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Combining Approaches to Improve Bounds on Convex Quadratic MINLP Problems¹

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ABSTRACT. *Bounds on the optimal value of a convex 0-1 quadratic programming problem with linear constraints can be improved by a preprocessing step that adds to the quadratic objective function terms which are equal to 0 for all 0-1 feasible solutions yet increase its continuous minimum. The continuous and the CHR bounds are improved if one first uses Plateau's QCR method (2005), or one of its predecessors, the eigenvalue method of Hammer and Rubin (1970) and the method of Billionnet and Elloumi (2007). We present some preliminary results for convex GQAP problems using the eigenvalue method of Hammer and Rubin.*

KEYWORDS: *Nonlinear integer programming, bounds, relaxation, SDP.*

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1. Introduction

In this paper we show how combining two recently developed techniques for mixed-integer quadratic optimization problems with linear constraints may substantially improve bounds over what each technique alone could produce.

The first technique is a special case of the primal relaxation for nonlinear mixed-integer programming problems introduced in Guignard (1994). This relaxation replaces part of the constraints by their integer convex hull. To be more specific, given the nonlinear integer problem $Max\{f(x)|Ax = b, Cx = d, x \in S\}$, where S contains the integrality conditions over x , the primal relaxation with respect to the constraints $Cx = d$ is the problem $Max\{f(x)|Cx = d, x \in Co\{y \in S|Ay = b\}\}$. In the linear case, this is equivalent to Lagrangean relaxation. In the nonlinear case, in general it is not. Contesse and Guignard (1995) showed that this relaxation can be solved by an augmented Lagrangean method, and this was successfully implemented by S. Ahn in his Ph.D. dissertation (1997). Albornoz (1998) and later, independently, Ahlatcioglu (2007), thought of using this relaxation without separating any constraint, i.e., of defining the convex hull relaxation (CHR) of the problem $Max\{f(x)|Ax = b, x \in S\}$ as $Max\{f(x)|x \in Co\{y \in S|Ay = b\}\}$. The advantage is that this relaxation can be solved very simply by using Frank and Wolfe's algorithm (1956) or, better, Von Hohenbalken's simplicial decomposition (1977), following an idea of Michelon and Maculan (1992) for solving directly the Lagrangean dual in the linear case, without resorting to Lagrangean multipliers.

A side benefit of this procedure is the generation of feasible integer points, which quite often provide a tight upper bound on the optimal value of the problem. Additionally, a feature added in the recent releases of CPLEX, the solution pool, gives access to (all if one chooses to) integer feasible points generated during any branch-and-bound run, and in the case of CHR, during the solution of the linearized 0-1 problems, one at each iteration of simplicial decomposition. This provides a larger pool of integer feasible solutions, and thus a higher probability of finding good solutions for the original quadratic problem, as one can sort these solutions according to a secondary criterion, in this case

the quadratic objective function. In the nonconvex case, this has been used as a heuristic for generating good feasible solutions (Pessoa et al., 2010).

If one wants to improve on the CHR bound, one has to realize how the bound is computed. The CHR relaxation computes its bound over the convex hull of all integer feasible points, but probably exhibits only a small portion of these. One cannot therefore use these points to construct the actual convex hull of all integer feasible solutions. Yet, the bound is equal to the optimum of the original objective function (notice that in principle it does not have to be quadratic as far as CHR is concerned), and thus there is no point in trying to generate valid cuts. The only improvement can come from using objective function properties, potentially combined with properties of the constraints. This is where the second technique, which we will generically refer to as QCR (for Quadratic Convex Reformulation), comes in.

This technique's initial aim was the convexification of a nonconvex quadratic function in 0-1 variables, using properties of the 0-1 variables, and if appropriate, linear equality constraints of a 0-1 quadratic model. It was pioneered by Hammer and Rubin (1970). They were convexifying a nonconvex quadratic function $f(x) = x^T Q x + c^T x$ of the 0-1 variables x_j , $j = 1, \dots, n$, by adding to it the null term $\sum_j \lambda(x_j^2 - x_j)$, so that the minimum over λ of the modified $f(x)$ for $x \in [0, 1]^n$ would be as large, i.e., as tight a bound as possible. They showed that taking λ equal to the smallest eigenvalue, λ_{min} , i.e., replacing Q_{jj} for all j by $Q_{jj} + \lambda_{min}$, would achieve this. Billionnet and Elloumi (2008) then showed that one could improve on this scheme by adding a term $\sum_j u_j(x_j^2 - x_j)$, where the u_j 's are the optimal dual variables of a certain semi-definite program. Finally, M.C. Plateau (2005) showed that, for a quadratic 0-1 programming problem with objective function $f(x)$ and with linear constraints, some of them equalities of the form $\sum_j a_{ij}x_j = b_i$, the best lower bound provided by the convexification of $f(x)$ coming from adding to it terms of the form $\sum_j u_j(x_j^2 - x_j)$ and $\sum_k (\sum_i \alpha_{ki}x_i) \left(\sum_j a_{kj}x_j - b_k \right)$, is obtained by using for u and α the dual variables of an enlarged SDP program. In her thesis, Plateau remarks that this convexification scheme can also be applied to func-

tions that are already convex in order to tighten lower bounds. In the rest of the paper, we will refer to this scheme as “de-convexification”, even though it keeps the functions convex, but in a sense, less so.

What we are proposing in this paper is to first de-convexify the quadratic objective function, using one of the techniques described above, and then to apply CHR to the resulting, already improved, model. Our intent is to eventually use the GAMS implementation of Plateau’s QCR method available in the GAMS model library, following a joint project between GAMS, M.C. Plateau, and a research group at the University of Pennsylvania. This will provide us with the best possible lifting of the lower bound before using CHR. This is work in progress (Guignard, Ahlatcioglu, Bussieck, Esen and Meeraus, 2010). What is shown here is that by using the weaker method of Hammer and Rubin before applying CHR, one already substantially improves the continuous lower bound as well as the CHR bound.

The reader is referred to Billionnet, Elloumi and Plateau (2008) for a more detailed explanation of QCR. In the next sections, we first briefly describe the CHR method following Ahlatcioglu and Guignard (2007), then present numerical results on the effect of combining both techniques, for convex quadratic assignment problems (GQAP).

2. The CHR algorithm

Consider the following nonlinear integer program (NLIP)

$$(NLIP) \quad \begin{array}{ll} \min & f(x) \\ \text{s.t.} & x \in S \end{array}$$

where $f(x)$ is a nonlinear convex function of $x \in R^n$, $S = \{x \in Y : Ax = b\}$, A is an $m \times n$ constraint matrix, b is a resource vector in R^m , Y is a subset of R^n specifying integrality restrictions on x .

Definition 2.1. We define the Convex Hull Relaxation of (NLIP) to be

$$(CHR) \quad \begin{array}{ll} \min & f(x) \\ \text{s.t.} & x \in Co(S) \end{array}$$

Problem (CHR) is in general not equivalent to (NLIP) when $f(x)$ is nonlinear, because an optimal solution of (CHR) may not be integer, and therefore not feasible for (NLIP). However, it is easy to see that (CHR) is indeed a relaxation to (NLIP).

This relaxation is a primal relaxation, in the x -space. It is actually a primal relaxation that does not “relax” any constraint. The difficulty in solving (CHR) comes from the implicit formulation of the convex hull. However the idea of decomposing the problem into a sub-problem and a master problem, first introduced by Frank & Wolfe (1956), and furthered by Von Hohenbalken with Simplicial Decomposition (1973), and Hearn et al. with Restricted Simplicial Decomposition (1987), provides an efficient way to solve (CHR) to optimality, by solving a sequence of linear integer problems and of essentially unconstrained nonlinear problems.

3. Applying simplicial decomposition to the CHR problem

3.1. Assumptions

In order for simplicial decomposition to guarantee a global optimal solution of (CHR), several conditions must be satisfied :

- 1) the feasible region must be compact and convex,
- 2) the objective function must be convex, and
- 3) (iii) the constraints must be linear.

3.2. The Subproblem

The first part of the decomposition problem is the sub-problem, which can be viewed as a feasible descent direction finding problem. At the k^{th} iteration of simplicial decomposition, given a feasible point x^k of (CHR), one must find a feasible descent direction in the polyhedron $Co\{Ax = b, x \in X\}$ by solving the linear programming problem

$$(CHS) \quad \begin{array}{ll} \min_y & \nabla f(x^k)^T (y - x^k) \\ \text{s.t.} & y \in Co(\{Ax \leq b, x \in Y\}) \end{array}$$

We will call x^k the linearization point. Unlike nonlinear problems, the linear programming problem (CHS) has an equivalent integer program, which we will call the Integer Programming Subproblem (IPS) :

$$\begin{aligned} \min \quad & \nabla f(x^k)^T(y - x^k) \\ (IPS) \quad \text{s.t.} \quad & Ay \leq b \\ & y \in Y. \end{aligned}$$

Problem (IPS) is usually much easier to solve than problem (NLIP). The solution to (IPS) will be an extreme point of the convex hull, unless x^k is optimal for the convex hull relaxation (CHR) problem. Thus, at each iteration we obtain an integer feasible point to the original (NLIP) problem. Convergence to the optimal solution will be discussed in section 4. If x^k is not optimal, we proceed to the master problem.

3.3. *The Master Problem*

The following nonlinear programming problem with one simple constraint is called the Master Problem (MP) :

$$\begin{aligned} (MP) \quad \min \quad & f(X\beta) \\ \text{s.t.} \quad & \sum_i \beta_i = 1, \beta_i \geq 0, i = 1, 2, \dots, r \end{aligned}$$

X is the $n \times r$ matrix comprised of a subset of extreme points of the convex hull, along with one of the current iterates x^k or a past iterate. There are r such points in X . Then at the master problem stage, (MP) is solved, which is a minimization problem over a $r - 1$ dimensional simplex. If the optimal solution of (CHR) is within this simplex, then the algorithm terminates. If not, the optimal solution β^* of (MP) will be used to compute the next iterate, x^{k+1} , which can be found using the formula :

$$x^{k+1} = \sum_i \beta_i^* \times X_i.$$

Then we go back to the subproblem, find another extreme point and increase the dimension of the simplex for (MP).

For some pathological cases, putting no restriction on r could potentially pose computational problems. Restricted simplicial decomposition, introduced by Hearn et al. (1987) puts a restriction on the number of extreme points that can be kept.

4. Convergence to the Optimal Solution of CHR

Because the objective function is convex, the necessary and sufficient optimality condition for x^k to be the global minimum is

$$\nabla f(x^k)^T (y^* - x^k) = 0$$

Lemma 2 of Hearn et al. (1987) proves that if x^k is not optimal, then $f(x^{k+1}) < f(x^k)$, so that the sequence is monotonically decreasing. Finally Lemma 3 of Hearn et al. (1987) shows that any convergent subsequence of x^k will converge to the global minimum. The algorithm used in this study follows the restricted simplicial decomposition (Hearn et al. 1987).

5. Calculating lower and upper bounds for convex GQAP problems

As stated in Definition 2.1, (CHR) is a relaxation to the (NLIP). Simplicial Decomposition finds

an optimal solution, say, x^* , to (CHR), and this provides a lower bound on $v(\text{NLIP})$:

$$LB_{CHR} = f(x^*)$$

On the other hand, at each iteration k of the subproblem an extreme point, y^{*k} , of the convex hull is found, which is an integer feasible point of (NLIP). Each point y^{*k} yields an Upper Bound (UB) on the optimal value of (NLIP), and the best upper bound on $v(\text{NLIP})$ can be computed as

$$UB_{CHR} = \min\{f(y^{*1}), f(y^{*2}), \dots, f(y^{*k})\}.$$

To demonstrate the ability of the CHR approach to compute bounds often significantly better than the continuous relaxation bounds, we implemented CHR to find a lower bound on the optimal value of convex GQAPs.

We used two types of data. First we adapted data for GQAPs from the literature, with problems of size 30x15, 35x15 and 30x20, and measured the improvement over the continuous bound by computing the ratio of

$$\frac{(\text{CHR bound} - \text{NLP bound})}{(\text{best feasible value found} - \text{NLP bound})}$$

as a measure of how much the gap is reduced when one replaces the NLP bound by the CHR bound. We computed the matrix of the objective function by premultiplying the original matrix Q by its transpose, where the entries of Q are products of a flow by a distance as given in the original GAP instances. These problems tend to have moderate integrality gaps. The improvement was in the range 43 to 99 %. The largest runtime on a fast workstation was 12 seconds.

The second data set uses again data from the linear GAP literature, and generates the objective function matrix as the product of a matrix by its transpose, but this matrix is now randomly generated with coefficients between -500 and +500. These tend to have large duality gaps and to be considerably more difficult to solve. We will describe in the next paragraph how one can partially reduce this gap.

6. A priori Improvement of Lower Bounds

For some of the convex data sets generated for GQAP, the gaps between the continuous and/or the CHR bound on the one hand, and the optimal value on the other, are very large. Since CHR computes a bound based on the convex hull of all 0-1 feasible solutions, there is nothing that can be done to improve that part of the model, like adding cuts or tightening inequalities. The only place where an improvement remains possible is the objective function.

The reason we mention the continuous relaxation bound is that we know that the CHR bound must be at least as good or better. If we can manage to increase the continuous bound, we might be able to increase the CHR bound as well.

Consider the convex function $f(x) = ux(x - 1)$, $x \in \{0, 1\}$, u a positive scalar. The problem is to minimize $f(x)$ subject to $x \in \{0, 1\}$. The function is zero for $x = 0$ or 1 , but it is negative in between. If one computes the continuous bound on $f(x)$ for $x \in [0, 1]$, one gets $u(1/2)(-1/2) = -u/4$, and if u is large, so is the integrality gap. Notice that one could however replace $f(x)$ by $g(x) = ex(x - 1)$ with $e > 0$, e very close to 0 , it would produce an equivalent problem $\min\{g(x)|x \in \{0, 1\}\}$. Indeed $g(x)$ coincides with $f(x)$ over the feasible set $\{0, 1\}$, yet it gives a much better lower bound equal to $-e/4$, and it is a convex function as long as $e > 0$, no matter how small.

If one has a convex objective function of n variables, the same kind of difficulty may occur, i.e., the continuous bound, and thus the integrality gap, may be very large because the value of the objective function drops substantially when the variables are allowed to be between 0 and 1 .

Convexification in its simplest form (Hammer and Rubin, 1970) adds terms of the form $u(x_{ij}^2 - x_{ij})$, with u real, to the quadratic objective function. To convexify a nonconvex quadratic function, one tends to add positive terms to the diagonal of the matrix, to make it positive semidefinite. Here as we start from already convex objective functions, we will subtract positive terms from the diagonal, as long as the objective function remains convex. This will not change the objective function for $x_{ij} \in \{0, 1\}$. We will call this backward process diagonal de-convexication, even though it leaves the problem convex.

A more sophisticated de-convexification is possible using semidefinite programming (see for instance Billionnet, El-loumi and Plateau (2008), as well as the GAMS website link <http://www.gams.com/modlib/libhtml/gqapsdp.htm> showing an application to GQAP using CSDP) but more expensive to setup. We will show here that subtracting a number slightly smaller than the smallest eigenvalue of the matrix already improves the continuous bound as well as the CHR bound for convex GQAPs. The joint implementation of

this de-convexification and CHR is in progress (Guignard, Ahlatcioglu, Bussieck, Esen and Meeraus, 2010).

7. Computational results

7.1. Instances with large integrality gaps.

To illustrate the diagonal de-convexification process, we will use generalized quadratic assignment instances with a large duality gap. We present results for two instances of size

Table 1

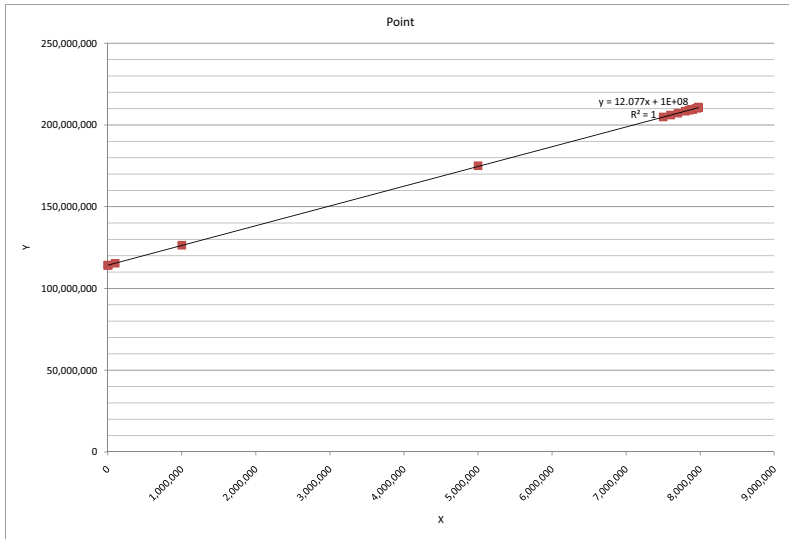
16 x 7	Continuous bound	CHR bound	RLT-1 bound	Optimal value or best feasible value	Smallest eigenvalue
Original convex function	114,187,401	139,645,033	185,918,839	577,900,705 (optimal)	
De-convexified function (HR)	210,434,185	232,950,970	185,918,839		7,977,050
De-convexified function (BE)	262,216,269				
20 x 10	Continuous bound	CHR bound	RLT-1 bound	Optimal value or best feasible value	Smallest eigenvalue
Original convex function	56,256,570	56,342,009	-424,138,807	469,555,787 (best found)	
De-convexified function (HR)	91,561,289	91,592,623	-424,138,807		2,129,919
De-convexified function (BE)	127,869,843				

16×7 and 20×10 respectively. 16×7 is the largest problem size that we were able to solve using CPLEX as a mixed-integer quadratic problem. Its objective function has no linear terms.

Table 1 compares bounds obtained before and after the de-convexification by eigenvalues (HR) and by Billionnet and Elloumi's approach (BE). Bounds from Plateau's QCR would be even better, and the CHR bound could of course be computed from that final model, implementation is in progress (Guignard, Bussieck, Esen and Meeraus 2010).

Figure 1 shows the increase in lower bound for problem 16×7 as one subtracts a larger and larger number from all

diagonal entries, until the matrix ceases to be positive-definite.



7.2. Large instances with smaller integrality gaps

Table 2 shows results for relatively large GQAP instances with smaller integrality gaps. The last two digits of an instance name are for identification, while the first four specify problem size, for instance 30x20 or 40x10. The gaps are computed from the best known integer feasible solution values (IFV) to-date. Replacing the continuous bound by the CHR bound almost bridges the gap in most cases. For these problems we did not try de-convexification, because the final gaps were usually very small.

Table 2. Continuous vs. CHR bound

Instance	Continuous bound	CHR bound	Best IFV	Improvement
30-20-35	28,996,191	29,210,393	29,267,194	79.04%
30-20-55	18,721,636	18,925,414	18,932,878	96.47%
30-20-75	24,882,925	25,273,194	25,299,161	93.76%
30-20-95	21,162,833	23,787,852	23,809,571	99.18%
35-15-35	32,750,712	32,769,891	32,795,216	43.09%
35-15-55	27,443,328	27,605,620	27,621,169	91.26%
35-15-75	30,638,516	30,920,476	30,928,923	97.09%
35-15-95	34,722,239	35,825,436	35,886,295	94.77%
50-10-75	56,103,056	56,606,460	56,615,187	98.30%
50-10-95	71,684,990	72,082,091	72,099,812	95.73%

8. Conclusion

The Convex Hull Relaxation (CHR), possibly combined with de-convexification as a preprocessing step, provides tight lower and upper bounds by (1) transforming a nonlinear integer optimization problem in one over the convex hull of all integer feasible solutions, and (2) replacing this problem by a sequence of integer linear programs and simple nonlinear continuous programs. The potential strength of the proposed algorithm is that the difficulty of the problems solved at each iteration stays relatively unchanged from iteration to iteration. It will be most suitable for those nonlinear integer problem types that would be much easier to solve with a linear objective function. One should expect that CHR will have a robust performance for large-scale problems if one has access to solvers able to handle large integer linear programs and simple nonlinear programs efficiently. Current experiments seem to confirm this behavior. Preceding the CHR bound computation by de-convexification of the quadratic objective function to a point where the function is still convex but has achieves its highest possible continuous bound is a very natural complement to CHR, as it concentrates on the objective function and possibly the linear equality constraints of the problem. There is indeed no obvious further improvement possible on the CHR bound coming solely from the constraint set, because this constraint set has already been maximally reduced to produce a formu-

lation equivalent to the minimization over the convex hull of integer feasible solutions. The positive results on CHR coupled with the HR deconvexification are already encouraging, and the initial experiments using Plateau's QCR method show a even larger improvement of the CHR bounds for problems with large gaps.

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