Bilinear GDP Relaxation Technique for nonconvex Quadratically Constrained Quadratic Programs

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Many problems in industry can be modeled as QCQP (e.g. scheduling of blending operations, water treatment networks, etc.)

These QCQPs are often non convex and NP hard to solve, leading to the need of global optimization techniques.

Although problems of small size can be handled, large scale models often find difficulties to be solved to global optimality.

Improvements on the solution methods for non convex QCQPs are still necessary
Solution of non-convex problems

- Classical optimization approaches to the global optimum problem result in local optimal solutions.
- Even in the case where a global solution is obtained, classical optimization cannot guarantee global optimality.

Deterministic global optimization techniques should be used.

Can we obtain a good relaxation for QCQP by using bilinear GDP?

(guaranteed global optimality)
Goal of this work

**GOAL:** Obtain tighter relaxations for **QCQP** by using **Bilinear GDP**
The QCQP Problem

General formulation of a Quadratically Constrained Quadratic Program:

\[
\text{QCQP: } \quad \min \begin{array}{l}
    x^TQ_0x + a_0^Tx \\
    x^TQ_ix + a_i^Tx = b_i, \quad i \in E \\
    x^TQ_ix + a_i^Tx \leq b_i, \quad i \in I
\end{array}
\]

where \( x \in \mathbb{R}^n \) and \( I \cup E = \{1, \ldots, m\} \)

Convex QCQP:

In the particular case when \( Q_i \succeq 0 \) for \( i \in I \) and \( i = 0 \), and \( Q_i = 0 \) for \( i \in E \) QCQP is a convex optimization problem

In general QCQP is a non-convex NP hard problem
QCQP Applications

Facility location problems

\[
\min \sum_i \sum_j \rho_{ij} \\
\text{s.t. } \rho_{ij} \geq \sigma_i \ \forall \ i, \forall \ j
\]

Where \( \rho_{ij} = (x_j - x_i)^2 + (y_j - y_i)^2 \) \( \forall \ i, j \)

Chemical Engineering Design problems

Water Treatment Network Design

Heat Exchanger Network Design

\[ \sum_{i \in S_k} \zeta_i = 1 \quad f_i = \zeta_i f_k \]

\[ C P f_i \Delta T_i = \Delta H \]
QCQP Solution Methods

Convex QCQP:

- **Interior Point Methods** have shown good performance, (Interior Point Methods in Convex programming, vol. 13 of Studies in Applied Mathematics, 1994)

  - Recast as a SDP (Semidefinite Program) and use an **Interior Point Method** (Vandenverghe and Boyd, 1996)

Non-Convex QCQP:

- For some particular cases there are specialized algorithms. (e.g. Minimization of a non-convex quadratic function over an sphere, Hager (2001)).

- In general use spatial branch and bound algorithms

Remarks:  
- Efficient spatial branch and bound algorithms need good relaxations

  - Good relaxations for non-convex QCQP can be obtained by using:
    1- **Semidefinite Programming** (Vandenverghe and Boyd, 1996)
    2- **Reformulation-Linearization Techniques** (Sherali and Alameddine, 1991)

The goal of this presentation is to show that by reformulating the QCQP as a bilinear GDP, good relaxations can also be derived
Bilinear Generalized Disjunctive Programs

How can we reformulate a QCQP as a Bilinear GDP?
QCQP reformulation as a bilinear GDP
(Bergamini & Grossmann, 2005)

Clearly both formulations define the same feasible region

\[ xy + x = \alpha \]
\[ x_{lo} \leq x \leq x_{up} \]
\[ y_{lo} \leq y \leq y_{up} \]

\[ f + x = \alpha \]
\[ f = xy \]
\[ x_{lo} \leq x \leq x^{*} \]
\[ y_{lo} \leq y \leq y_{up} \]
\[ Y_{1,2} \{True,False\} \]

How do we obtain good relaxations for Bilinear GDP?
Relaxation of bilinear GDP
(Ruiz & Grossmann, 2007)

Example:

Bilinear GDP  →  Linear GDP  →  Reformulated Linear GDP  →  Tighter LP

Bilinear terms relaxation (McCormick envelopes)  Basic Steps  Convex Hull Relaxation
Traditional QCQP Relaxation Technique

Illustrative Example

\[
\begin{align*}
xy & \leq \alpha \\
ax + by & \leq c \\
x_{lo} & \leq x \leq x_{up} \\
y_{lo} & \leq y \leq y_{up}
\end{align*}
\]

McCormick Envelopes

Traditional Approach

\[
\begin{align*}
f & \leq \alpha \\
f & \leq xy_{lo} + yx_{up} - y_{lo}x_{up} \\
f & \leq xy_{up} + yx_{lo} - y_{up}x_{lo} \\
f & \geq xy_{up} + yx_{up} - x_{up}y_{up} \\
f & \geq xy_{lo} + yx_{lo} - x_{lo}y_{lo}
\end{align*}
\]

\[
\begin{align*}
ax + by & \leq c \\
x_{lo} & \leq x \leq x_{up} \\
y_{lo} & \leq y \leq y_{up}
\end{align*}
\]
Bilinear GDP Relaxation proposed

**Proposed Relaxation**

\[ \begin{align*}
xy & \leq \alpha \\
ax + by & \leq c \\
x_{lo} & \leq x \leq x_{up} \\
y_{lo} & \leq y \leq y_{up}
\end{align*} \]

**Bilinear GDP Reformulation**
(Bergamini & Grossmann)

\[ \begin{align*}
Y_1 & \\
Y_2 & \\
\begin{cases}
    f = xy & \\
    x \leq x^* \leq x_{up} & \\
    y \leq y_{lo} & \\
    y \leq y_{up} & \\
\end{cases}
\end{align*} \]

**McCormick Relaxation**

\[ \begin{align*}
f & \leq \alpha \\
ax + by & \leq c \\
f & \leq \alpha \\
ax + by & \leq c \\
\begin{cases}
y \leq y_{lo} & \\
y \leq y_{up} & \\
x \leq x_{lo} & \\
x \leq x_{up} & \\
\end{cases}
\end{align*} \]

**Basic Steps**
(Sawaya & Grossmann)

\[ \begin{align*}
Y_{lo} & \leq Y \leq Y_{up} \\
Y_{1,2} & \{True,False\}
\end{align*} \]

The convex hull relaxation leads to a **tighter** linear program.
Comparison between the traditional relaxation and the proposed approach

\[ f \leq \alpha \]
\[ f \leq ax + by \leq c \]
\[ x_{lo} \leq x \leq x_{up} \]
\[ y_{lo} \leq y \leq y_{up} \]

Clearly the relaxation given by the traditional approach is dominated by the bilinear GDP relaxation
Summary of the methodology proposed

• **Step 1**: Reformulate the QCQP as a Bilinear GDP by defining each bilinear term through a disjunction.

• **Step 2**: Relax the bilinear terms by using the McCormick envelopes considering the bounds defined in each disjunct.

• **Step 3**: Apply a set of “basic steps” by introducing the linear and (linearized) bilinear constraints inside the disjunctions.

• **Step 4**: Relax the new obtained bilinear GDP using the convex hull relaxation.
The improvement in the relaxation is clear but still there are some questions to answer...

### Computational Results

<table>
<thead>
<tr>
<th>Problem characteristics</th>
<th>Solution</th>
<th>McCormick Relaxation</th>
<th>Bilinear GDP Relaxation</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>Lower Bound</td>
<td>Lower Bound</td>
</tr>
<tr>
<td>mi</td>
<td>mb</td>
<td>n</td>
<td>nb</td>
</tr>
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<td>3</td>
<td>9</td>
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### Number of nodes

<table>
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<tr>
<th></th>
<th>BARON + BGDP Relaxation</th>
<th>BARON (standard)</th>
<th>Improvement</th>
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<tbody>
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Conclusions and Remarks

• Non-convex QCQP are present in many fields (e.g. optimization of systems that include blending, splitting, distillation, etc.).

• Non-convex QCQP are usually solved by spatial branch and bound methods and hence good relaxations are necessary.

• Bilinear GDP relaxation has shown to improve the relaxation given by the traditional approaches (by using McCormick envelopes)

• The side effect of good relaxations is often the increase of the size of the problems. Hence, wise implementations should be carried out...

• This method has many parameters that we can/should define (i.e. 1- Grid Size and Type 2- Set of Bilinear Terms 3- Set of Constraints, etc). But how?

• Efficient algorithms that take advantage of the relaxation obtained by Bilinear GDP relaxation still need to be developed....