Bilinear GDP Relaxation Technique for nonconvex Quadratically Constrained Quadratic Programs

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Motivation

- **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***

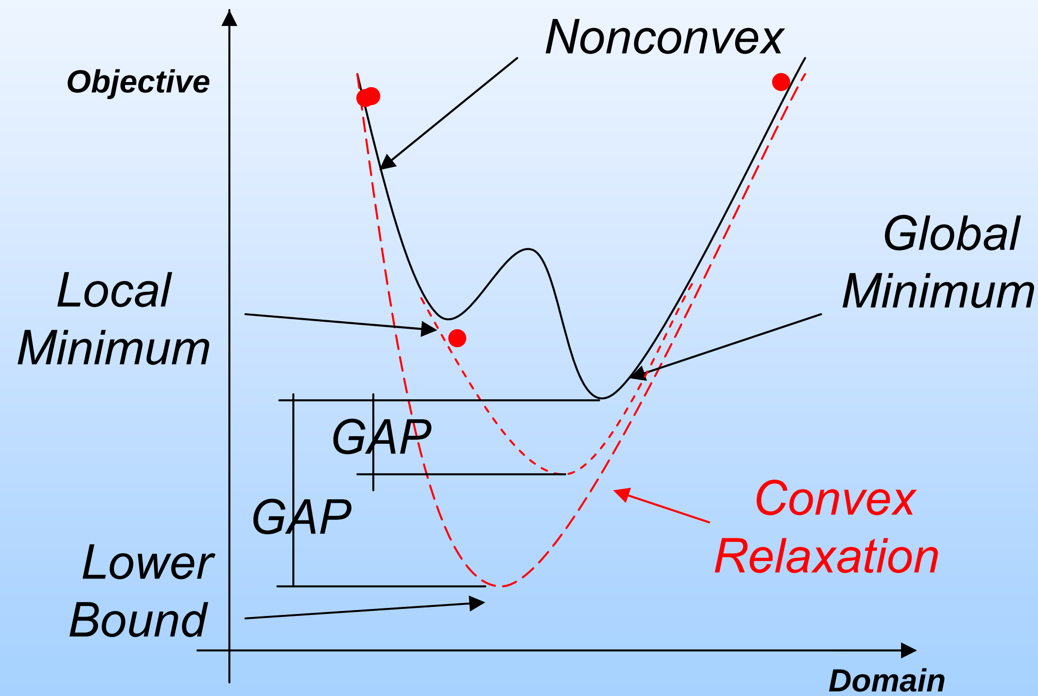
Solution of non-convex problems

- **Classical optimization approaches** used to solve nonconvex problems usually lead to **local optimal solutions**

- **Deterministic optimization approaches** often find the global optimum by **approximating** sequentially the nonconvex problem with a convex **relaxation**
- Even in the case where a global solution is obtained **classical optimization cannot guarantee global optimality**

Finding better **relaxations** is one of the **key** elements in **Global Optimization algorithms**

- The **tighter** the **relaxation** the **closer** the **gap** between the lower bound and the global optimal solution



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

(guaranteed global optimality)

Goal of this work

QCQP can be reformulated as a bilinear GDP
(Bergamini & Grossmann, 2005)

Good relaxations for bilinear GDP are known
(Ruiz & Grossmann, 2007)

Bilinear GDP relaxation for QCQP

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

The QCQP Problem

General formulation of a Quadratically Constrained Quadratic Program:

QCQP:

$$\min \quad \boxed{x^T Q_0 x + a_0^T x} \longrightarrow \text{Quadratic objective function}$$

$$\boxed{\begin{array}{ll} x^T Q_i x + a_i^T x = b_i\,, & i \in E \\ x^T Q_i x + a_i^T x \le b_i\,, & i \in I \end{array}} \longrightarrow \text{Quadratic constraints}$$

$$l \le x \le u$$

$$\text{where } x \in R^n \text{ and } I \cup E = \{1, \ldots, m\}$$

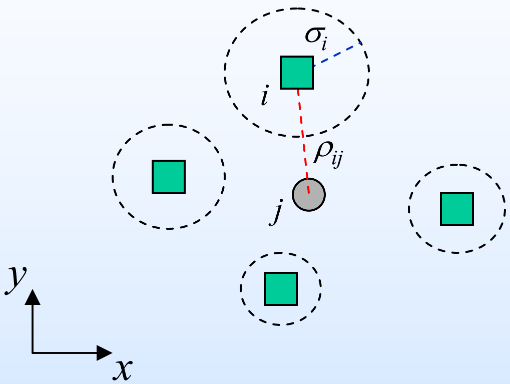
Convex QCQP:

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



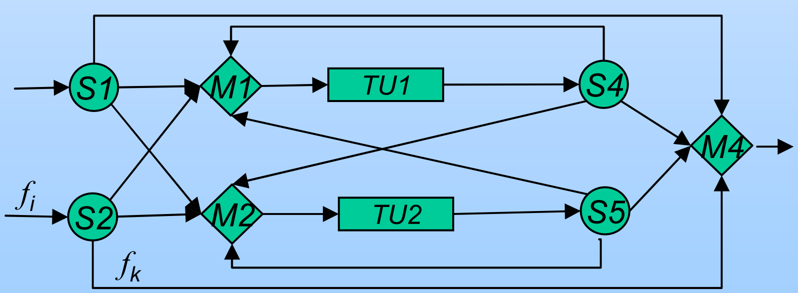
$$\min \quad \sum_i \sum_j \rho_{ij}$$

$$s.t. \quad \rho_{ij} \geq \sigma_i \quad \forall i, \forall j$$

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

Chemical Engineering Design problems

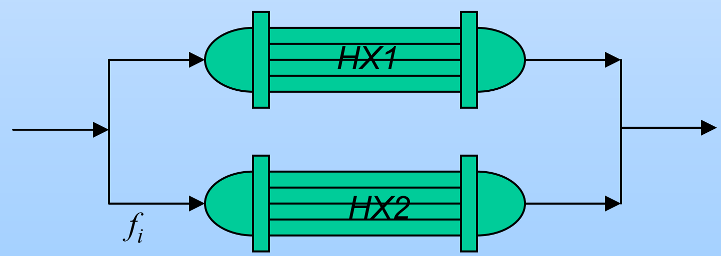
Water Treatment Network Design



Splitter Model

$$\sum_{i \in S_k} \zeta_i^k = 1 \qquad f_i = \zeta_i^k f_k$$

Heat Exchanger Network Design



Heat Exchanger Model

$$CPf_i \Delta T_i = \Delta H$$

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

$$Min\ \ Z = \boxed{f(x)} + \sum_{k \in K} c_k$$ → **Objective Function**

$$s.t.\ \ \boxed{g(x)} \le 0$$ → **Global Constraints**

$$\bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ \boxed{r_{ik}(x)} \le 0 \\ c_k = \gamma_{ik} \end{bmatrix}$$ → **Disjunctions** $k \in K$

$$\Omega(Y) = True$$ → **Logic Propositions**

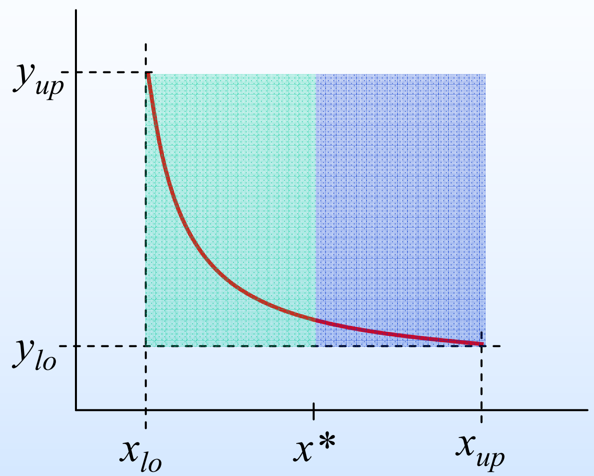
$$x \in R^n, c_k \in R, Y_{ik} \in \{True, False\} \qquad i \in D_k\ ,\ k \in K$$

Bilinearities

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***

QCQP

$$\boxed{xy} + x = \alpha$$

$$x_{lo} \le x \le x_{up}$$

$$y_{lo} \le y \le y_{up}$$

Bilinear GDP

$$f + x = \alpha$$

$$\begin{bmatrix} Y_1 \\ f = xy \\ x_{lo} \le x \le x^* \\ y_{lo} \le y \le y_{up} \end{bmatrix} \veebar \begin{bmatrix} Y_2 \\ f = xy \\ x^* \le x \le x_{up} \\ y_{lo} \le y \le y_{up} \end{bmatrix}$$

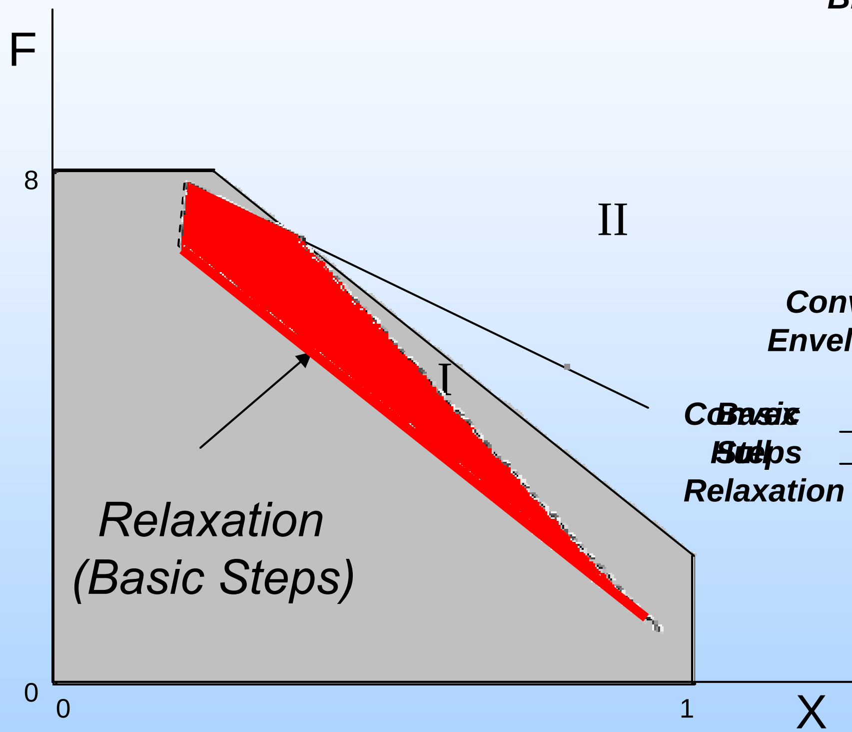
$$Y_{1,2}\ \{True, False\}$$

*How do we obtain **good relaxations** for **Bilinear GDP** ?*

Relaxation of bilinear GDP

(Ruiz & Grossmann, 2007)

Example:



Bilinear Terms

Max Z = $\theta P X - \gamma F - CP$

s.t. $P \le d$

Convex Envelopes

Basic Steps Relaxation

$$\left[\begin{array}{c} Y_{11} \\ P \le F.X^{LO} + F^{UP}.X - F^{UP}.X^{LO} \\ P \le F.X^{UP} + F^{LO}.X - F^{LO}.X^{UP} \\ P \ge F.X^{LO} + F^{LO}.X - F^{LO}.X^{LO} \\ P \ge F.X^{UP} + F^{UP}.X - F^{UP}.X^{UP} \\ F = \alpha_1 X + \beta_1 \\ X_1^{LO} \le X \le X_1^{UP} \\ CP = Cp_1 \end{array}\right] \vee \left[\begin{array}{c} Y_{21} \\ P \le d \\ P \le F.X^{UP} + F^{LO}.X - F^{LO}.X^{UP} \\ P \le F.X^{LO} + F^{UP}.X - F^{UP}.X^{LO} \\ P \ge F.X^{LO} + F^{LO}.X - F^{LO}.X^{LO} \\ P \ge F.X^{UP} + F^{UP}.X - F^{UP}.X^{UP} \\ F = \alpha_2 X + \beta_2 \\ X_2^{LO} \le X \le X_2^{UP} \\ CP = Cp_2 \end{array}\right]$$

$Y_{11} \vee Y_{21} = True$

$CP, X, F \in R$

$F^{LO} \le F \le F^{UP}$

$Y_{11}, Y_{21} \in \{True, False\}$

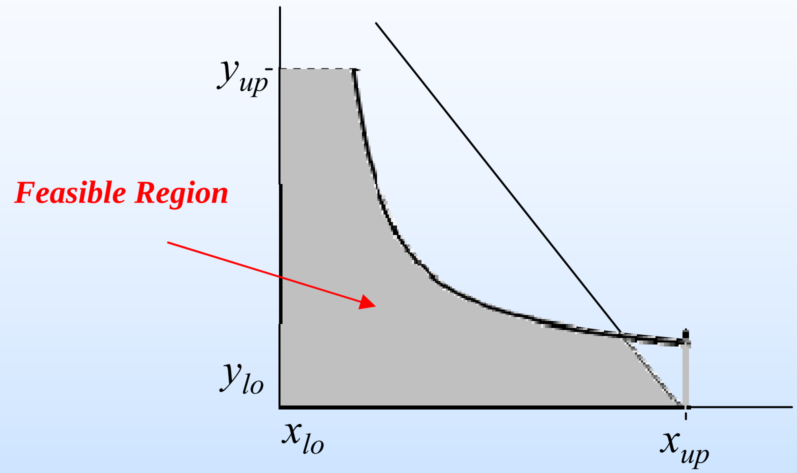
Bilinear GDP → *Linear GDP* → *Reformulated Linear GDP* → *Tighter LP*

Bilinear terms relaxation (McCormick envelopes) — *Basic Steps* — *Convex Hull Relaxation*

Traditional QCQP Relaxation Technique

Illustrative Example

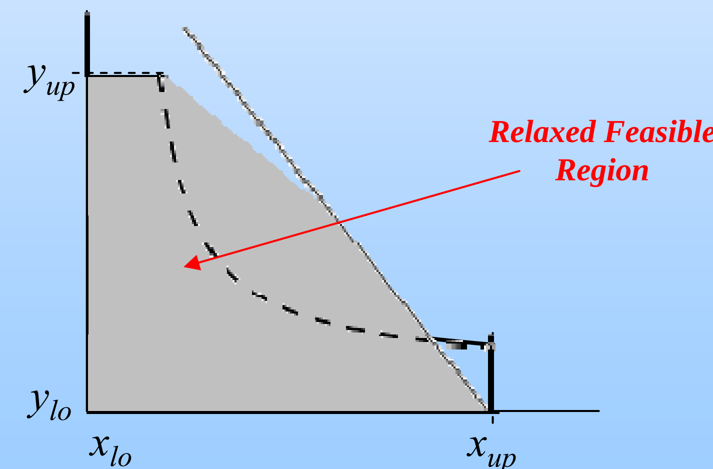
$$\boxed{xy} \le \alpha$$
$$ax + by \le c$$
$$x_{lo} \le x \le x_{up}$$
$$y_{lo} \le y \le y_{up}$$



McCormick Envelopes

Traditional Approach

$$f \le \alpha$$
$$\boxed{\begin{aligned} f &\le xy_{lo} + yx_{up} - y_{lo}x_{up} \\ f &\le xy_{up} + yx_{lo} - y_{up}x_{lo} \\ f &\ge xy_{up} + yx_{up} - x_{up}y_{up} \\ f &\ge xy_{lo} + yx_{lo} - x_{lo}y_{lo} \end{aligned}}$$
$$ax + by \le c$$
$$x_{lo} \le x \le x_{up}$$
$$y_{lo} \le y \le y_{up}$$



Bilinear GDP Relaxation proposed

Proposed Relaxation

$$
\begin{gathered}
xy \le \alpha \\
ax+by \le c \\
x_{lo} \le x \le x_{up} \\
y_{lo} \le y \le y_{up}
\end{gathered}
$$

Bilinear GDP Reformulation
(Bergamini & Grossmann)

$$
\begin{gathered}
f \le \alpha \\
ax+by \le c \\
\begin{bmatrix} Y_1 \\ f = xy \\ x_{lo} \le x \le x^* \end{bmatrix} \veebar \begin{bmatrix} Y_2 \\ f = xy \\ x^* \le x \le x_{up} \end{bmatrix} \\
y_{lo} \le y \le y_{up} \\
Y_{1,2}\ \{True, False\}
\end{gathered}
$$

McCormick Relaxation

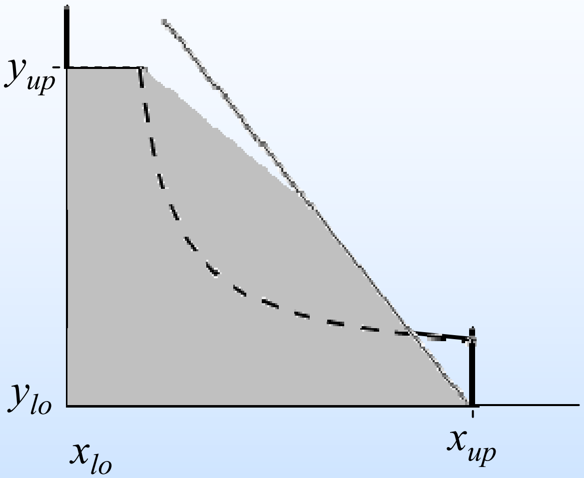
$$
\begin{gathered}
f \le \alpha \\
ax+by \le c \\
\begin{bmatrix} Y_1 \\ f \le xy_{up} + yx_{lo} - x_{lo}y_{up} \\ f \le xy_{lo} + yx^* - y_{lo}x^* \\ f \ge xy_{lo} + yx_{lo} - y_{lo}x_{lo} \\ f \ge yx^* + xy_{up} - x^*y_{up} \\ x_{lo} \le x \le x^* \end{bmatrix} \veebar \begin{bmatrix} Y_2 \\ f \le xy_{up} + yx^* - x^*y_{up} \\ f \le xy_{lo} + yx_{up} - y_{lo}x_{up} \\ f \ge xy_{lo} + yx^* - y_{lo}x^* \\ f \ge yx_{up} + xy_{up} - x_{up}y_{up} \\ x^* \le x \le x_{up} \end{bmatrix} \\
y_{lo} \le y \le y_{up} \\
Y_{1,2}\ \{True, False\}
\end{gathered}
$$

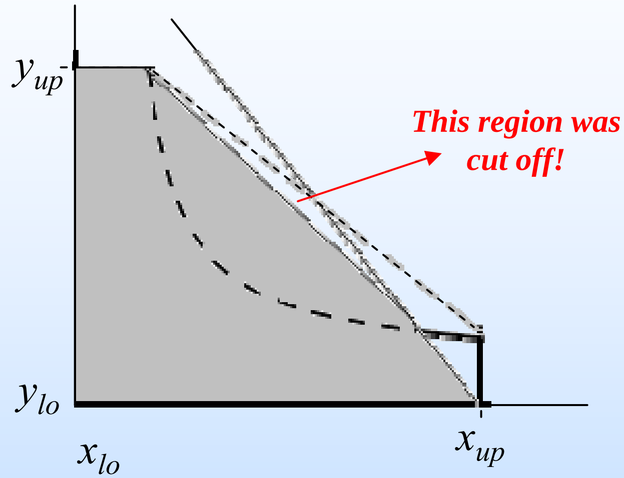
Basic Steps
(Sawaya & Grossmann)

$$
\begin{gathered}
\begin{bmatrix} Y_1 \\ ax+by \le c \\ f \le \alpha \\ f \le xy_{up} + yx_{lo} - x_{lo}y_{up} \\ f \le xy_{lo} + yx^* - y_{lo}x^* \\ f \ge xy_{lo} + yx_{lo} - y_{lo}x_{lo} \\ f \ge yx^* + xy_{up} - x^*y_{up} \\ x_{lo} \le x \le x^* \end{bmatrix} \veebar \begin{bmatrix} Y_2 \\ ax+by \le c \\ f \le \alpha \\ f \le xy_{up} + yx^* - x^*y_{up} \\ f \le xy_{lo} + yx_{up} - y_{lo}x_{up} \\ f \ge xy_{lo} + yx^* - y_{lo}x^* \\ f \ge yx_{up} + xy_{up} - x_{up}y_{up} \\ x^* \le x \le x_{up} \end{bmatrix} \\
y_{lo} \le y \le y_{up} \\
Y_{1,2}\ \{True, False\}
\end{gathered}
$$

The convex hull relaxation leads to
*a **tighter** linear program*

Comparison between the traditional relaxation and the proposed approach





$$f \le \alpha$$
$$f \le xy_{lo} + yx_{up} - y_{lo}x_{up}$$
$$f \le xy_{up} + yx_{lo} - y_{up}x_{lo}$$
$$f \ge xy_{up} + yx_{up} - x_{up}y_{up}$$
$$f \ge xy_{lo} + yx_{lo} - x_{lo}y_{lo}$$
$$ax+by \le c$$
$$x_{lo} \le x \le x_{up}$$
$$y_{lo} \le y \le y_{up}$$

$$\left[\begin{array}{c} Y_1 \\ ax+by \le c \\ f \le \alpha \\ f \le xy_{up} + yx_{lo} - x_{lo}y_{up} \\ f \le xy_{lo} + yx^* - y_{lo}x^* \\ f \ge xy_{lo} + yx_{lo} - y_{lo}x_{lo} \\ f \ge yx^* + xy_{up} - x^* y_{up} \\ x_{lo} \le x \le x^* \end{array}\right] \underline{\vee} \left[\begin{array}{c} Y_2 \\ ax+by \le c \\ f \le \alpha \\ f \le xy_{up} + yx^* - x^* y_{up} \\ f \le xy_{lo} + yx_{up} - y_{lo}x_{up} \\ f \ge xy_{lo} + yx^* - y_{lo}x^* \\ f \ge yx_{up} + xy_{up} - x_{up}y_{up} \\ x^* \le x \le x_{up} \end{array}\right]$$

Convex hull relaxation

$$y_{lo} \le y \le y_{up}$$
$$Y_{1,2}\ \{True, False\}$$

*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**.

Computational Results

	Problem characteristics				Solution	McCormick Relaxation	Bilinear GDP Relaxation	
	ml	*mb*	*n*	*nb*		**Lower Bound**	**Lower Bound**	**Grid Size**
Quesada	4	7	5	9	-116491.47	-479594.5	-461071.79	3
ex2_1_9	1	0	10	22	-0.38	-2.2	-1.5	3
ex3_1_1	3	3	8	5	7049.38	2533.2	2592	10
ex5_2_2_case2	3	3	9	2	-600	-1200	-1200	10

	Number of nodes		
	BARON + BGDP Relaxation	*BARON (standard)*	*Improvement*
Quesada	11	17	**35%**
ex5_2_2_case2	19	27	**30%**
ex2_1_9*	1399	1813	**23%**
ex3_1_1*	45	180	**75%**

The improvement in the relaxation is clear but still there are some questions to answer…

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* ***<u>need to be developed</u>****….*