Bound constraints for Point Packing in a Square

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1 Introduction

In this paper we present a conjecture about the bounds on the variables for the Point Packing in a Square (PPS) problem. There exist several formulations for this problem, most of them are introduced in [1]; in order to semplify the following presentation, we use this formulation:

> *Place n points in the unit square such that the minimum pairwise distance is maximal.*

This problem can be formulated this way:

$$\max \alpha \tag{1}$$
$$\forall i < j \leq n \quad (x_i - x_j)^2 + (y_i - y_j)^2 \geq \alpha \tag{2}$$
$$\forall i \leq n \quad x_i \leq 1 \tag{3}$$
$$\forall i \leq n \quad y_i \leq 1 \tag{4}$$
$$\forall i \leq n \quad x_i \geq 0 \tag{5}$$
$$\forall i \leq n \quad y_i \geq 0 \tag{6}$$
$$\alpha \geq 0. \tag{7}$$

The positive variable α is the square of the minimum pairwise distance between the points. Constraints (2) are the distance inequalities, while inequalities (3)-(6) mean that the points are inside the unit square.

When we try to solve PPS by means of solvers which implement the spatial Branch-and-Bound algorithm [2,3], like Couenne [4] or BARON [5], we notice

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that it is not easy to decrease the value of the upper bound on α during the computation. In next Section, we will show that it depends also on the bound on the variables, and we propose a method to obtain better results by modifying the inequalities (3)-(6).

After that, in Section 3 we present some computational results, while in Section 4 there are the conclusions and the future work.

2 Bounds on the variables

PPS is a nonlinear nonconvex problem; when we try to solve it by means of spatial Branch-and-Bound, usually the root node corresponds to a linear relaxation of the problem, whose optimal solution represents an upper bound for the original problem. For the formulation (1)-(7) the relaxation is the following (as explained in [6,7]).

$$
\begin{aligned}
&\max \alpha && (8)\\
\forall i < j \leq n \quad & -l(i,j) \geq \alpha && (9)\\
\forall i \leq n \quad & x_i \leq 1 && (10)\\
\forall i \leq n \quad & y_i \leq 1 && (11)\\
\forall i \leq n \quad & x_i \geq 0 && (12)\\
\forall i \leq n \quad & y_i \geq 0 && (13)\\
& \alpha \geq 0. && (14)
\end{aligned}
$$

where $l(i,j) = -(Lx_i - Ux_j + Ux_i - Lx_j)(x_i - x_j) - (Ly_i - Uy_j + Uy_i - Ly_j)(y_i - y_j) + (Lx_i - Ux_j)(Ux_i - Lx_j) + (Ly_i - Uy_j)(Uy_i - Ly_j)$ is the convex envelope of the nonlinear part of constraint (2) while L and U represent respectively the lower and upper bounds on the variables (in this case, $L = 0$ and $U = 1$ for all the variables).

Proposition 2.1 *The optimal solution of the problem* (8)-(14) *is* $\alpha^* = 2$.

Proof. It is easy to see that when all the lower bounds have the same value L, and the upper bounds have the same value U, then $-l(i,j) = 2(U - L)^2$. The problem of maximizing α, with the constraints $\forall i < j \leq n \quad \alpha \leq 2(U - L)^2$, has obviously optimal solution $\alpha^* = 2(U - L)^2$. Since $L = 0$ and $U = 1$, then the optimal solution of (8)-(14) is $\alpha^* = 2$. □

The bound provided by the previous relaxation is not very good: since α is the square of the minimum distance between the points, the upper bound on the distance is $\sqrt{2}$, that is the optimal solution obtained when there are only 2 points in the square, placed in two opposite vertices. Furthermore, this bound does not depend on the number of points n, nor on the value of the variables x and y: due to the fact that all the lower (upper) bounds have the same value, in the linear relaxation $l(i,j)$ all the coefficients of the terms containing x and y become 0.

In order to improve the bound on α, we should change the value of lower and upper bounds for some variables; thus, the corresponding terms containing x

		Original formulation		Bounds constraints formulation	
n	d^*	LB	UB	LB	UB
9	0.5	0.000098	1.414213	**0.300463**	**0.707107**
10	0.421279	0.000098	1.414213	**0.396156**	**0.707107**
11	0.398207	0.000099	1.414213	0.000099	**0.707107**
12	0.388730	0.000099	1.414213	**0.360065**	**0.707107**
13	0.366096	0.000098	1.414213	**0.339654**	**0.502948**
14	0.348915	0.000098	1.414213	**0.340830**	**0.502874**
15	0.341081	0.000098	1.414213	**0.334524**	**0.502793**
16	0.333333	0	1.414213	**0.290033**	**0.502793**
17	0.306153	0	1.414213	**0.000099**	**0.502793**
18	0.300462	0	1.414213	**0.252819**	**0.502793**
19	0.289541	0.000047	1.414213	**0.252337**	**0.502793**
20	0.286611	0	1.414213	**0.276468**	**0.502793**

and y in the linear relaxation do not disappear. The following conjecture refers to that idea.

Conjecture 2.2 *Consider an instance of PPS with n points. Divide the unit square in k^2 equal subsquares, with $k = \arg\min_s \left|\frac{n}{2} - s^2\right|$, $s \in \left\{\left\lceil\sqrt{\frac{n}{2}}\right\rceil, \left\lfloor\sqrt{\frac{n}{2}}\right\rfloor\right\}$. There is at least one point of the optimal solution in each subsquare.*

The meaning of this conjecture is that we can change the value of the bounds for k^2 points. For example, consider the case with $n = 9$: here, $k = 2$, so there are 4 subsquares. According to the conjecture, we can place one point in each subsquare; for instance, if we put the point i is in the bottom left subsquare, we can modify the bounds provided by (3)-(4) obtaining $x_i \leq 0.5$ and $y_i \leq 0.5$.

In order to change other bounds, we can use these properties of the optimal solution, as remarked in [8]:

- at least $n_x = \lceil\frac{n}{2}\rceil$ points are on the left half of the square (x bounds property);
- among the previous n_x points, at least $n_y = \lceil\frac{n_x}{2}\rceil$ are on the bottom half (y bounds property).

After dividing the square in k^2 subsquares, we have placed in the left half of the square $\eta < n_x$ points, so for others $n_x - \eta$ points we can change the upper bounds on the variable x from 1 to 0.5, according to x bounds property. A similar idea can be used for the y bounds property.

3 Results

In this Section we present the values of the upper and lower bounds for some instances of the PPS problem obtained at the root node, using Couenne, with and without the bound constraints presented in the previous section. Furthermore, we present the values of the optimal distance $d^* = \sqrt{\alpha^*}$ for these solutions (which can be found in `http://www.packomania.com` and [1]).

4 Conclusions and future work

In this paper we showed the effect of the bounds constraints: the upper bounds obtained are better, as well as the lower bounds (namely the best solutions found). Moreover, we can see an improvement of the upper bounds from the instance $n = 12$ (where $k = 3$) to the instance $n = 13$ (where $k = 4$).

The future work has three main directions: first, we want to prove the conjecture presented in this paper. Second, we want to try other kinds of subdivision of the square. Finally, we will try to adapt these ideas for other formulations of this problem where some symmetry breaking constraints are used [9,10].

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