Fast computation of bounds in constrained quadratic integer programming

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Optimization, Game Theory, and Data Analysis
60 years of Manuel ☺
Wien, December 21, 2018

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Constrained Integer Quadratic Programming

Given a symmetric matrix Q, find

$$\begin{aligned} \min \quad & x^\top Qx + c^\top x = q(x) \\ & Ax = b \\ & x_i \in \{l_i, \ldots, u_i\} \quad i = 1, \ldots, n \end{aligned} \tag{CIQP}$$

with A $m \times n$ matrix, $b \in \mathbb{R}^m$.

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StQP

$$\begin{aligned} \min \quad & x^\top Qx = q(x) \\ & e^T x = 1 \\ & x_i \geq 0 \quad i = 1, \dots, n \end{aligned}$$

Foreword

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StQP is ....

- nonlinear enough to be hard
- smooth enough to be appealing
- combinatorics related to connect continuous and discrete communities
- copositive enough ......to think positive !

However **Integer StQP is easy**

In this talk I focus on the how to define lower bounds for CIQP that

- can be computed quickly
- can be embedded effectively in a fast branch-and-bound procedure

This is a review of a joint research with Christoph Buchheim, Marianna De Santis, Mauro Piacentini and (new entry) Giorgio Grani




Branch and bound algorithm

Branch...

- **Branching rule:**
  - ▷ The order in which **primal** variables are fixed is **predetermined** (suitable for small domains $\{l, \ldots, u\}$)
- [Buchheim, Caprara, Lodi - Math. Progr. (2012)]

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  - ▷ Once all the integer variables are fixed, an **integer feasible solution** is found and the current upper bound can be eventually updated

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...and Bound

- **Upper bound (incumbent) computation:**
  - ▷ Once all the integer variables are fixed, an **integer feasible solution** is found and the current upper bound can be eventually updated
- **Lower bound computation:**
  - ▷ **Solve** the **dual problem of a continuous relaxation**

Drawing inspiration from unconstrained case

Consider the unconstrained case with $Q \not\succeq 0$

$$\begin{array}{ll} \min & x^\top Q x + c^\top x \\ & x \in \{l, \dots, u\}^n \end{array} \qquad \text{(IQP)}$$

The **continuous relaxation** of this problem,

$$\begin{array}{ll} \min & q(x) = x^\top Q x + c^\top x \\ \text{s.t.} & l \le x \le u \\ & x \in \mathbb{R}^n \end{array}$$

is an **NP-hard problem** in the case $Q \not\succeq 0$.

Continuous relaxation of the problem

Find an ellipsoid

$$\mathcal{E}(H)$$

such that

$$[l, u] \subseteq \mathcal{E}(H) = \{x \in \mathbb{R}^n \mid (x - x^0)^\top H(x - x^0) \leq 1\},$$

where $H \succeq 0$ and x^0 denotes the center of the ellipsoid.

Obtain a lower bound by solving

$$\begin{array}{ll} \min & q(x) = x^\top Q x + c^\top x \\ & x \in \mathcal{E}(H) \,. \end{array}$$

Ellipsoidal relaxation

$$\begin{array}{ll} \min & q(x) = x^\top Q x + c^\top x \\ \text{s.t.} & x \in \mathcal{E}(H) \, . \end{array}$$

- (Global) minimize a non-convex $q(x)$ over $\mathcal{E}(H)$ can be done efficiently: in P
  [Vavasis, 1991], [Ye, 1991]
- Strong duality holds
  [Conn, Gould, Toint - SIAM (2000)]; [Moré - OMS (1993)]; [Rendl, Wolkowicz - MP (1997)]; [Pong, Wolkowicz - COAP (2014)]; ...
- Efficient algorithm that provides dual bound

$$(Q + \lambda H)x = -c \qquad \lambda \geq 0 \qquad Q + \lambda H \succeq 0$$

[Moré, Sorensen - SIAM J. Sci. Statist. Comput. (1983)]

We look for the best ellipsoid

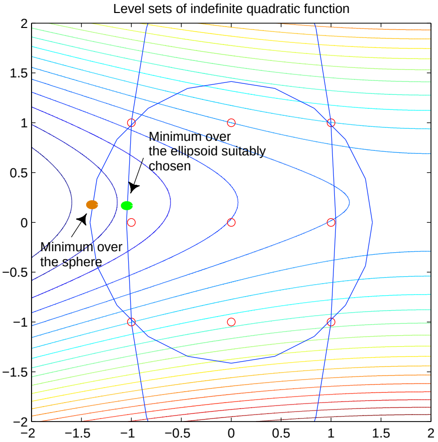

Figure : Different choices of the ellipsoid $\mathcal{E}(H)$ give rise to different bounds.

We look for the best ellipsoid

In a preprocessing phase, we compute an approximated solution of the following problem:

$$\max_{H \in \mathcal{H}_{diag}} \; q^*(H)$$

where $\mathcal{H}_{diag}$ defines a closed simplex in $\mathbb{R}^n$

$$\mathcal{H}_{diag} := \left\{ H \succeq 0 \mid H = \mathrm{Diag}(h), \; \sum_{i=1}^{n} h_i = 1 \right\},$$

and

$$q^*(H) := \min_{x \in \mathbb{R}^n} \{ q(x) \mid x^\top H x = 1 \} .$$

Fixing order matters!

Consider fixing e.g. $n,\ n-1, \dots, k, \dots, 3,\ 2,\ 1$
Nodes in the branching tree at the same level k (when k variabes have been fixed) share the same quadratic part

$$\begin{pmatrix} q_{11} & \cdots & q_{1k} \\ q_{21} & \cdots & q_{2k} \\ \vdots & \vdots & \vdots \\ q_{k-1,1} & \cdots & q_{k-1,k-1} \end{pmatrix}$$

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Diagonalization of Q_k for all k

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Exploit convexity

- Fixing may lead to quadratic problem at the node with $Q_I \succeq 0$.
- By the **convexity** we can improve **cut off** of nodes

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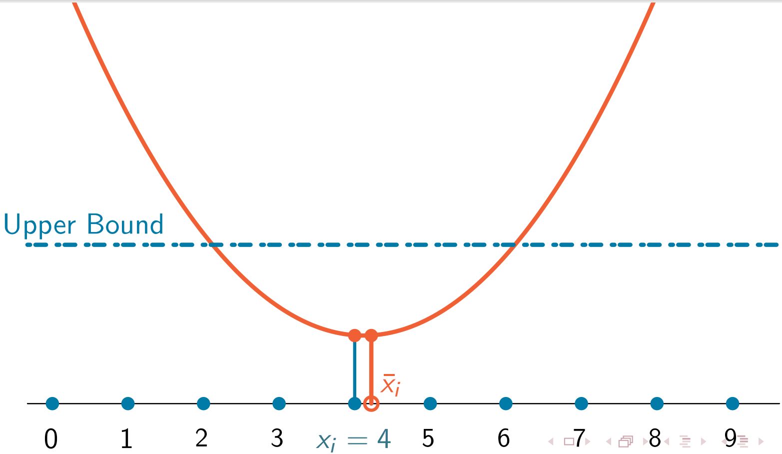

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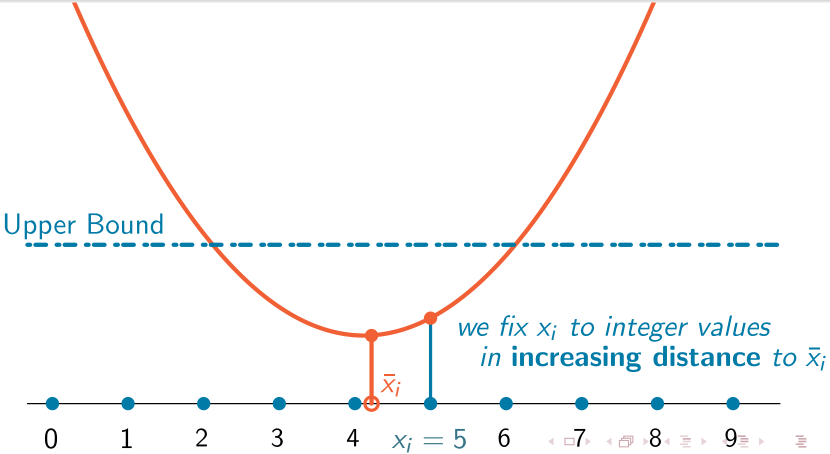

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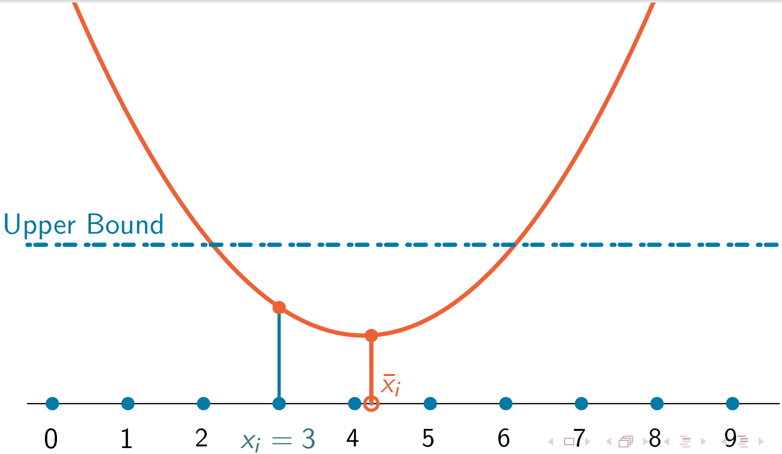

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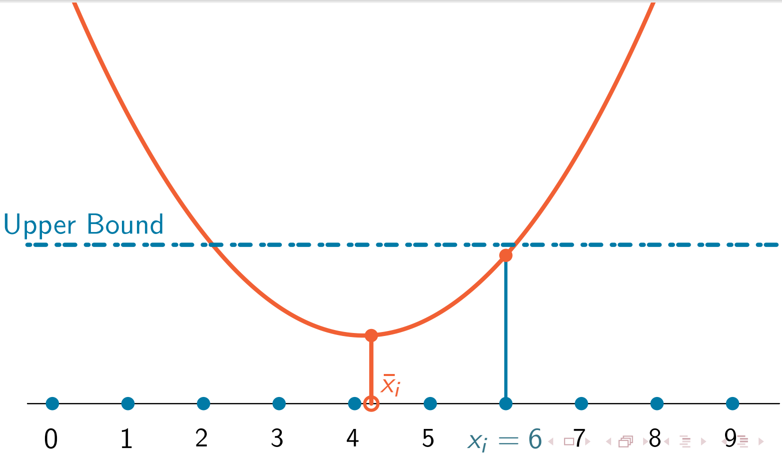

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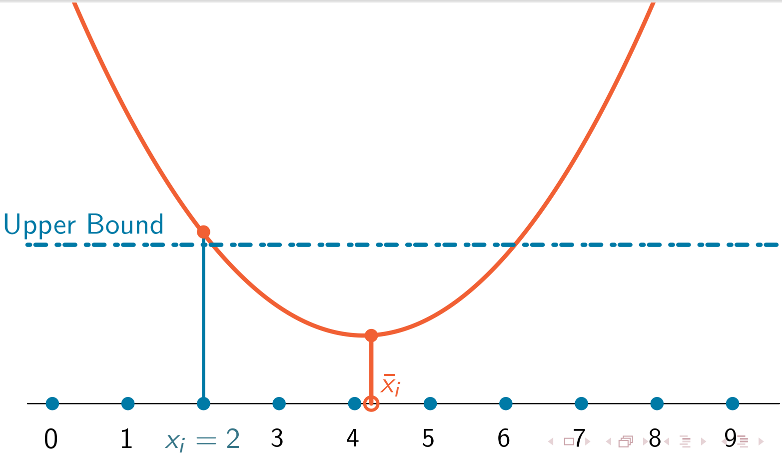

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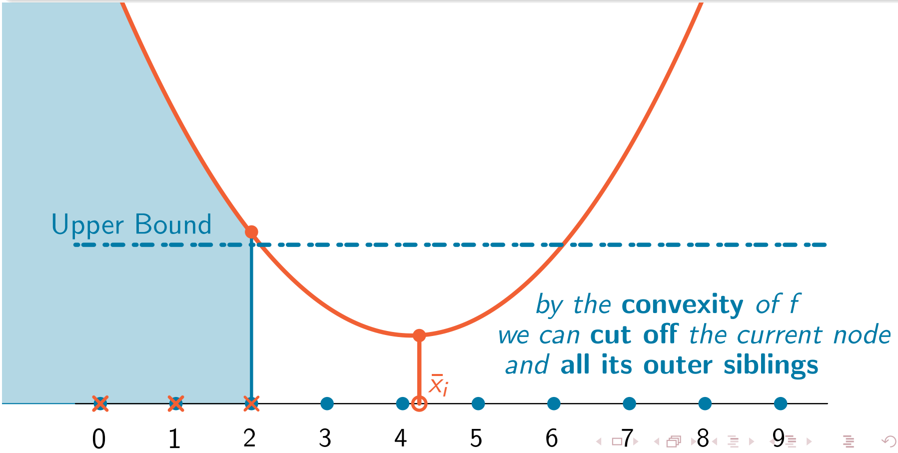

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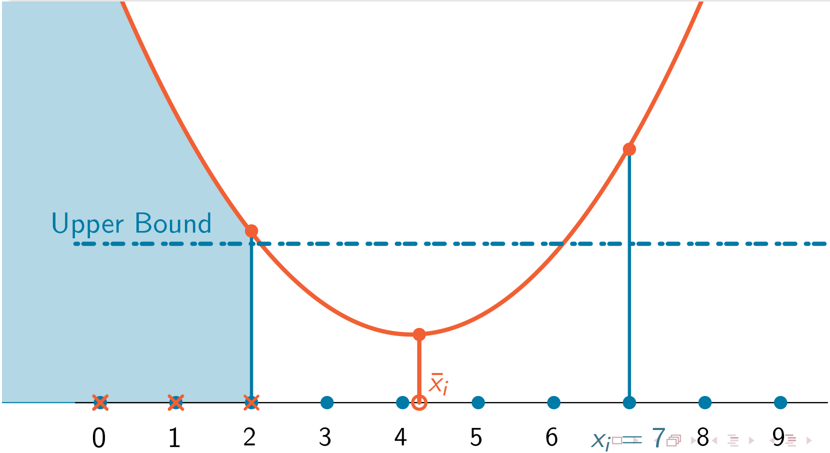

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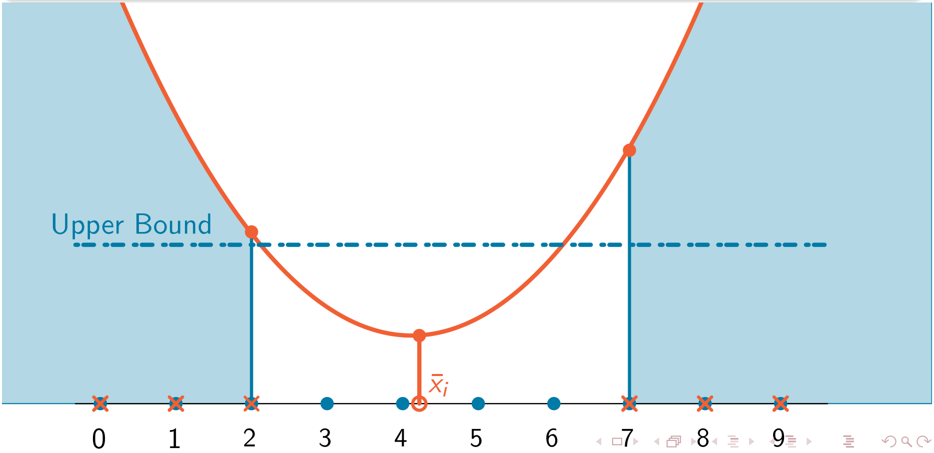

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Preprocessing and warm start are crucial elements that speed up the process B&B

HOW TO EXTEND THE APPROACH TO THE PRESENCE OF LINEAR EQUALITY CONSTRAINTS?

$$\begin{aligned} \min \quad & x^\top Q x + c^\top x \\ & \mathbf{Ax{=}b} \\ & x \in \{l, \ldots, u\}^n \end{aligned} \tag{CIQP}$$

Constrained case: relaxations

Consider non-convex CIQP ($Q \nsucceq 0$)
Again continuous relaxation to $x \in [l, u]^n \supset \{l, \ldots, u\}^n$ is still NP-hard

Constrained case: relaxations

Consider non-convex CIQP ($Q \not\succeq 0$)
Again continuous relaxation to $x \in [l, u]^n \supset \{l, \ldots, u\}^n$ is still NP-hard
Trivially we get

$$\{x : Ax = b,\ \{l, \ldots, u\}^n\} \subseteq [l, u]^n \subseteq \mathcal{E}(H)$$

and a bound is obtained by solving

$$\min_{x \in \mathcal{E}(H)} q(x)$$

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Linear constraints are "forgotten".

Can we do better ?

The elimination approach: relax and reduce

At each node a bound is obtained by solving

$$\begin{aligned} \min \quad & q(x) = x^\top Qx + c^\top x \\ & Ax = b \\ & x \in \mathcal{E}(H) \end{aligned} \tag{TQP}$$

where the axis parallel ellipsoid satisfies

$$[l, u] \subseteq \mathcal{E}(H) = \{x \in \mathbb{R}^n \mid (x - x^0)^\top H(x - x^0) \leq 1\},$$

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Tackling the linear constraints $Ax = b$

- By elimination: by using the familiar partitioning of x into basic and non-basic variables x_B and x_N, thus $Bx_B + Nx_N = b$.
- By exact penalization

The reduced problem

The x_B variables can be eliminated via substituting

$$x_B = B^{-1}b - B^{-1}Nx_N$$

After some algebra, we get the smaller problem in the non-basic variables $x_N \in \mathbb{R}^k$ $(k = n - m)$

$$\begin{aligned} f^*_{proj}(H) = \min \quad & x_N^\top \widetilde{Q} x_N + \widetilde{c}^\top x_N + d \\ & (x_N - x_N^0)^\top \widetilde{H}(x_N - x_N^0) \leq \alpha \\ & x_N \in \mathbb{R}^k \ , \end{aligned}$$

where

$$\begin{aligned} \widetilde{Q} &= Q_{NN} + N^\top B^{-\top} Q_{BB} B^{-1} N - Q_{BN}^\top B^{-1} N - N^\top B^{-\top} Q_{BN} \\ \widetilde{H} &= H_{NN} + N^\top B^{-\top} H_{BB} B^{-1} N - H_{NB} B^{-1} N - N^\top B^{-\top} H_{BN} \end{aligned}$$

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  All time-consuming calculations concerning these n different matrices can be performed in a preprocessing phase.

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- Light Cons: Vectors $\widetilde{c}, d, \alpha$ depend on the values at which the variables have been fixed but they can be updated in an incremental fashion.
- Cons: $\widetilde{H}$ is no more diagonal and depends on the original H in a difficult way
- Optimizing the bound

$$\max_{H \in \mathcal{H}_{diag}} f^*_{proj}(H)$$

  may be not straightforward

Penalty approach

[Poljak,Rendl,Wolkowitcz - JOGO(1995)]

Theorem

There exists $\bar{M} \in \mathbb{R}$ *such that, for all* $M \geq \bar{M}$

$$\begin{array}{ll} \min & x^\top Q x + c^\top x \\ \text{s.t.} & Ax = b \\ & l \leq x \leq u \\ & x \in \mathbb{Z}^n \end{array} \quad = \quad \begin{array}{ll} \min & x^\top Q x + c^\top x + M\|Ax - b\|^2 \\ \text{s.t.} & l \leq x \leq u \\ & x \in \mathbb{Z}^n \end{array}$$

The value of M can be found using

$$\bar{M} = ub - lb > 0,$$

where

$$ub = q(\hat{x})$$

where $\hat{x}$ is a feasible integer point $\hat{x} \in \{l, u\} \cap \{x \in \mathbb{R}^n : Ax = b\}$;

$$lb = q(\tilde{x}) = \min_{x \in C} q(x) \qquad \text{for any}$$

with C such that $C \supseteq X \cap \mathcal{F}$.

e.g. $C = \mathcal{E}(H) \supseteq [l, u]^n$ so that

$$\begin{aligned} lb = \quad \min \quad & x^\top Qx + c^\top x \\ \text{s.t.} \quad & x \in \mathcal{E}(H) \end{aligned}$$

Relaxation

It is a box constrained problem over integer variables

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \quad & x^\top(Q + MA^TA)x + (c - 2MA^Tb)^\top x + M\|b\|^2 \\ & x \in \{l, \dots, u\}^n \end{aligned} \qquad \text{(BQP)}$$

Relaxation

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$$x\in\{l,\dots,u\}^n$$

Choose an axis-parallel ellipsoid $\mathcal{E}(H)$

$$\{l,\dots,u\}^n\subseteq\mathcal{E}(H)=\{x\in\mathbb{R}^n \mid (x-x^0)^\top H(x-x^0)\leq 1\}$$

The value

$$f^*_{pen}(H,M)=\min_{x\in\mathcal{E}(H)} x^\top(Q+MA^TA)x+(c-2MA^Tb)^\top x+M\|b\|^2$$

gives a bound.

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- Pros: the approach for the box integer quadratic case directly applied
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  Linear constraints are taken into account in the shape of the objective function.
- Cons: shape of the ellipsoid does not "follow" the shape of the linear constraint: the bound may be bad
- Pros: The best (or a better) bound with parallel axis ellipsoid can be found by solving (approximately) by a subgradient approach

$$\max_{H \in \mathcal{H}_{diag}} \; f^*_{pen}(H, M)$$

Projection versus penalty

Which one gives better bound ?

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Let $H \succ 0$ such that $\{l, \dots, u\}^n \subseteq \mathcal{E}(H)$.

$$\begin{array}{ll} \min & q(x) \\ & Ax = b \\ & x^\top H x \leq 1 \end{array} \quad = \quad \lim_{M \to \infty} \quad \begin{array}{ll} \min & q(x) + M\|Ax - b\|^2 \\ & x^\top H x \leq 1. \end{array}$$

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Which one gives better bound ?

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As a sideproduct of such result, we get that for $M > 0$ and $H \succ 0$ the lower bound computed by the penalty approach is less (weaker) or equal than the one computed by the projection approach.

SOME NUMERICAL RESULTS

Numerical experience

- (GQIP) Penalty formulation embedded in the B&B scheme defined in [Buchheim, De Santis, Palagi, Piacentini, SIOPT 2013]
- Comparison with the MIQP solver of `CPLEX 12.6`

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Benchmark:

- constrained integer quadratic instances from `http://cedric.cnam.fr/~lamberta/Library/eiqp_iiqp.html`
  - Dimension $n = 20, 30, 40$
  - only one constraint, consisting in a linear equation with all positive entries $a^\top x = b$
  - three different right hand side b;
  - $[0, u]$, and $u = 1, 2, 10$;
  - For each dimension 15 instances are available: total of 405 instances.
- We consider **3h** as **time limit**
- Average over the successfully solved instances are reported (Time and ♯ nodes)

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It is not StQP, but....

it is the easiest generalization which is meaningful with integer variables

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Comparison with the MIQP solver of CPLEX 12.6

[0,1]				
n	Alg	Sol	Time	♯ nodes
20	GQIP	15	0.01	3501.40
	CPLEX	15	0.51	123.47
30	GQIP	15	0.09	17938.47
	CPLEX	15	1.98	314.07
40	GQIP	15	1.15	169471.40
	CPLEX	15	7.50	640.20
[0,2]				
n	Alg	Sol	Time	♯ nodes
20	GQIP	15	0.05	34303.47
	CPLEX	15	131.42	191111.20
30	GQIP	15	3.18	1066773.87
	CPLEX	2	5957.31	2847726.00
40	GQIP	11	63.28	10085272.82
	CPLEX	1	1554.17	239087.00
[0,10]				
n	Alg	Sol	Time	♯ nodes
20	GQIP	1	32.98	18428173.00
	CPLEX	15	18.77	9339.00
30	GQIP	0	–	–
	CPLEX	14	1203.30	130090.64
40	GQIP	0	–	–
	CPLEX	6	2864.64	151549.00

Table : Results for instances with $b = \frac{u}{2} \sum_{i=1}^{n} a_i$.

Comparison with the MIQP solver of CPLEX 12.6

[0,1]				
n	Alg	Sol	Time	♯ nodes
20	GQIP	15	**0.01**	3501.40
	CPLEX	15	0.51	123.47
30	GQIP	15	**0.09**	17938.47
	CPLEX	15	1.98	314.07
40	GQIP	15	**1.15**	169471.40
	CPLEX	15	7.50	640.20

[0,2]				
n	Alg	Sol	Time	♯ nodes
20	GQIP	15	**0.05**	34303.47
	CPLEX	15	131.42	191111.20
30	GQIP	**15**	3.18	1066773.87
	CPLEX	**2**	5957.31	2847726.00
40	GQIP	**11**	63.28	10085272.82
	CPLEX	**1**	1554.17	239087.00

[0,10]				
n	Alg	Sol	Time	♯ nodes
20	GQIP	**1**	32.98	18428173.00
	CPLEX	**15**	18.77	9339.00
30	GQIP	**0**	–	–
	CPLEX	**14**	1203.30	130090.64
40	GQIP	**0**	–	–
	CPLEX	**6**	2864.64	151549.00

Table : Results for instances with $b = \frac{u}{2}\sum_{i=1}^{n} a_i$.

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THANK YOU

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Happy 60^o Manuel