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SYMMETRY BREAKING IN PACKING EQUAL SPHERES IN A UNIT CUBE

Ali Djebid [1], Brahim Oukacha[2], Karim Benalia[3]

[1] Laboratory of Operational Research and Mathematics of Decision, Faculty of Sciences, University Mouloud Mammeri of Tizi Ouzou , 15000 Tizi-Ouzou, Algeria.

e-mail : ali.djebid@ummto.dz

[2] Laboratory of Operational Research and Mathematics of Decision, Faculty of Sciences, University Mouloud Mammeri of Tizi Ouzou , 15000 Tizi-Ouzou, Algeria.

e-mail : brahim.oukacha@ummto.dz

[3]Department of Mathematical Sciences, Faculty of Hydrocarbons and Chemistry, University of Boumerdes, Boumerdes 35000, Algeria.

e-mail : k.benalia@univ-boumerdes.dz

Abstract

The structure of symmetric solutions for some optimization problems leads to a notable increase in computation time and memory consumption for most solving algorithms. To address this disadvantage, various symmetry breaking methods have been developed over the past decades. Among them, the addition of symmetry breaking constraints to the problem formulation. In this work, we propose new symmetry breaking constraints for the packing problem of equal spheres in a unit cube. We also show that the integration of these constraints leads to a narrowing of the original formulation. The numerical results highlight a significant performance improvement, both in computing time and memory usage.

Math. Subject Classification: 90C20, 90C26, 90C57.

Key Words and Phrases: Exploiting symmetry, Symmetry, Reformulation, Spheres packing.

1. Introduction

Symmetry has quickly become a fundamental concept in many scientific fields, as it improves both theoretical knowledge and practical performance. In recent years, much research effort has focused on detecting and eliminating symmetries in various domains. Among the first areas to take an interest in exploiting symmetry during resolution was propositional logic, particularly through the satisfiability (SAT) problem and propositional calculus [2,14]. These were then generalized to constraint programming [5] and subsequently integrated into broader frameworks such as mathematical programming [8,9,10], mixed integer non-linear programming (MINLP) [7], and mixed integer linear programming (MILP) [12].

Geometric object packing problems are known to be very difficult to solve in practice. In this study, we are interested in exploiting symmetry in the packing problem where the objects are equal spheres and the packing region is a unit cube. As the problem of packing equal circles

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into a square [4,3,6]. The problem of packing equal spheres [6,15] admits symmetries that arise from the geometry of the configurations (rotation and reflection of the cube) and the problem formulation. Besides, packing equal spheres in a unit cube (PESC) also generates a completely symmetric group of the order of the number of objects since they are identical. This strong symmetry significantly increases the redundancy in the search space, which can lead to a significant increase in computation time for Branch and Bound (BB) algorithm.

Thus, it is possible to significantly reduce the size of the search space by eliminating redundant or equivalent solutions [11]. This approach not only speeds up computation times but also improves the robustness and scalability of optimization methods, particularly in the case of large-scale or highly combinatorial problems. Furthermore, explicitly considering symmetry can guide the design of more compact mathematical formulations, facilitate the generation of valid cuts, and improve the performance of heuristics and metaheuristics. An effective approach is to introduce symmetry-breaking constraints (SBCs) into the initial formulation of the problem. These constraints aim to reduce the search space by eliminating certain symmetric solutions while ensuring that at least one optimal solution is preserved.

In this paper, we present new SBCs to the problem of PESC. These constraints consist in ordering the spheres with respect to all axes. The rest of the paper is organized as follows: The section 2 presents the mathematical formulation of the PESC and introduces algebraic notions of symmetry. The section 3 is dedicated to symmetry detection. The section 4 proposes fixed, strong SBCs and new sets of mixed SBCs. The experimental results are detailed in section 5, and show that adding these SBCs significantly improves the performance of the BB algorithm. Finally, section 6 concludes this document.

2. Background and notations

We begin by presenting the mathematical formulation of the problem of PESC adapted from [6], before reviewing some basic definitions concerning groups.

2.1 Formulation of packing equal spheres in a unit cube

This problem consists of finding the maximum radius r of the spheres, such that each pair of spheres must not overlap and the N spheres must be placed in the interior of the unit cube. The variables $x^i = (x_1^i,\ x_2^i,\ x_3^i)$, $i \leq N$ determine the coordinates of the center of the i^{th} sphere. The model we are going to study is a quadratically constrained non-convex quadratic program which is written in the following form:

$$(P)\begin{cases}\max\ r & (1)\\ \left\|x^i - x^j\right\|^2 \geq\ 4r^2, \qquad \forall\ 1 \leq i < j \leq N & (2)\\ r \leq x_d^i \leq 1 - r\ ,\ \ i \leq N\ , 1\ \leq d \leq 3 & (3)\\ r \geq 0 & (4)\end{cases}$$

Where the norm $\|\ .\ \|$ is taken to be the euclidean norm. Constraint (1) represents the objective function that maximizes the minimum distance between the spheres center. Constraints (2)

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represents the quadratic constraints that ensure the non-overlapping between any pair of distinct spheres. Constraints (3) ensure that the spheres are inside the unit cube. The constraints (4) is the non negativity constraint. In everything that follows, $\mathcal{F}(P)$ is the feasible region and $\mathcal{G}(P)$ is the global solution set.

2.2 Symmetries

We will go over some definitions and notations for the groups used, for more details see [9,10,13].

For a set $\mathrm{I} = \{1,\ 2, \dots, n\}$, S_n and C_n are the symmetric and cyclic group of order n. A permutation $\pi\ \in\ S_n$ is represented by an n-vector, with π_i the image of i under π. The identity permutation is the permutation $\pi \in\ S_n$ such that $\pi_i = i$ for $i = 1,\ 2, \dots, n$. Given a vector $V = \{v_1, v_2, \dots, v_n\}\ \in\ \mathbb{R}^n$ and a permutation $\pi\ \in\ S_n$ act on V by permuting its coordinates as follows: $\pi(V) = \left(v_{\pi(1)}, v_{\pi(2)}, \dots, v_{\pi(n)}\right)$

For a set of permutations S, $\langle S \rangle$ is defined to be the smallest group containing all permutation in S. The group $\langle S \rangle$ is the group generated by S. For a group G that acts on a set X, $XG = \{xg |\ x \in X, g\ \in G\}$, we denote by xG if $X = \{x\}$ the orbit of x in G, where $orb(x, G) = \{x \in\ \mathbb{R}^n\ |\ y = g(x),\ \ g \in G\}$. For a subset $Y \subseteq X$ we let $Stab(Y, G\ ) = \{g \in G\ |\ g(Y) = Y\}$, the setwise stabilizer of Y in G. For any permutation $\pi\ \in\ S_n$, let $\Gamma(\pi)$ be the set of its disjoint cycles σ such that $\pi =\ \prod_{\sigma\ \in \Gamma(\pi)} \sigma$.

Let G_1 and G_2 be two groups. A homomorphism from G_1 into G_2 is any application h that satisfies $\forall\ \sigma, \pi\ \in\ G_1, h(\sigma\pi) = h(\sigma)h(\pi)$.Two groups are isomorphic when there is a group morphism between them that is bijective.

3. Detection of symmetries

In this section, we discuss a procedure to find the symmetries of PESC. Conceptually, we look for a set of permutations that act on the indices of variables and leave the formulation invariant and give the same solutions during the research process.

Definition 1. *Solution symmetries are the set of permutations that act on the solutions without influencing the set of solutions.*

Definition 2. *Formulation symmetries are permutations of variables that leave the problem formulation invariant.*

These permutations affect all permissible solutions to problem (P), while preserving the fundamental objective of the initial formulation.

Definition 3. *Formulation group G_P of (P) is the group of permutations which keeps the formulation of (P) invariant.*

Definition 4. *Solution group of (P) is the group of all permutations, which keeps the set G_P invariant, it is defined as $G_P^* = stab(\mathcal{G}(P),\ S_n)$.*

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However, to clearly illustrate the group of formulation of problem (P). Let $\{1, 2, \dots, N\}$ be the set of the spheres indices. We denote by S_n the symmetric group of order N, the group of all permutations of N spheres. C_3 the cyclic group of order 3, group of rotations of the unit cube i.e. permutation of axes x_1, x_2 and x_3. we conjecture that the formulation group G_P of packing equal spheres in a unit cube is isomorphic to $C_3 \times S_N$.

Theorem 5. *The formulation group G_P of the problem of packing N identical spheres in a unit cube is isomorphic to $C_3 \times S_N$.*

Proof. The proof to this theorem can be easily adapted from Costa et al [3].

4. Elimination of symmetries

In this section, we study three types of constraints aimed at eliminating symmetries: (i). fixing constraints (Fixing SBCs), which consist of arbitrarily fixing certain decision variables; (ii). strong symmetry breaking constraints (Strong SBCs), as presented in [10] and (iii). mixed symmetry breaking constraints (Mixed SBCs).

Definition 6. *Given a permutation $\pi \in S_n$ acting on the component indices of the vectors in a given set $X \subseteq \mathbb{R}^n$, the constraints $g(x) \leq 0$ are symmetry breaking constraints with respect to π and x if there is $y \in X$ such that $g(\pi y) \leq 0$.*

Definition 7. *Given a group G_P , $g(x) \leq 0$ are symmetry breaking constraints w.r.t G_P and x if there Is $y \in XG_P$ such that $g(y) \leq 0$.*

After adding symmetry breaking constraints to the initial formulation of the problem, we obtain another formulation of the problem called narrowing.

Definition 8. *A narrowing (Q) of (P) is such that, there is a function $g: \mathcal{F}(Q) \longrightarrow \mathcal{F}(P)$ for which $g(\mathcal{G}(Q)) \subseteq g(\mathcal{G}(P))$ and (Q) is infeasible only if (P) is.*

4.1 Fixed SBCs

When a problem has symmetries, it is often possible to fix certain variables in order to eliminate redundancies due to solutions that are equivalent by symmetry. For example, in the problem of packing identical spheres, the formulation and solutions remain invariant by permutation of the sphere indices. We can then, without loss of generality, arbitrarily choose one sphere and fix it relative to the others, since any configuration can always be reduced to the fixed configuration by a symmetric transformation.

Proposition 9. *The constraints $x_1^i \leq x_1^j$ for i fixed, $j = 1,2, \dots, N$ and $i \neq j$ is the set of symmetry breaking constraints.*

Proof. Let $X^* = (x_1^i, x_2^i, x_3^i, r)$ be an optimal solution $X^* \in \mathcal{G}(P)$ that satisfies the constraints of proposition 9 and σ a permutation of G_P such that $\sigma(x_1^i) = x_1^j$. Since the spheres are identical, then $\sigma(X^*, r) = \sigma(x_1^i, x_2^i, x_3^i, r) = (x_1^j, x_2^j, x_3^j, r) = Y^*$.

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Thus, by adding constraints $x_1^i \leq x_1^j$ for i fixed, $j = 1, \dots, N$ and $i \neq j$ to the formulation of the problem, and since they verify X^*, they make Y^*unfeasible. Hence, $x_1^i \leq x_1^j$ for i fixed, $j = 1, \dots, N$ and $i \neq j$ is the set of symmetry breaking constraints.

Since the spheres are identical, we can fix one of them among the N. Furthermore, this sphere can be fixed relative to an arbitrary axis, such as the x_2-axis or the x_3-axis.

4.2 Strong SBCs

The principle of strong SBCs is to order the spheres along one of the axes. In our case and by Theorem 5, we can order the indices of spheres with respect to the x_1 axis.

Proposition 10. *The constraints* $\forall\, i \leq N-1,\ x_1^i \leq x_1^{i+1}$ *are symmetry breaking constraints with respect to* $\pi \in G_P$*,* $\mathcal{G}(P)$*.*

Proof. If (x_1^i, x_2^i, x_3^i, r) is an optimal solution of the problem (P) and a permutation σ_i acts on the set of indices of the spheres then there exists a permutation $\pi \in G_P$ such that $\pi(x_1^i, x_2^i, x_3^i, r) = (\pi x_1^i, \pi x_2^i, \pi x_3^i, r)$ verifies the constraints of the proposition.

The spheres can always be ordered with respect to the other axis as follows: $\forall\, i \leq N-1,\ x_2^i \leq x_2^{i+1}$ or , $x_3^i \leq x_3^{i+1}$respectively.

4.3 Mixed SBCs

In this subsection, we propose a new mixed SBCs for packing the equal spheres problem in a unit cube. These constraints are introduced at the same time on all x_1, x_2 and x_3 axes. But let's ensure that there exists at least one optimal solution of $\mathcal{G}(P)$ is validated by the G_P group. For that, we consider a parameter $\alpha = \sqrt[3]{N}$ where N represents the number of spheres to be packed in the unit cube and 3 is the dimension d of the problem. Let $m \in \{1, 2, \dots, N'\}$ where $N' = \left\lceil \frac{N}{\alpha} \right\rceil$ and for each $i \in \{1, 2, \dots, N''\}$, where $N'' = \left\lfloor \frac{N}{m} \right\rfloor$. This gives us the following sets.

$$C_i^{x_1} = \{x_1^j \leq x_1^{j+1}, \forall\, j \leq N-1 \wedge j \neq mi\}.$$

$$C_i^{x_2} = \left\{x_2^{k-(m-1)} \leq x_2^{k+1}, \forall\, k \leq N-1 \wedge k = mi\right\}.$$

$$C_i^{x_3} = \left\{x_3^{k-(m-2)} \leq x_3^{k+1}, \forall\, k \leq N-1 \wedge k = mi\right\}.$$

Now show that for all $i \in \{1,2,\dots,N''\}$, $\forall m \in \{1,2,\dots,N'\}$, $P \cup C_i^{x_1} \cup C_i^{x_2} \cup C_i^{x_3}$ forms a narrowing.

Theorem 11. *Let* $m \in \{1,2,\dots,N'\}$ *and for all* $\in \{1,2,\dots,N''\}$, (Q_i) *is a narrowing of* (P).

Proof. Let $m \in \{1,2,\dots,N'\}$ and $(x_1^i, x_2^i, x_3^i, r^o) \in \mathcal{G}(P)$ an optimal solution, suppose now that for a permutation $\pi \in S_N$ we have $\pi(x_1^i, x_2^i, x_3^i, r^o) = (\pi x_1^i, \pi x_2^i, \pi x_3^i, r^o)$ where π acts only on a vector in $\mathbb{R}^n$ by permutation of the spheres between them, so $\pi(x_1^i, x_2^i, x_3^i, r^o) \in \mathcal{G}(P)$.

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The constraints $\forall\ i \leq N-1,\ x_1^i \leq x_1^{i+1}$ are known to be SBCs for the sphere packing problem. For all $i \leq N-1$ and $k = mi$, if $x_2^{k-(m-1)} \leq x_2^{k+1}$ and $x_3^{k-(m-2)} \leq x_3^{k+1}$ the result holds. Otherwise suppose that $x_2^{k-(m-1)} > x_2^{k+1}$ and $x_3^{k-(m-2)} > x_3^{k+1}$. Thus, consider the following permutations on the indices of the spheres $\sigma_i = \prod_{l=0}^{m}(i+l, i+m+l)$ that act on the x_2 axis, and $\tau_i = \prod_{l=0}^{m}(i+l+1, i+m+l)$ that act on the x_3 axis. Both permutations are in S_N; $\sigma_i(x_1^i, x_2^i,\ x_3^i, r^o)$ and $\tau_i(x_1^i, x_2^i,\ x_3^i, r^o)$ have the following properties:

1. For $l = 0$ we have the two cycles $(i, i+m)$and $(i+1, i+m)$ then $x_2^i \leq x_2^{i+m}$ and $x_3^{i+1} \leq x_3^{i+m}$ respectively.

2. For all $l \leq m-2$, the permutation σ_i, we have $\sigma_i\ x_1^{i+l} = x_1^{i+m+l} \leq x_1^{i+m+l+1} = \sigma_i x_1^{i+l+1}$ hence $\sigma_i\ x_1^{i+l} \leq \sigma_i x_1^{i+l+1}$ and $\sigma_i\ x_1^{i+m+l} = x_1^{i+m+1} \leq x_1^{i+m+1+1} = \sigma_i x_1^{i+m+l+1}$ hence $\sigma_i\ x_1^{i+m+l} \leq \sigma_i x_1^{i+m+l+1}$.

The permutation τ_i we have $\tau_i\ x_1^{i+l+1} = x_1^{i+m+l} \leq x_1^{i+m+l+1} = \tau_i x_1^{i+l+1+1}$ hence $\tau_i\ x_1^{i+l+1} \leq \tau_i x_1^{i+l+2}$ and $\tau_i\ x_1^{i+m+l} = x_1^{i+l+1} \leq x_1^{i+l+1+1} = \tau_i x_1^{i+m+l+1}$ hence $\tau_i\ x_1^{i+m+l} \leq \tau_i x_1^{i+m+l+1}$.

3. $\forall j \neq m(i-1)+1$ and $\forall j \neq m(i-1)+2$ then σ_i and τ_i respectively fixed $x_1^j \leq x_1^{j+1}$.

Thus $\sigma_i(x_1^i, x_2^i,\ x_3^i, r^o)$ and $\tau_i(x_1^i, x_2^i,\ x_3^i, r^o)$ apparent to $\mathcal{G}(P)$ and satisfied the constraints of (Q_i).

Proposition 12. *The set constraints* $\zeta_i = C_i^{x_1} \cup C_i^{x_2} \cup C_i^{x_3}$ *are mixed symmetry breaking constraints for all* $i \in \{1, 2, \ldots, N^{"}\}$.

Proof. Let $(x_1^i, x_2^i,\ x_3^i, r^o) \in \mathcal{G}(P)$. As $\sigma_i = \prod_{l=0}^{m}(i+l\ , i+m+l\ )$ and $\tau_i = \prod_{l=0}^{m}(i+l+1\ , i+m+l\ )$ are permutation to disjoint cycles. Then the permutations ρ_i formed by σ_i and τ_i generate the symmetric group acting on the spheres indices. Thus there exist a permutation $\pi \in G_P$ such that $\pi(x_1^i, x_2^i,\ x_3^i, r^o) = (\pi x_1^i, \pi\ x_2^i,\ \pi x_3^i, r^o)$ verifies the constraints ζ_i.

5. Experiments

For the experimental results, we use the AMPL modeling language, executed on a computer equipped with an Intel® CoreTM i5-8250U processor clocked at 1.80 GHz and 8 GB of RAM, running on Windows. AMPL integrates several free non-linear programming solvers, among which the Couenne solver [1].

In Table 1, we present the simulation results for the four formulations with and without symmetry breaking constraints. The first line contains the instance of the problem of packing equal spheres into a unit cube with N: number of spheres and r^*: maximum radius. The second to fifth lines contain the formulations of the problem, and each column indicates the number of nodes in the search tree of the BB algorithm, denoted nb, and the execution time of the solver. We set the maximum execution time of the solver to 12 hours.

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Table 1: Solving of instances with the Couenne solver and $m = 2$.

Instances	N	2	3	4	5	6
	r^*	0.316987	0.292893	0.292893	0.263932	0.257359
Original	nb	0	34	364	-	-
	$Time$	0.162	1.304	3.108	-	-
FSBCs	nb	0	0	6	1067952	-
	$Time$	0.019	0.28	1.064	1626.38	-
SSBCs	nb	0	8	6	20354	-
	$Time$	0.016	0.36	0.865	149.078	-
MSBCs	nb	0	2	0	37504	1906674
	$Time$	0.013	0.092	0.029	54.856	6921.435

We note in Table 1 that the number of nodes in the search tree is smaller for the MSBCs formulation, except for the $N = 5$ instance, where the SSBCs formulation gives fewer nodes, $nb = 20354$ compared to $nb = 1067952$ and $nb = 37504$ for the FSBCs and MSBCs formulations, respectively. However, the time required for the solver to return a solution is better for the formulation with mixed SBC constraints. We also note that for $N = 5$, we obtain no results in 12 hours for the original formulation, and that for the instance $N = 6$, we obtain a result only for the formulation with mixed SBC constraints and no results even for the FSBCs and SSBCs formulations.

The table 2 presents the results obtained after executing the Couenne solver on several instances of the problem. The m and i to see the influence of the instance of the problem. The N is the number of spheres, r^* is the maximum radius obtained by the solver. nb is the number of nodes of the branch and bound algorithm and time is the solver execution time in seconds. We have limited the CPU time to 2 hours.

Table 2: Variation of parameters m and n.

N	m	i	r^*	Nb	Time
	1	1	0.292893	18	0.505
3		2	0.292893	18	0.539
	2	1	0.292893	2	0.119
	1	1	0.292893	2	0.189
		2	0.292893	0	0.039
4		3	0.292893	2	0.149

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	2	1	0.292893	0	0.029
	3	1	0.292893	0	0.031
5	1	1	0.263932	66734	90.121
		2	0.263932	148214	193.866
		3	0.263932	215172	276.837
		4	0.263932	65538	88.375
	2	1	0.263932	76784	109.689
		2	0.263932	37504	54.856
	3	1	0.263932	92198	125.732
6	1	1	0.257359	1906674	6921.435
		2	0.257359	1488168	7200
		3	0.257359	1236873	7200
	2	1	0.257359	1421001	7200
		2	0.257359	1355560	7200
	3	1	0.257359	1364772	7200
	4	1	0.257359	1366459	7200

According to Table 2, the best results are obtained by different parameters m and i versus computation time. The best times for $N = 3$, $N = 4$, $N = 5$ and $N = 6$ are given by $(m, i) = (2, 1)$, $(m, i) = (2, 2)$ and $(m, i) = (1, 1)$, respectively. While the smallest number of noted in the search tree for instances of size $N = 3$, $N = 4$, $N = 5$ and $N = 6$ is obtained by $(m, i) = (2,1)$, $(m, i) = (1,2) = (2, 1) = (3, 1)$,$(m, i) = (2,2)$ and $(m, i) = (1, 3)$ respectively. Note also that for instance $N = 6$ the solver, returned an optimal solution in a CPU time equal to 6921.435 and for $(m, i) = (1, 1)$.

6. Conclusion

In this article, we explored the application of mathematical programming symmetry breaking techniques to the problem of packing equal spheres into a unit cube. Based on the fixed SBCs and Strong SBCs, we proposed new mixed SBCs, designed to better break the symmetric structure of the problem. The experimental results, obtained using the Couenne non-linear solver, show that these mixed constraints outperform conventional formulations and existing strong-sense and fixed-sense constraints, both in terms of computation time and reduction in the number of nodes explored in the Branch and Bound algorithm's search tree.

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