SDP versus RLT for Nonconvex QCQP

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1 The QCQP Problem

We consider a Quadratically Constrained Quadratic Programming problem of the form:

QCQP: max
$$x^T Q_0 x + a_0^T x$$

s.t. $x^T Q_i x + a_i^T x \leq b_i$, $i \in \mathcal{I}$
 $x^T Q_i x + a_i^T x = b_i$, $i \in \mathcal{E}$
 $l \leq x \leq u$,

where $x \in \Re^n$ and $\mathcal{I} \cup \mathcal{E} = \{1, \ldots, m\}$. The matrices Q_i are assumed to be symmetric. If $Q_i \leq 0$ for $i = 0, Q_i \geq 0$ for $i \in \mathcal{I}$ and $Q_i = 0$ for $i \in \mathcal{E}$, then QCQP is a convex optimization problem. In general however QCQP is NP-hard.

QCQP is a well-studied problem in the global optimization literature with many applications, frequently arising from Euclidean distance geometry.

2 RLT and SDP Relaxations

Relaxations of QCQP based on Semidefinite Programming (SDP) and the Reformulation-Linearlization Technique (RLT) both relax product terms $x_i x_j$ to an element X_{ij} of an $n \times n$ matrix X. The two relaxations differ in the form of the constraints on X.

Semidefinite Programming

The SDP relaxation of QCQP may be written

SDP: min
$$Q_0 \bullet X + a_0^T x$$

s.t. $Q_i \bullet X + a_i^T x \leq b_i, \quad i \in \mathcal{I}$
 $Q_i \bullet X + a_i^T x = b_i, \quad i \in \mathcal{E}$
 $l \leq x \leq u, \quad X - xx^T \succeq 0.$

It is very well known that the condition $X - xx^T \succeq 0$ is equivalent to

$$\tilde{X} := \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succeq 0,$$

and therefore SDP may be alternatively written in the form

SDP: min
$$\tilde{Q}_0 \bullet \tilde{X}$$

s.t. $\tilde{Q}_i \bullet \tilde{X} \le 0$, $i \in \mathcal{I}$
 $\tilde{Q}_i \bullet \tilde{X} = 0$, $i \in \mathcal{E}$
 $l \le x \le u$, $\tilde{X} \succeq 0$,

where

$$\tilde{Q}_i := \begin{pmatrix} -b_i & a_i^T/2 \\ a_i/2 & Q_i \end{pmatrix}.$$

Reformulation-Linearization Technique

The RLT relaxation of QCQP is based on forming products of the bound constraints $x_i - l_i \ge 0$ and $u_i - x_i \ge 0$, i = 1, ..., n. Forming all such possible products, and relaxing product terms $x_i x_j$ to X_{ij} , results in the system of constraints

$$X_{ij} - l_i x_j - l_j x_i \geq -l_i l_j,$$

$$X_{ij} - u_i x_j - u_j x_i \geq -u_i u_j,$$

$$X_{ij} - l_i x_j - u_j x_i \leq -l_i u_j,$$

$$X_{ij} - l_j x_i - u_i x_j \leq -l_j u_i,$$

i, j = 1, ..., n. Note that for i = j the two upper bounds on X_{ii} are the same. Using the fact that $X_{ij} = X_{ji}$, the result is an ordinary Linear Programming (LP) problem with n(n+1)/2 variables and a total of m + n(2n+3) constraints. For the purpose of interpretation it is helpful to write the constraints on X_{ij} in the alternative form

$$X_{ij} \geq x_i x_j - (x_i - l_i)(x_j - l_j), X_{ij} \geq x_i x_j - (u_i - x_i)(u_j - x_j), X_{ij} \leq x_i x_j + (x_i - l_i)(u_j - x_j), X_{ij} \leq x_i x_j + (u_i - x_i)(x_j - l_j).$$

Comparison between SDP and RLT

To compare the SDP and RLT relaxations it is useful to consider the principal submatrix of \tilde{X} corresponding to two variables x_i and x_j . Taking i = 1 and j = 2 w.l.o.g., let

$$\tilde{X}^{12} = \begin{pmatrix} 1 & x_1 & x_2 \\ x_1 & X_{11} & X_{12} \\ x_2 & X_{12} & X_{22} \end{pmatrix}.$$

It is then straightforward to show that the condition $\tilde{X}^{12} \succeq 0$, from SDP, is equivalent to the constraints

$$X_{ii} \geq x_i^2, \quad i = 1, 2,$$

$$X_{12} \leq x_1 x_2 + \sqrt{(X_{11} - x_1^2)(X_{22} - x_2^2)},$$

$$X_{12} \geq x_1 x_2 - \sqrt{(X_{11} - x_1^2)(X_{22} - x_2^2)}.$$

Proposition. Consider the SDP and RLT constraints on X_{11} , X_{22} and X_{12} for values of x_i satisfying $l_i \leq x_i \leq u_i$, i = 1, 2. Then:

1. SDP implies no upper bound on X_{ii} , i = 1, 2 compared to the RLT upper bounds

$$X_{ii} \le x_i^2 + (x_i - l_i)(u_i - x_i).$$

2. The SDP lower bounds $X_{ii} \ge x_i^2$, i = 1, 2 dominate the RLT lower bounds

$$X_{ii} \ge x_i^2 - (x_i - l_i)^2, \quad X_{ii} \ge x_i^2 - (u_i - x_i)^2.$$

3. The SDP bounds on X_{12} dominate the RLT bounds on X_{12} if for i = 1, 2

$$X_{ii} \le x_i^2 + (x_i - l_i)^2, \quad X_{ii} \le x_i^2 + (u_i - x_i)^2.$$

Proof of part 3: Assume that $X_{ii} \leq x_i^2 + (x_i - l_i)^2$, i = 1, 2. Then

$$(x_i - l_i)^2 \geq X_{ii} - x_i^2, \quad i = 1, 2$$

$$(x_i - l_i) \geq \sqrt{X_{ii} - x_i^2}, \quad i = 1, 2$$

$$(x_1 - l_1)(x_2 - l_2) \geq \sqrt{(X_{11} - x_1^2)(X_{22} - x_2^2)}.$$

It follows that the SDP lower bound

$$X_{12} \ge x_1 x_2 - \sqrt{(X_{11} - x_1^2)(X_{22} - x_2^2)}$$

can be no worse than the RLT lower bound

$$X_{12} \ge x_1 x_2 - (x_1 - l_1)(x_2 - l_2).$$

The analysis for the other RLT bounds is similar. \Box

Remark. If $x_i = (l_i + u_i)/2$, i = 1, 2 then the SDP bounds on X_{12} dominate the RLT bounds for all X_{ii} that satisfy the RLT upper bounds in part 1. In this case can compute that the 3-dimensional volume of the intersection of the SDP and RLT constraints on X_{11}, X_{22}, X_{12} is $(u_1 - l_1)^3(u_2 - l_2)^3/72$, compared to $(u_1 - l_1)^3(u_2 - l_2)^3/8$ for RLT constraints alone. So for these "midpoint" values of x_i , adding SDP decreases volume by a factor of 9.



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



Figure 2: RLT versus SDP+RLT regions, $0 \le x \le e, x_1 = .1, x_2 = .5$.



Figure 3: RLT versus SDP+RLT regions, $0 \le x \le e, x_1 = .1, x_2 = .9$.



Figure 4: RLT versus SDP+RLT regions, $0 \le x \le e, x_1 = .9, x_2 = .99$.

3 Computational Results I: Box-constrained QP

Consider 15 box-constrained QP problems with n = 30, from Vandenbussche and Nemhauser (2003). Density of Q_0 varies from 60% to 100%. Compare bounds from Vandenbussche and Nemhauser polyhedral relaxation PS, BARON, RLT, SDP, and SDP+RLT. (Results for BARON are at root after tightening - courtesy of Dieter Vandenbusshe. SDP includes upper bound on diagonal components X_{ii} .)

Problem	Optimal	Bound value				SDP+	Gap to optimal value				SDP+
instance	value	RLT	BARON	\mathbf{PS}	SDP	RLT	RLT	BARON	\mathbf{PS}	SDP	RLT
30-60-1	706.00	1454.75	1430.20	1405.25	768.12	714.67	106.06%	102.58%	99.04%	8.80%	1.23%
30-60-2	1377.17	1699.50	1668.51	1637.00	1426.94	1377.17	23.41%	21.15%	18.87%	3.61%	0.00%
30-60-3	1293.50	2047.00	2006.83	1966.00	1370.13	1298.21	58.25%	55.15%	51.99%	5.92%	0.36%
30-70-1	654.00	1569.00	1547.43	1525.50	746.43	674.00	139.91%	136.61%	133.26%	14.13%	3.06%
30-70-2	1313.00	1940.25	1888.67	1836.25	1375.07	1313.00	47.77%	43.84%	39.85%	4.73%	0.00%
30-70-3	1657.40	2302.75	2251.55	2199.50	1719.77	1657.55	38.94%	35.85%	32.71%	3.76%	0.01%
30-80-1	952.73	2107.50	2072.29	2036.50	1050.76	965.25	121.21%	117.51%	113.75%	10.29%	1.31%
30-80-2	1597.00	2178.25	2158.29	2138.00	1622.81	1597.00	36.40%	35.15%	33.88%	1.62%	0.00%
30-80-3	1809.78	2403.50	2376.47	2349.00	1836.79	1809.78	32.81%	31.31%	29.79%	1.49%	0.00%
30-90-1	1296.50	2423.50	2385.44	2346.75	1348.48	1296.50	86.93%	83.99%	81.01%	4.01%	0.00%
30-90-2	1466.84	2667.00	2623.11	2578.50	1527.87	1466.84	81.82%	78.83%	75.79%	4.16%	0.00%
30-90-3	1494.00	2538.25	2499.69	2460.50	1516.81	1494.00	69.90%	67.32%	64.69%	1.53%	0.00%
30-100-1	1227.13	2602.00	2541.99	2481.00	1285.74	1227.13	112.04%	107.15%	102.18%	4.78%	0.00%
30-100-2	1260.50	2729.25	2699.12	2668.50	1365.32	1261.08	116.52%	114.13%	111.70%	8.32%	0.05%
30-100-3	1511.05	2751.75	2704.14	2655.75	1611.11	1513.08	82.11%	78.96%	75.76%	6.62%	0.13%
Ave	rage						76.94%	73.97%	70.95%	5.58%	0.41%

Table 1: Comparison of bounds for indefinite box-constrained QP Problems

4 Computational Results II: Circle Packing

Consider the problem of maximizing the radius of n non-overlapping circles packed into the unit square in \Re^2 . Via a simple, well-known transformation this is equivalent to the "point packing" problem

$$\max \theta \text{s.t.} \quad (x_i - x_j)^2 + (y_i - y_j)^2 \ge \theta, \quad 1 \le i < j \le n \quad 0 \le x \le e, \quad 0 \le y \le e.$$

Note that:

- 1. The variable θ represents the minimum squared distance separating n points in the unit square. The corresponding radius for n circles that can be packed into the unit square is $\sqrt{\theta}/[2(1+\sqrt{\theta})]$.
- 2. The problem formulation involves no terms of the form $x_i y_j$. As a result, the RLT and SDP bounds can both be based on matrices X and Y relaxing xx^T and yy^T , respectively.
- 3. Let $n_x = \lceil n/2 \rceil$, $n_y = \lceil n_x/2 \rceil$. By symmetry could assume $.5 \le x_i \le 1, i = 1, \ldots, n_x$ and $.5 \le y_i \le 1, i = 1, \ldots, n_y$.





radius = 0.174457630187 density = 0.669310826841 distance = 0.535898384862 contacts = 14



radius = 0.170540688701 density = 0.730963825254 distance = 0.517638090205 contacts = 20 © R.SPECHT 10-58P-1999

N = 11

N = 9



radius = 0.166666666667 density = 0.785398163397 distance = 0.50000000000 contacts = 24

N = 1010 circles in the unit square

radius = 0.148204322565 density = 0.690035785264 @ X.Secor distance = 0.421279543984 contacts = 21



radius = 0.142399237696 density = 0.700741577756 distance = 0.398207310237 contacts = 20

N = 1212 circles in the unit square



Conjecture. Consider the RLT and SDP relaxations of the point packing problem for $n \ge 2$, where the SDP relaxation includes the upper bounds on X_{ii} and Y_{ii} . Then:

- 1. The optimal value for the RLT relaxation is 2.
- 2. The optimal value for the SDP relaxation is $1 + \frac{1}{n-1}$ and adding the RLT constraints does not change this value.
- 3. For $n \ge 5$ the optimal value for the RLT relaxation using symmetry is $\frac{1}{2}$.
- 4. For $n \ge 5$ the optimal value for the SDP relaxation using symmetry is

$$.25 + \frac{1}{4\lfloor (n-1)/4 \rfloor},$$

equal to $.25 + \frac{1}{n-1}$ if n-1 is divisible by 4.

Additional RLT constraints based on order

Note that one could assume w.l.o.g. that $x_1 \ge x_2 \ge \ldots \ge x_n$. Adding these constraints alone has no effect on the SDP or RLT relaxations. However, one can generate new RLT constraints by taking products of these constraints with each other and/or the original bound constraints. To limit the number of additional constraints, we consider the inequalities

$$x_i \ge x_{i+1} \quad i = 1, \dots, n-1$$

and the constraints that result from products with the upper and lower bounds on x_i and x_{i+1} . This gives a total of 5(n-1) additional constraints. (If the tightened bounds based on symmetry are also used then the first n_y components of x are treated as a separate block from the remaining $n - n_y$ components.)

Conjecture. Consider the RLT and SDP relaxations of the point packing problem for $n \ge 2$, where the SDP relaxation includes the upper bounds on X_{ii} and Y_{ii} . Then:

- 1. The optimal value for the RLT relaxation with the additional order constraints is $1 + \frac{1}{n-1}$.
- 2. For $n \geq 5$ the optimal value for the RLT relaxation using symmetry and the additional order constraints is

$$.25 + \frac{1}{4\lfloor (n-1)/4 \rfloor}.$$

3. For $n \ge 9$ the optimal value for the SDP relaxation using symmetry and the additional order constraints is strictly less than that of the RLT relaxation using symmetry and the additional order constraints.



5 What Next?

- 1. Lower bound on volume reduction (X_{ii}, X_{jj}, X_{ij}) for RLT+SDP compared to RLT.
- 2. Alternative treatment of symmetry/order in point packing problem.
- 3. Dynamic generation of constraints for RLT+SDP.
- 4. Additional Euclidean distance problems (protein folding local refinement).