \text{proj}(QPB_n \cap \{\tilde{Y} \mid y_{ii} = x_i,\ i = 1, \ldots, n\})$.

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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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- 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!

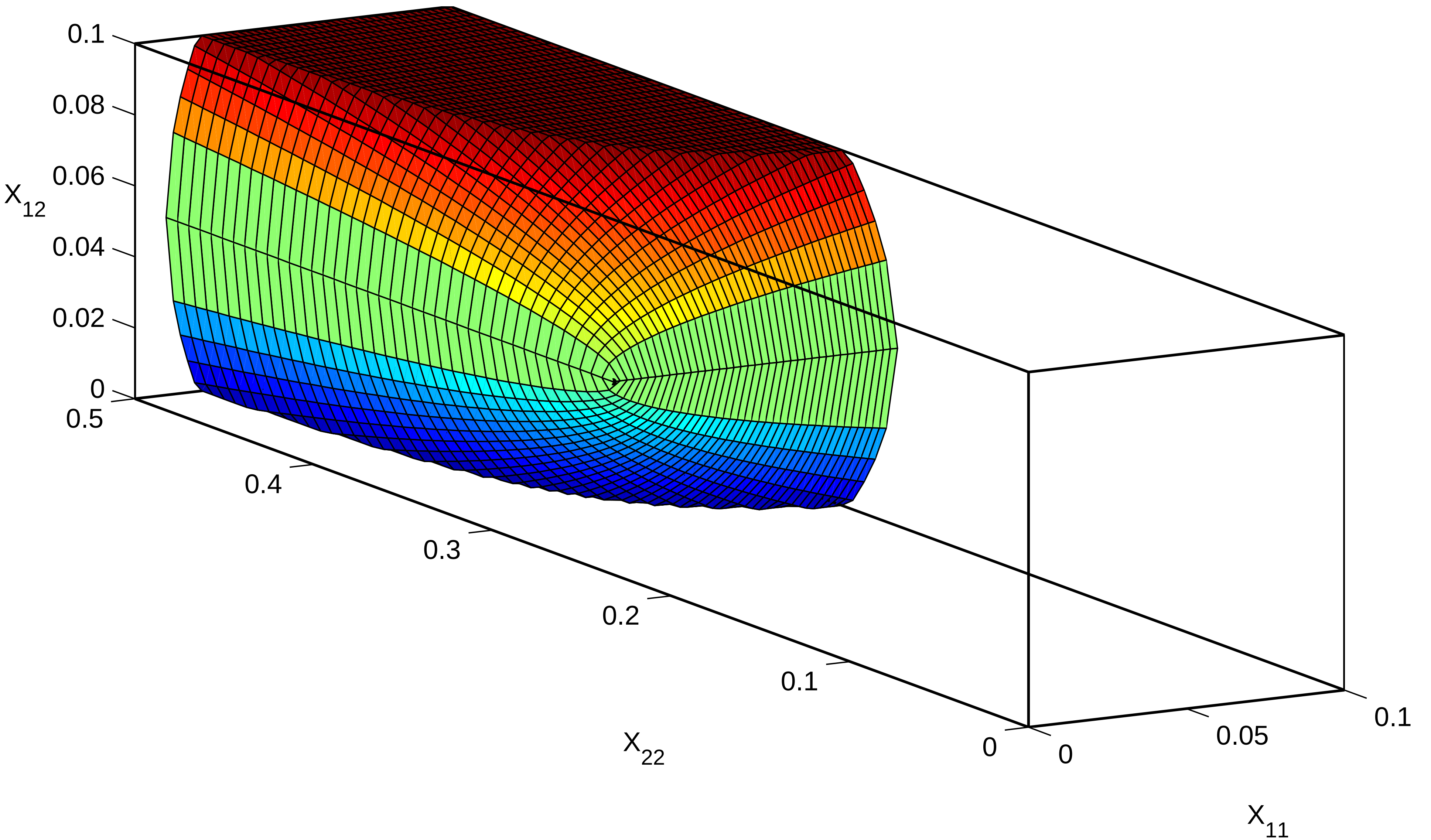

Figure 4: RLT versus PSD $\cap$ RLT regions, $0 \leq x \leq e$, $x_1 = .1$, $x_2 = .5$.

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

	Objective Value				Cuts Added		% Gaps to OPT		
Problem	OPT	PSD	PSD+RLT	PSD+RLT+TRI	RLT	TRI	PSD	PSD+RLT	PSD+RLT+TRI
20-100-1	706.50	739.39	706.52	706.50	197	55	4.655%	0.002%	0.000%
20-100-2	856.50	900.20	857.97	856.50	184	172	5.102%	0.171%	0.000%
20-100-3	772.00	785.51	772.00		168		1.750%	0.000%	
30-060-1	706.00	768.12	714.68	706.00	371	777	8.799%	1.229%	0.000%
30-060-2	1377.17	1426.94	1377.17		381		3.614%	0.000%	
30-060-3	1293.50	1370.13	1298.26	1293.50	394	288	5.924%	0.368%	0.000%
30-070-1	654.00	746.43	674.00	654.00	369	784	14.133%	3.058%	0.000%
30-070-2	1313.00	1375.07	1313.00		449		4.727%	0.000%	
30-070-3	1657.40	1719.77	1657.57	1657.40	452	442	3.763%	0.010%	0.000%
30-080-1	952.73	1050.76	965.25	952.73	365	718	10.290%	1.315%	0.000%
30-080-2	1597.00	1622.81	1597.00		376		1.616%	0.000%	
30-080-3	1809.78	1836.79	1809.78		317		1.492%	0.000%	
30-090-1	1296.50	1348.48	1296.50		370		4.009%	0.000%	
30-090-2	1466.84	1527.87	1466.84		344		4.160%	0.000%	
30-090-3	1494.00	1516.81	1494.00		420		1.527%	0.000%	
30-100-1	1227.13	1285.74	1227.13		356		4.777%	0.000%	
30-100-2	1260.50	1365.32	1261.11	1260.50	427	465	8.316%	0.048%	0.000%
30-100-3	1511.05	1611.11	1513.15	1511.05	377	265	6.622%	0.139%	0.000%
40-030-1	839.50	876.60	839.50		656		4.419%	0.000%	
40-030-2	1429.00	1496.83	1429.00		889		4.747%	0.000%	
40-030-3	1086.00	1156.52	1086.00		705		6.494%	0.000%	
40-040-1	837.00	956.09	863.09	837.00	710	1966	14.228%	3.117%	0.000%
40-040-2	1428.00	1452.53	1428.00		600		1.718%	0.000%	
40-040-3	1173.50	1269.83	1180.85	1173.50	745	1427	8.209%	0.626%	0.000%
40-050-1	1154.50	1276.79	1160.44	1154.50	797	1608	10.592%	0.515%	0.000%
40-050-2	1430.98	1517.51	1436.05	1430.98	788	961	6.047%	0.354%	0.000%
40-050-3	1653.63	1747.31	1653.63		680		5.665%	0.000%	

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

	Objective Value				Cuts Added		% Gaps to OPT		
Problem	OPT	PSD	PSD+RLT	PSD+RLT+TRI	RLT	TRI	PSD	PSD+RLT	PSD+RLT+TRI
40-060-1	1322.67	1481.96	1352.92	1322.67	696	1722	12.043%	2.287%	0.000%
40-060-2	2004.23	2099.58	2004.23		739		4.758%	0.000%	
40-060-3	2454.50	2508.68	2454.50		701		2.207%	0.000%	
40-070-1	1605.00	1663.98	1605.00		584		3.675%	0.000%	
40-070-2	1867.50	1931.34	1867.50		650		3.418%	0.000%	
40-070-3	2436.50	2522.71	2436.50		828		3.538%	0.000%	
40-080-1	1838.50	1936.17	1838.50		615		5.312%	0.000%	
40-080-2	1952.50	2012.92	1952.50		639		3.094%	0.000%	
40-080-3	2545.50	2638.34	2545.89	2545.50	755	742	3.647%	0.015%	0.000%
40-090-1	2135.50	2262.51	2135.50		763		5.948%	0.000%	
40-090-2	2113.00	2268.86	2113.75	2113.00	731	336	7.376%	0.035%	0.000%
40-090-3	2535.00	2594.26	2535.00		598		2.338%	0.000%	
40-100-1	2476.38	2557.23	2476.38		673		3.265%	0.000%	
40-100-2	2102.50	2216.62	2106.37	2102.50	707	1251	5.428%	0.184%	0.000%
40-100-3	1866.07	2037.31	1908.19	1866.07	664	1732	9.176%	2.257%	0.000%
50-030-1	1324.50	1389.09	1324.50		903		4.877%	0.000%	
50-030-2	1668.00	1755.68	1671.33	1668.00	831	233	5.257%	0.200%	0.000%
50-030-3	1453.61	1565.76	1454.88	1453.61	830	180	7.715%	0.087%	0.000%
50-040-1	1411.00	1483.01	1411.00		1017		5.103%	0.000%	
50-040-2	1745.76	1881.33	1749.46	1745.76	868	509	7.766%	0.212%	0.000%
50-040-3	2094.50	2176.98	2094.50		1081		3.938%	0.000%	
50-050-1	1198.41	1417.77	1302.24	1200.14	723	1531	18.304%	8.664%	0.144%
50-050-2	1776.00	1942.53	1789.58	1776.00	867	667	9.377%	0.765%	0.000%
50-050-3	2106.10	2268.04	2121.93	2106.10	937	933	7.689%	0.752%	0.000%
60-020-1	1212.00	1297.42	1212.00		1199		7.048%	0.000%	
60-020-2	1925.50	2010.57	1925.50		1319		4.418%	0.000%	
60-020-3	1483.00	1604.60	1491.06	1483.00	1040	735	8.200%	0.543%	0.000%
						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

$$y_{ii} \le x_i \iff x_i - y_{ii} \ge 0.$$

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

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If $\lambda_i > 4\Delta$, conclude that

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

Note that for QPB, can set $\delta_i = .5$ for any i such that $q_{ii} \leq 0$. Indicate such i in tabular output by writing $-\delta_i$.

Example: Consider problem 30-060-3 with PSD and RLT constraints. Gap to optimality is 0.37%.

Table 3: Solution output for 30-060-3 using PSD and RLT

x	z_d	z_l	z_u	δ	l	u
0.9994	90.8803	0	0.0010	-0.4447	0	1
0.9996	42.7392	0	0.0012	0.3727	0	1
0.8994	44.7452	0	0	-0.3794	0	1
0.7672	38.2900	0	0	-0.3550	0	1
0.9800	60.3003	0	0	-0.4139	0	1
0.9988	99.7733	0	0.0005	-0.4499	0	1
0.9844	41.4727	0	0	0.3682	0	1
0.9991	95.5775	0	0.0007	-0.4476	0	1
0.1477	23.5807	0	0	-0.2207	0	1
0.9881	27.2218	0	0.0001	0.2750	0	1
0.2371	15.8647	0	0	0	0	1
0.9991	90.5048	0	0.0006	-0.4445	0	1
0.9565	25.5004	0	0	-0.2527	0	1
0.9999	98.1925	0	0.0042	0.4491	0	1
0.0285	1.1118	0	0	0	0	1
0.1784	41.0107	0	0	-0.3664	0	1
0.9853	49.4844	0	0	-0.3925	0	1
0.9997	62.0796	0	0.0017	-0.4166	0	1
0.4921	18.4713	0	0	0	0	1
0.1046	21.0579	0	0	0.1568	0	1
0.0449	32.2790	0	0	0.3209	0	1
0.0011	33.7484	0.0005	0	-0.3307	0	1
0.0344	33.8963	0	0	-0.3316	0	1
0.9969	33.5803	0	0.0002	-0.3296	0	1
0.0971	3.2503	0	0	0	0	1
0.0173	41.1413	0	0	0.3669	0	1
0.9748	48.3384	0	0	-0.3896	0	1
0.9749	56.0286	0	0	0.4065	0	1
0.9758	79.3920	0	0	-0.4361	0	1
0.9112	26.7175	0	0	0.2690	0	1

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What to do?

Dumb idea: Add explicit bounds $\epsilon \le x_i \le 1 - \epsilon$, $\epsilon > 0$.

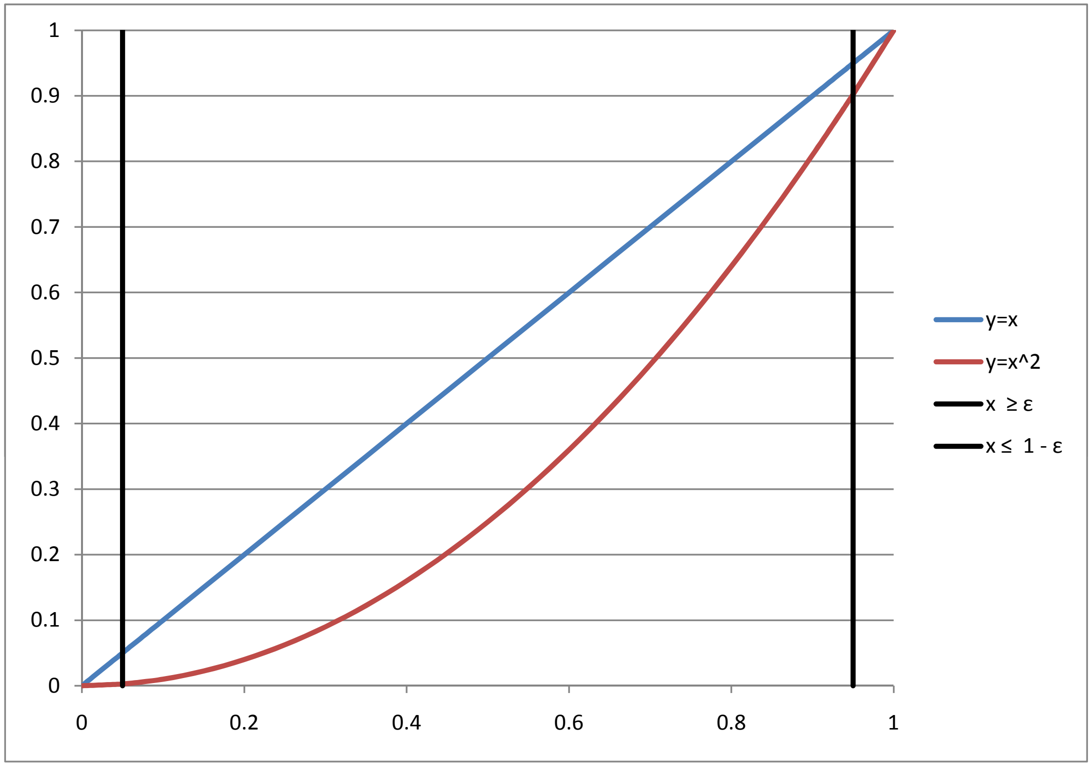

Figure 5: Tightened bound constraints using $\epsilon = .05$.

- Using $\epsilon > 0$ is *restriction* of original problem, but if constraints are tight can recover rigorous bound using Lagrange multipliers.

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Consider 30-060-3 with $\epsilon = .02$. Gap increases from 0.37% to 0.57%, but 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, $\epsilon = .02$

x	z_d	z_l	z_u	δ	l	u
0.9800	122.0003	0	66.5356	-0.4352	1	1
0.9800	68.0193	0	72.3112	0.3759	0.8978	1
0.8624	44.0950	0	0	-0.2870	0	1
0.6876	39.7575	0	0	-0.2531	0	1
0.9678	70.5789	0	0.0001	-0.3811	0	1
0.9800	122.5487	0	27.3048	-0.4355	1	1
0.9758	72.6318	0	0.0004	0.3850	0	1
0.9800	82.2755	0	60.2789	-0.4002	1	1
0.1965	27.3298	0	0	0	0	1
0.9711	42.5011	0	0.0002	0.2758	0	1
0.2380	22.5653	0	0	0	0	1
0.9800	91.9245	0	25.5476	-0.4118	1	1
0.9608	41.0645	0	0.0001	-0.2646	0	1
0.9800	51.3008	0	85.3841	0.3254	0.9134	1
0.0569	10.6306	0	0	0	0	1
0.2358	46.1886	0	0	-0.2999	0	1
0.9689	66.6622	0	0.0002	-0.3730	0	1
0.9800	51.3913	0	27.077	-0.3258	1	1
0.4823	26.9097	0	0	0	0	1
0.1110	26.7362	0	0	0	0	1
0.0852	38.1760	0	0	0.2374	0	1
0.0200	39.6029	15.4382	0	-0.2517	0	0
0.0756	33.6005	0	0	-0.1732	0	1
0.9800	71.7403	0	25.4883	-0.3834	1	1
0.1066	22.5000	0	0	0	0	1
0.0281	52.8366	0.0002	0	0.3318	0	1
0.9532	63.3240	0	0.0001	-0.3651	0	1
0.9519	70.3034	0	0.0001	0.3806	0	1
0.9639	77.2046	0	0.0001	-0.3928	0	1
0.8712	29.5291	0	0	0	0	1

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- Fix variables and re-solve with $\epsilon = 0$. Get exact optimal solution.
- 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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- 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.)
- Application to problems with constraints. Expect good effect of cuts from BQP_n on problems where multiple bound constraints are tight.

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