Packing circles in a square: a theoretical comparison of various convexification techniques

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Abstract

We consider the problem of packing congruent circles with the maximum radius in a unit square. As a mathematical program, this problem is a notoriously difficult nonconvex quadratically constrained optimization problem which possesses a large number of local optima. We study several convexification techniques for the circle packing problem, including polyhedral and semi-definite relaxations and assess their strength theoretically. As we demonstrate both theoretically and numerically, when embedded in branch-and-cut based global solvers, the current state-of-the-art bounding techniques are only effective for small-size circle packing problems.

Key words: Circle packing problem, Non-overlapping constraints, Polyhedral relaxations, Semi-definite relaxations, Boolean quadric polytope.

1 Introduction

The problem of finding the maximum radius \( r \) of \( n \) identical non-overlapping circles that fit in a unit square is a classic problem in discrete geometry. It is well-known that this problem can be equivalently stated as:

"Locate \( n \) points in a unit square, such that the minimum distance between any two points is maximal."

Denote by \((x_i, y_i), i \in \{1, \ldots, n\}\) the coordinate of the \(i\)th point to be located in the unit square. It then follows that the above problem can be stated as the following optimization problem:

\[
\text{(CP)} \quad \text{maximize} \quad \gamma \\
\text{subject to} \quad (x_j - x_i)^2 + (y_j - y_i)^2 \geq \gamma, \quad 1 \leq i < j \leq n, \\
\quad x \in [0, 1]^n, \quad y \in [0, 1]^n,
\]

where \( \gamma \) denotes the minimum squared pair-wise distance of the points in the unit square. The corresponding radius \( r \) for \( n \) circles that can be packed into the unit square is then given by \( r = \sqrt{\frac{\gamma}{2(1+\sqrt{\gamma})}} \). Throughout this paper, we refer to Problem (CP) as the Circle packing problem. In spite of its simple formulation, the Circle packing problem is a difficult nonconvex optimization problem with a large number of locally optimal solutions. This nonconvexity is due to the presence of the non-overlapping constraints defined by (1). In fact, non-overlapping constraints appear in a variety of applications including circular cutting, communication networks and facility layout problems (see [2] for a detailed review of industrial applications).

The Circle packing problem and its variants have been studied extensively by the optimization community; several customized stochastic and deterministic algorithms have been proposed to find high quality solutions for this problem (cf. [11] for a review of the existing optimization techniques). Yet, we are unable to solve Problem (CP) to global optimality for \( n > 10 \) with any of the state-of-the-art general-purpose global solvers [8, 6, 13] within a few hours of CPU-time. This surprisingly poor performance is mainly due to the generation of weak upper bounds on the optimal value of \( \gamma \), which in turn is caused by our inability to effectively convexify a collection of non-overlapping constraints.

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In this paper, we perform a systematic study of the existing techniques to convexify a nonconvex set defined by a collection of non-overlapping constraints. We consider various polyhedral and semi-definite relaxations of the Circle packing problem; interestingly, we are able to solve these relaxations analytically and conduct a theoretical assessment of their relative strength. Moreover, we investigate the effect of symmetry-breaking constraints based on tightened variable bounds and/or order constraints on the quality of these relaxations. As we detail in the following sections, the best polyhedral and semi-definite relaxations are obtained via a certain combination of the two types of symmetry-breaking constraints.

In Section 2, we consider relaxations of Problem (CP) obtained by replacing each non-overlapping constraint with its convex hull over the corresponding domain. We refer to such relaxations as single-row polyhedral relaxations of the Circle packing problem. We demonstrate that the upper bounds given by such relaxations are quite weak, confirming their ineffectiveness when embedded in global solvers. In Section 3, we propose tighter polyhedral relaxations of Problem (CP) by convexifying multiple non-overlapping constraints simultaneously. Namely, we consider a reformulation of the Circle packing problem whose relaxation is closely related to the Boolean quadric polytope [7], a well-studied polytope in combinatorial optimization. By building upon existing results on the facial structure of the Boolean quadric polytope, we present multi-row polyhedral relaxations of the Circle packing problem whose quality is significantly better than single-row counterparts. In Section 4, we examine the strength of semi-definite programming (SDP) relaxations for the Circle packing problem. We show that the upper bounds achieved by these relaxations are identical or worse than the bounds obtained by the proposed polyhedral relaxations. Finally, in Section 5, we incorporate our best multi-row polyhedral relaxations in the global solver BARON [8] and demonstrate their impact on the convergence rate of the branch-and-cut tree for Circle packing problems with $3 \leq n \leq 20$.

2 Single-row polyhedral relaxations

The basic approach. Perhaps the most intuitive approach to obtain a polyhedral relaxation for the Circle packing problem is to replace the nonconvex set defined by a single non-overlapping constraint by its convex hull. Denote by $\text{conv}(C)$ the convex hull of a nonconvex set $C$ and denote $\text{conc}_X f$ the concave envelope of the function $f$ over the convex set $X$. It is simple to show that the concave envelope of a convex quadratic of the form $f(u) = (u_1 - u_2)^2$ over the box $u \in \mathcal{H} = [0, 1]^2$ is given by $\text{conc}_H f(u) = \min\{u_1 + u_2, 2 - u_1 - u_2\}$. As the non-overlapping constraints are separable in $x$ and $y$ variables, we have

$$\text{conv}\{x_i, x_j, y_i, y_j, \gamma : (x_j - x_i)^2 + (y_j - y_i)^2 \geq \gamma, x \in [0, 1]^2, y \in [0, 1]^2\} = \{ (x_i, x_j, y_i, y_j, \gamma : \text{conc}_H f(x) + \text{conc}_H f(y) \geq \gamma, x \in [0, 1]^2, y \in [0, 1]^2\}$$

It then follows that the following linear program (LP) provides an upper bound on the optimal value of Problem (CP):

\[
\begin{align*}
\text{(TW)} \quad & \text{maximize} & & \gamma \\
& \text{subject to} & & x_i + x_j + y_i + y_j \geq \gamma \\
& & & -x_i - x_j + y_i + y_j + 2 \geq \gamma \\
& & & x_i + x_j - y_i - y_j + 2 \geq \gamma \\
& & & -x_i - x_j - y_i - y_j + 4 \geq \gamma \\
& & & 0 \leq x \leq 1, 0 \leq y \leq 1.
\end{align*}
\]

We now show that the optimal value of Problem (TW) is $\gamma^* = 2$ for all $n \geq 2$. From the constraint set of the above LP, consider the set of four inequalities associated with a pair of points indexed by $(i, j)$. Together with the lower and upper bounds on $x$ and $y$ variables, over this particular constraint set, the maximum of $\gamma$ is attained when all four inequalities are binding, implying $x_i + x_j = 1$ and $y_i + y_j = 1$. It follows that $\gamma^* \leq 2$. In addition, the point $\bar{x}_i = \bar{y}_i = \frac{1}{2}$, for $i = 1, \ldots, n$, with $\bar{\gamma} = 2$ is feasible for (TW). Hence, $\gamma^* = 2$ for all $n \geq 2$.

Remark 1. Define $X_{ij} = x_ix_j$ (resp. $Y_{ij} = y_iy_j$), for all $1 \leq i \leq j \leq n$. We replace the set \{(x_i, x_j, X_{ij}) : X_{ij} \geq x_ix_j, x \in [0, 1]^2\} (resp. \{(y_i, y_j, Y_{ij}) : Y_{ij} \geq y_iy_j, y \in [0, 1]^2\}) by its convex hull for all $1 \leq i < j \leq n$. Similarly, we replace the set \{(x_i, X_{ii}) : X_{ii} \leq x_i^2, x \in [0, 1]\} (resp. \{(y_i, Y_{ii}) : Y_{ii} \leq y_i^2, y \in [0, 1]\}) by its
convex hull for all \(1 \leq i \leq n\) to obtain the following relaxation of the feasible region of Problem (CP) in the lifted space \((x, y, X, Y, \gamma)\):

\[
S = \left\{ (x, y, X, Y, \gamma) : \begin{array}{l}
X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \ X_{ij} \geq 0, \\
x_{ij} \geq x_i + x_j - 1, \ Y_{ij} \geq 0, \ Y_{ij} \geq y_i + y_j - 1, \ \forall 1 \leq i < j \leq n, \ X_{ii} \leq x_i, \\
Y_{ii} \leq y_i, \ \forall 1 \leq i \leq n \end{array} \right\}.
\]

It is simple to verify that the projection of \(S\) onto the \((x, y, \gamma)\) space is given by the constraint set of Problem (TW). This lifted relaxation is often referred to as the first-level Reformulation Linearization Technique (RLT) relaxation \([10]\) of the Circle packing problem and is utilized by most of the general-purpose global solvers to find upper bounds for this problem.

Clearly, the Circle packing problem is highly symmetric. It has been observed that utilizing symmetry-breaking constraints is beneficial for solving this problem to global optimality \([1, 3]\). In the following, we present sharper polyhedral relaxations for Problem (CP) by utilizing a couple of simple symmetry-breaking type constraints.

**Tight variable bounds.** Let \(n_x = \lceil n/2 \rceil\) and \(n_y = \lceil n_x/2 \rceil\). By symmetry, we can assume that at any optimal solution of Problem (CP)

\[
0 \leq x_i \leq \frac{1}{2}, \quad i = 1, \ldots, n_x,
\]

and

\[
0 \leq y_i \leq \frac{1}{2}, \quad i = 1, \ldots, n_y.
\]

Utilizing the above bounds on \(x\) and \(y\) variables and replacing each bivariate quadratic by its concave envelope over the corresponding box we obtain the following relaxation of Problem (CP):

\[
\text{(TWbd)} \quad \text{maximize} \quad \gamma \\
\text{subject to} \quad \begin{array}{l}
x_i + x_j + y_i + y_j \geq 2\gamma \\
x_i + x_j - y_i - y_j + 1 \geq 2\gamma \\
x_i - x_j + y_i + y_j \geq 1 \geq 2\gamma \\
x_i - x_j - y_i - y_j + 2 \geq 2\gamma \\
1 \leq i < j \leq n_y \quad (i)
\end{array}
\]

\[
\begin{array}{l}
x_i + x_j + y_i + 2y_j \geq 2\gamma \\
x_i + x_j - 3y_i + 2 \geq 2\gamma \\
x_i - x_j + y_i + 2y_j + 1 \geq 2\gamma \\
x_i - x_j - 3y_i + 3 \geq 2\gamma \\
1 \leq i \leq n_y < j \leq n_x \quad (ii)
\end{array}
\]

\[
\begin{array}{l}
x_i + 2x_j + y_i + 2y_j \geq 2\gamma \\
x_i + 2x_j - 3y_i + 2 \geq 2\gamma \\
x_i - x_j + y_i + 2y_j + 2 \geq 2\gamma \\
x_i - x_j - 3y_i + 4 \geq 2\gamma \\
1 \leq i \leq n_y < n_x < j \quad (iii)
\end{array}
\]

\[
\begin{array}{l}
x_i + x_j + 2y_i + 2y_j \geq 2\gamma \\
x_i + x_j - 2y_i - 2y_j + 4 \geq 2\gamma \\
x_i - x_j + 2y_i + 2y_j + 1 \geq 2\gamma \\
x_i - x_j - 2y_i - 2y_j + 5 \geq 2\gamma \\
1 \leq n_y < i < j \leq n_x \quad (iv)
\end{array}
\]

\[
\begin{array}{l}
x_i + 2x_j + 2y_i + 2y_j \geq 2\gamma \\
x_i + 2x_j - 2y_i - 2y_j + 4 \geq 2\gamma \\
x_i - 3x_i + 2y_i + 2y_j + 2 \geq 2\gamma \\
x_i - 3x_i - 2y_i - 2y_j + 6 \geq 2\gamma \\
1 \leq n_y \leq n_x < j \quad (v)
\end{array}
\]

\[
\begin{array}{l}
x_i + x_j + y_i + y_j \geq \gamma \\
x_i + x_j - y_i - y_j + 2 \geq \gamma \\
x_i - x_j + y_i + y_j + 2 \geq \gamma \\
x_i - x_j - y_i - y_j + 4 \geq \gamma \\
1 \leq i < j \leq n \quad (vi)
\end{array}
\]
Suppose that \( n \geq 5 \), so that \( n_y \geq 2 \); i.e., there exists at least one pair \((i, j)\) satisfying inequalities (i) defined above; from these inequalities, it follows that \( \gamma^* \leq \tilde{\gamma} = \frac{4}{3} \). In addition, if \( \tilde{\gamma} \) is attained, we have \( x_i + x_j = \frac{4}{3} \) and \( y_i + y_j = \frac{1}{3} \) for all \( 1 \leq i < j \leq n_y \). We now show that \( \gamma \) is a sharp upper bound by providing a feasible point of Problem (TW\text{bnd}) that attains this bound. Let \( \tilde{x}_i = \tilde{y}_i = \frac{1}{3} \) for \( 1 \leq i \leq n_y \) and \( \tilde{x}_i = \tilde{y}_i = \frac{1}{2} \) for \( n_y < i \leq n \). Observe that \( \tilde{x}_i = \tilde{y}_i = \frac{1}{3} \) and \( \tilde{x}_j = \tilde{y}_j = \frac{1}{2} \) for all \((i, j)\) satisfying the conditions of constraint sets (ii) and (iii). In addition, the left-hand side of constraints (ii) is smaller than that of (iii) at any point with \( x_i \leq \frac{1}{3} \). Using a similar argument we conclude that if the constraint set (iv) is satisfied at \((\tilde{x}, \tilde{y})\) then (v) and (vi) hold too. Hence, it suffices to check the validity of (ii) and (iv) at \((\tilde{x}, \tilde{y}, \gamma)\). It is simple to verify that the value of the left-hand side of the first two inequalities of (ii) (resp. (iv)) is equal to 2.0 (resp. 3.0), while the value of the last two is equal to \( \frac{4}{3} \) (resp. 2.0). Thus, the optimal value of Problem (TW\text{bnd}) is given by \( \gamma^* = \frac{4}{3} \).

**Remark 2.** An equivalent formulation of Problem (TW\text{bnd}) in a lifted space can be obtained by utilizing the first-level RLT constraints of the Circle packing problem over the domain defined by (2) and (3). That is, the projection of the set \( S_{\text{bnd}} \) defined by the following inequalities

\[
\begin{align*}
X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} & \geq \gamma, \quad 1 \leq i < j \leq n \\
X_{ij} & \geq 0, \quad Y_{ij} \geq 0, \quad 1 \leq i < j \leq n \\
X_{ii} & \leq x_i, \quad Y_{ii} \leq y_i, \quad 1 \leq i \leq n \\
X_{ij} & \geq x_i/2 + x_j/2 - 1/4, \quad 1 \leq i < j \leq n_x \\
X_{ij} & \geq x_i + x_j/2 - 1/2, \quad 1 \leq i \leq n_x < j \\
X_{ij} & \geq x_i + x_j - 1, \quad X_{ij} \leq x_i, \quad n_x < i < j \leq n \\
Y_{ij} & \geq y_i/2 + y_j/2 - 1/4, \quad 1 \leq i < j \leq n_y \\
Y_{ij} & \geq y_i + y_j/2 - 1/2, \quad 1 \leq i \leq n_y < j \\
Y_{ij} & \geq y_i + y_j - 1, \quad n_y < i < j \leq n,
\end{align*}
\]

onto the \((x, y, \gamma)\) space coincides with the feasible region of Problem (MT\text{bnd})

**Order constraints.** Next, we study the impact another type of symmetry breaking constraints on the quality of single-row polyhedral relaxations for the Circle packing problem. Clearly, we can always impose an order on \( x \) (or \( y \)) variables by adding the inequalities

\[
0 \leq x_1 \leq x_2 \leq \cdots \leq x_n \leq 1,
\]

(4) to Problem (CP). Subsequently, we replace each bivariate quadratic of the form \( f(x) = (x_j - x_i)^2 \), by its concave envelope over the triangular region \( 0 \leq x_i \leq x_j \leq 1 \), and each bivariate quadratic of the form \( f(y) = (y_j - y_i)^2 \), by its concave envelope over the unit hypercube to obtain the following relaxation of (CP):

\[
\text{(TWord)} \quad \text{maximize} \quad \gamma \\
\text{subject to} \quad \begin{align*}
x_j - x_i + y_i + y_j & \geq \gamma \\
x_j - x_i - y_i - y_j + 2 & \geq \gamma
\end{align*}, \quad 1 \leq i < j \leq n \\
0 \leq x_1 \leq \cdots \leq x_n \leq 1 \\
0 \leq y \leq 1.
\]

To find the optimal value of Problem (TWord), we first find an upper bound on its objective function value by considering a specific subset of the constraints and subsequently show that this upper bound is indeed sharp by providing a feasible point of (TWord) that attains the same objective value. Consider the following inequalities

\[
\begin{align*}
x_{i+1} - x_i + y_i + y_{i+1} & \geq \gamma \\
x_{i+1} - x_i - y_i - y_{i+1} + 2 & \geq \gamma
\end{align*}, \quad 1 \leq i < n
\]

We would like to find the maximum value of \( \gamma \) over the region defined by these inequalities together with the lower and upper bounds on \( x \) and \( y \) variables. Let \((\tilde{x}, \tilde{y}, \tilde{\gamma})\) denote the optimal solution of this auxiliary
The optimal value of the above problem is attained at $\tilde{x}$.

We can strengthen this relaxation by utilizing the order constraints given by (TWord), we obtain

$$\tilde{x}_i + \tilde{x}_{i+1} = 1, \quad \forall i \in \{1, \ldots, n-1\},$$

which in turn implies $\tilde{y}_i = \tilde{y}_i = \ldots = \tilde{y}_{2k+1}$ and $\tilde{y}_2 = \tilde{y}_4 = \ldots = \tilde{y}_{2k}$ for all $k \in \{1, \ldots, \lfloor n/2 \rfloor \}$. Furthermore, $\tilde{x}_{i+1} - \tilde{x}_i + \tilde{x}_i + \tilde{x}_{i+1} = \tilde{x}_{i+2} - \tilde{x}_i + \tilde{y}_i + \tilde{y}_{i+2}$ for all $i = 1, \ldots, n - 2$. Since $\tilde{y}_i = \tilde{y}_{i+2}$, it follows that $\tilde{x}_{i+1} - \tilde{x}_i = \tilde{x}_{i+2} - \tilde{x}_i$ or equivalently $\tilde{x}_{i+1} = \Delta x$ for $i = 1, \ldots, n - 1$. Thus, $\tilde{\gamma}$ can be found by solving the following problem:

$$\text{maximize} \quad 1 + \Delta x$$
$$\text{subject to} \quad x_{i+1} - x_i \geq \Delta x, \quad 1 \leq i < n$$
$$0 \leq x_1, x_n \leq 1.$$

The optimal value of the above problem is attained at $\tilde{x}_i = \frac{i - 1}{n - 1}$, $i = 1, \ldots, n$ and is given by $\tilde{\gamma} = 1 + \frac{1}{n-1}$. Next, we utilize $(\tilde{x}, \tilde{y}, \tilde{\gamma})$ to construct a feasible solution of (TWord). Substituting $(\tilde{x}, \tilde{y}, \tilde{\gamma})$ in the remaining constraints of (TWord), we obtain

$$1 - \frac{i - 1}{n - 1} \leq \tilde{y}_i + \tilde{y}_i \leq 1 + \frac{i - 1}{n - 1}$$
for all $j > i + 1$. It follows that $(\tilde{x}, \tilde{y}, \tilde{\gamma})$ is feasible for (TWord), provided that

$$1 - \frac{1}{n - 1} \leq \tilde{y}_i + \tilde{y}_i \leq 1 + \frac{1}{n - 1}, \quad \forall j > i + 1$$

Two cases arise:

(i) if $i$ is an even (resp. odd) number and $j$ is odd (resp. even), then by (5) we have $\tilde{y}_i + \tilde{y}_i = 1$ and condition (6) is clearly satisfied,

(ii) if $i$ and $j$ are both even (or odd) numbers, then by (5) we have $\tilde{y}_i + \tilde{y}_i = 2\tilde{y}_i$. Therefore, inequality (6) simplifies to $\frac{1}{2}(1 - \frac{1}{n-1}) \leq \tilde{y}_i \leq \frac{1}{2}(1 + \frac{1}{n-1})$, $i = 1, \ldots, n$.

Hence, a feasible solution of (TWord) with $\tilde{\gamma} = 1 + \frac{1}{n-1}$ can be obtained by letting $\tilde{x}_i = \frac{i - 1}{n - 1}$, and $\tilde{y}_i = \frac{1}{2}$ for all $i = 1, \ldots, n$, implying that the optimal value of Problem (TWord) is given by:

$$\gamma^* = 1 + \frac{1}{n - 1}.$$

**Remark 3.** Consider the first-level RLT relaxation of the feasible region of Problem (CP) defined in Remark 1. We can strengthen this relaxation by utilizing the order constraints given by (4) to generate the following RLT-type constraints:

$$X_{ii} \leq X_{ij},$$
$$x_i - X_{ij} \leq x_j - X_{jj},$$

$$1 \leq i < j \leq n.$$

Suppose that we add the above inequalities to the set $S$ defined in Remark 1. Then it can be shown that the projection of this new set onto the $(x, y, \gamma)$ space is given by the feasible region of (TWord). We should remark that using inequalities (4) together with the bounds on $x$ variables, one can construct many more RLT-type inequalities. However, it can be shown that all such inequalities are redundant in the sense that they do not improve the quality of the bound obtained by the corresponding relaxation.

**Best single-row polyhedral relaxations** It is not surprising that combining the two aforementioned symmetry-breaking constraints leads to a stronger relaxation of Problem (CP). In the following, we analyze the quality of the bound given by such a relaxation. Suppose that $n \geq 5$ so that $n_y \geq 2$. Let $x_i \leq \frac{1}{2}$ for $i = 1, \ldots, n_x$ and $\gamma_i \leq \frac{1}{2}$ for $i = 1, \ldots, n_y$. If we impose these restricted bounds on both $x$ and $y$ variables, then $x_{n_y} \leq x_{n_y+1}$ is no longer valid. Thus, we impose the order constraints as follows

$$x_i \leq x_{i+1}, \quad \forall i \in \{1, \ldots, n - 1\} \setminus \{n_y\}.$$
Subsequently, we replace each quadratic term by its concave envelope over the corresponding rectangular, triangular or trapezoidal domain to obtain the following relaxation:

\[(\text{TWcomb}) \quad \text{maximize} \quad \gamma \]
\[\text{subject to} \quad \begin{align*}
    x_j - x_i + y_i + y_j &\geq 2\gamma, & 1 \leq i < j \leq n_y & \quad (i) \\
    x_j - x_i - y_i - y_j + 1 &\geq 2\gamma \\
    x_i + x_j + y_i + 2y_j &\geq 2\gamma \\
    x_i + x_j - 3y_i + 2 &\geq 2\gamma \\
    -x_i - x_j + y_i + 2y_j + 1 &\geq 2\gamma \\
    -x_i - x_j - 3y_i + 3 &\geq 2\gamma \\
    x_i + 2x_j + y_i + 2y_j &\geq 2\gamma \\
    x_i + 2x_j - 3y_i + 2 &\geq 2\gamma \\
    -3x_i + y_i + 2y_j + 2 &\geq 2\gamma \\
    -3x_i - 3y_i + 4 &\geq 2\gamma \\
    x_j - x_i + 2y_i + 2y_j &\geq 2\gamma \\
    x_j - x_i - 2y_i - 2y_j + 4 &\geq 2\gamma \\
    x_j - x_i + 2y_i + 2y_j &\geq 2\gamma \\
    2x_j - 3x_i + 2y_i + 2y_j &\geq 2\gamma \\
    2x_j - 3x_i - 2y_i - 2y_j + 4 &\geq 2\gamma \\
    x_j - x_i + y_i + y_j &\geq \gamma \\
    x_j - x_i - y_i - y_j + 2 &\geq \gamma \\
\end{align*} \quad , \quad \begin{align*}
    1 \leq i \leq n_y < j < n_x \quad (ii) \\
    1 \leq i \leq n_y < n_x < j \quad (iii) \\
    1 \leq i < j \leq n_x \quad (iv) \\
    n_y < i < j < n_x \quad (v) \\
    n_x < i < j < n \quad (vi) \quad \begin{align*}
    0 \leq x \leq 1, 0 \leq y \leq 1.
\end{align*} \quad \begin{align*}
\end{align*}
\]

As in the previous case, to characterize an optimal solution of Problem (TWcomb), we first infer an upper bound on its objective value using the constraint set (i) and subsequently show that this upper bound is sharp by providing a corresponding feasible solution. Consider the following inequalities present the constraint set (i):

\[
\begin{align*}
    x_{i+1} - x_i + y_i + y_{i+1} &\geq 2\gamma \\
    x_i - x_i - y_i - y_{i+1} + 1 &\geq 2\gamma,
\end{align*}
\]

for all \(1 \leq i < n_y\). It follows that \(\gamma^* \leq \tilde{\gamma} = \frac{1}{4}(1 + \frac{1}{n_y-1})\), and this upper bound is attained when \(x_{i+1} - x_i = \frac{1}{2(n_y-1)}\) and \(y_i + y_{i+1} = \frac{1}{2}\) for all \(i < n_y\). Now, consider the point \(\tilde{x}_i = \frac{i-1}{2(n_y-1)}, \tilde{y}_i = \frac{1}{4}\) for \(i = 1, \ldots, n_y\) and \(\tilde{x}_i = \tilde{y}_i = \frac{1}{2}\) for \(i = n_y + 1, \ldots, n\), and \(\tilde{\gamma} = \frac{1}{4}(1 + \frac{1}{n_y-1})\). We show that \((\tilde{x}, \tilde{y}, \tilde{\gamma})\) is feasible for the above LP. For the constraint sets (ii) and (iii), we have \(\tilde{x}_i = \frac{i-1}{2(n_y-1)}, \tilde{y}_i = \frac{1}{4}\) and \(\tilde{x}_j = \tilde{y}_j = \frac{1}{2}\). In addition, (ii) implies (iii) at any point with \(x_i \leq \frac{1}{2}\). Similarly, it can be shown that (v) implies (iv) and (vi). Thus, it suffices to verify the validity of (ii) and (v) at \((\tilde{x}, \tilde{y}, \tilde{\gamma})\). Clearly, \(\tilde{\gamma} \leq \frac{1}{2}\). First, consider the constraint set (ii); for this subset, we have \(\tilde{x}_i + \tilde{x}_j \leq 1\). In addition, \(\tilde{y}_i + 2\tilde{y}_j = 2 - 3\tilde{y}_i = \frac{4}{3} > 2\tilde{\gamma}\). Thus, (ii) holds at this point. For the constraint set (v) we have \(\tilde{x}_i = \tilde{x}_j = \tilde{y}_i = \tilde{y}_j = \frac{1}{2}\). Thus, the left-hand side of the first two inequalities is equal to 2.0, while the left-hand side of the last two inequalities is equal to \(\frac{4}{3}\), which in turn implies (v) holds at \((\tilde{x}, \tilde{y}, \tilde{\gamma})\). Hence, the optimal value of Problem (TWcomb) is given by

\[
\gamma^* = \frac{1}{4}(1 + \frac{1}{n_y-1}).
\]

Remark 4. Define the set \(\mathcal{I} = \{(i, j) : 1 \leq i < j \leq n_y\} \cup \{(i, j) : n_y + 1 \leq i < j \leq n\}\). An equivalent extended formulation for Problem (TWcomb) can be obtained by adding the following RLT-type constraints to the set \(\mathcal{S}_{\text{comb}}\) defined in Remark 2:

\[
\begin{align*}
    X_{ii} &\leq X_{ij}, \quad \forall (i, j) \in \mathcal{I} \\
    \frac{x_i}{2} - X_{ij} &\leq \frac{x_j}{2} - X_{jj}, \quad \forall (i, j) \in \mathcal{I} \quad \text{with} \quad j \leq n_x \\
    x_i - X_{ij} &\leq x_j - X_{jj}, \quad \forall (i, j) \in \mathcal{I} \quad \text{with} \quad j > n_x.
\end{align*}
\]
Remark 5. In order to combine the order constraints (4) with the tighter variables bounds (2) and (3), we eliminated the order constraint $x_{ny} \leq x_{ny} + 1$, while keeping the rest of the symmetry-breaking constraints unchanged. There is an alternative method to combine these two types of symmetry-breaking constraints: we can impose the order constraints in their original form as defined by (4) as well as tighter variable bounds on $x$ variables as defined by (2), but do not impose any tighter bounds on $y$ variables. Subsequently, to obtain a relaxation of the Circle packing problem, we replace each bivariate quadratic with its concave envelope over the corresponding domain. It can be shown that the optimal value of this relaxation is $\gamma^* = 1 + \frac{1}{4(n_y - 1)}$, which is strictly larger than the optimal value of Problem (MTcomb). Hence, we do not pursue this approach throughout the paper.

We summarize the results of this section in the following theorem. We should remark that Anstreicher [1] conjectured these upper bounds and verified them numerically for $3 \leq n \leq 50$.

Theorem 1. Consider the single-row polyhedral relaxations of the Circle packing problem defined above:

(i) Let $n \geq 2$. Then the optimal value of Problem (TW) is attained at $x_i^* = y_i^* = \frac{1}{2}$, $i = 1, \ldots, n$, and is equal to
$$\gamma^* = 2.$$ 

(ii) Let $n \geq 2$. Then the optimal value of Problem (TWord) is attained at $x_i^* = \frac{i-1}{n-1}$, $y_i^* = \frac{1}{2}$, for all $i = 1, \ldots, n$, and is equal to
$$\gamma^* = 1 + \frac{1}{n-1}.$$ 

(iii) Let $n \geq 5$. Then an optimal solution of Problem (TWbnd) is given by $x_i^* = y_i^* = \frac{1}{4}$ for $1 \leq i \leq n_y$, and $x_i^* = y_i^* = \frac{1}{2}$ for $n_y + 1 \leq i \leq n$ and its optimal value is equal to
$$\gamma^* = \frac{1}{2}.$$ 

(iv) Let $n \geq 5$. Then the optimal value of Problem (TWcomb) is
$$\gamma^* = \frac{1}{4} \left( 1 + \frac{1}{\lfloor (n-1)/4 \rfloor} \right),$$
and an optimal solution is attained at $x_i^* = \frac{i-1}{2(n_y - 1)}$, $y_i^* = \frac{1}{4}$, for $1 \leq i \leq n_y$, and $x_i^* = y_i^* = \frac{1}{2}$ for $n_y + 1 \leq i \leq n$.

3 Multi-row polyhedral relaxations

In this section, we introduce stronger polyhedral relaxations of the Circle packing problem by convexifying multiple non-overlapping constraints simultaneously. This is in contrast with the polyhedral relaxations studied in the Section 2, where the feasible region defined by a single constraint was replaced by its convex hull over rectangular or triangular domains. We start by introducing a reformulation of Problem (CP) which will be crucial for the later developments:

$$(\text{CPr}) \quad \text{maximize} \quad \gamma \\
\text{subject to} \quad (x_j - x_i)^2 + (y_j - y_i)^2 \geq \beta_{ij}, \quad 1 \leq i < j \leq n, \quad \beta_{ij} \geq \gamma, \quad 1 \leq i < j \leq n, \quad x \in [0,1]^n, \quad y \in [0,1]^n.$$ 

Denote by $\mathcal{X}$ the feasible region of Problem (CPr) and define the sets
$$\mathcal{P} = \{(x, y, \beta, \gamma) : (x_j - x_i)^2 + (y_j - y_i)^2 \geq \beta_{ij}, \quad \forall 1 \leq i < j \leq n, \quad x, y \in [0,1]^n\}$$
and
\[ \mathcal{K} = \{(x, y, \beta, \gamma) : \beta_{ij} \geq \gamma, \forall 1 \leq i < j \leq n, x, y \in \mathbb{R}^n \}. \]

Clearly, \( \text{conv}(\mathcal{X}) = \text{conv} (\mathcal{P} \cap \mathcal{K}) \) and \( \mathcal{K} \) is a convex cone. This in turn implies \( \text{conv}(\mathcal{P}) \cap \mathcal{K} \supseteq \text{conv}(\mathcal{X}) \), and hence \( \text{conv}(\mathcal{P}) \cap \mathcal{K} \) is potentially a good relaxation for the feasible region of the Circle packing problem. In the following, we characterize the convex hull of \( \mathcal{P} \). To this end, consider the set
\[ \mathcal{Q} = \left\{(x, y, X, Y) : x_i^2 \geq X_{ii}, y_i^2 \geq Y_{ii}, \forall 1 \leq i \leq n, \right. \]
\[ \left. X_{ij} \geq x_ix_j, \ Y_{ij} \geq y_iy_j, \forall 1 \leq i < j \leq n, \ x, y \in [0, 1]^n \right\}. \]

To characterize \( \text{conv}(\mathcal{P}) \), it suffices to characterize \( \text{conv}(\mathcal{Q}) \), as \( \mathcal{P} \) is the image of \( \mathcal{Q} \) under a linear mapping \( \mathcal{L} \), and we have \( \text{conv}(\mathcal{P}) = \text{conv}(\mathcal{L}\mathcal{Q}) = \mathcal{L}\text{conv}(\mathcal{Q}) \). Now consider the set \( \hat{\mathcal{Q}} \) denote by \( \mathcal{Q}_x \) (resp. \( \mathcal{Q}_y \)), the set obtained by dropping the inequalities containing \((y, Y)\) variables (resp. \((x, X)\) variables) from the description of \( \mathcal{Q} \). It then follows that \( \text{conv}(\mathcal{Q}) = \text{conv}(\mathcal{Q}_x) \cap \text{conv}(\mathcal{Q}_y) \). Let \( \mathcal{Q}_x \) denote the projection of \( \mathcal{Q}_x \) onto the \((x, X)\) space and define the two sets
\[ \mathcal{Q}^{b}_x = \{(x, X) : X_{ij} \geq x_ix_j, \forall 1 \leq i < j \leq n, \ x \in [0, 1]^n \} \]
and
\[ \mathcal{Q}^{c}_x = \{(x, X) : X_{ii} \leq x_i^2, \forall 1 \leq i \leq n, \ x \in [0, 1]^n \}. \]

Clearly, \( \text{conv}(\mathcal{Q}^{b}_x) = \{(x, X) : X_{ii} \leq x_i, \forall 1 \leq i \leq n, \ x \in [0, 1]^n \} \). Moreover, \( \text{conv}(\mathcal{Q}_x) = \text{conv}(\mathcal{Q}^{b}_x) \cap \text{conv}(\mathcal{Q}^{c}_x) \), as the projection of each point in the convex hull of \( \{(x_i, X_{ii}) : X_{ii} \leq x_i^2, x_i \in [0, 1] \} \) onto the \( x_i \) space can be uniquely written as a convex combination of the two end points of [0, 1].

Now consider the convex hull of \( \mathcal{Q}^{b}_x \). It is simple to show that \( \text{conv}(\mathcal{Q}^{b}_x) \) is polyhedral and the projection of its vertices onto the space of \( x \) variables coincides with the vertices of the unit hypercube. It then follows that \( \text{conv}(\mathcal{Q}^{b}_x) \) is a relaxation of the Boolean quadratic polytope [7] defined as
\[ BQP = \text{conv}\{(x, X) : X_{ij} = x_ix_j, \forall 1 \leq i < j \leq n, \ x \in \{0, 1\}^n \}. \]

In fact, the facets of \( \text{conv}(\mathcal{Q}^{b}_x) \) are precisely those of the Boolean quadric polytope of the form \( ax + bX \leq c \) with \( b_{ij} \leq 0 \), for all \( 1 \leq i < j \leq n \). To see this, first note that both \( \text{conv}(\mathcal{Q}^{b}_x) \) and \( BQP \) have the same set of vertices; however, while the Boolean quadric polytope is bounded, \( \text{conv}(\mathcal{Q}^{b}_x) \) is an unbounded polyhedron whose recession cone is given by \( \{X_{ij} \geq 0, \forall 1 \leq i < j \leq n\} \). It then follows that a facet-defining inequality for \( BQP \) defines a facet of \( \text{conv}(\mathcal{Q}^{b}_x) \) if and only if it is valid for \( \text{conv}(\mathcal{Q}^{b}_x) \). To see this, suppose that \( ax + bX \leq c \) defines a facet of the Boolean quadric polytope and \( b_{ij} > 0 \) for some \( 1 \leq i < j \leq n \). Consider a point \( (\hat{x}, \hat{X}) \in BQP \). It then follows that we can construct a point in \( \text{conv}(\mathcal{Q}^{b}_x) \) by making the value of \( \hat{X}_{ij} \) arbitrarily large while keeping all other components unchanged, so as to violate \( ax + bX \leq c \). Symmetrically, we obtain a characterization of \( \text{conv}(\mathcal{Q}^{c}_y) \).

Hence, the following relaxation of Problem (CPr)
\[
\text{maximize} \quad \gamma \\
\text{subject to} \quad (x, y, \beta, \gamma) \in \text{conv}(\mathcal{P}) \cap \mathcal{K}
\]
can be equivalently written as
\[
\text{(MT)} \quad \text{maximize} \quad \gamma \\
\text{subject to} \quad X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \ 1 \leq i < j \leq n \\
(x, X) \in \text{conv}(\mathcal{Q}^{b}_x) \\
(y, Y) \in \text{conv}(\mathcal{Q}^{c}_y) \\
X_{ii} \leq x_i, \ Y_{ii} \leq y_i, \ 1 \leq i \leq n.
\]

We now analyze the quality of the bound given by the above relaxation. First, note that there exist optimal solutions of Problem (MT) at which all inequalities (9) are binding, as otherwise we can increase the \( \beta_{ij} \) corresponding to any inactive constraint without decreasing the objective value. Moreover, at such
Summing up over that are facet-defining for $\text{conv}(Q)$, we can also assume that $X_{ii} = x_i$ and $Y_{ii} = y_i$ for all $1 \leq i \leq n$. Finally, due to the symmetry of the constraint set of Problem (MT) in $(x, X)$ and $(y, Y)$ variables, there exist optimal solutions with

$$x_i - 2X_{ij} + x_j = y_i - 2Y_{ij} + y_j = \frac{\gamma}{2}, \quad \forall 1 \leq i < j \leq n.$$ 

Summing up over $x_i - 2X_{ij} + x_j = \gamma/2$ for all $1 \leq i < j \leq n$, we obtain

$$\frac{(n-1)}{2} \sum_{i=1}^{n} x_i - \sum_{1 \leq i < j \leq n} X_{ij} = \frac{n(n-1)}{8} \gamma.$$ 

Thus, an optimal solution of (MT) can be obtained by solving the following problem:

$$(\text{MTx}) \quad \text{maximize} \quad \frac{8}{n(n-1)} \left( \frac{(n-1)}{2} \sum_{i=1}^{n} x_i - \sum_{1 \leq i < j \leq n} X_{ij} \right)$$

subject to

$$(x, X) \in \text{conv}(Q^b)$$

$$x_i - 2X_{ij} + x_j = x_j - 2X_{jk} + x_k, \quad \forall 1 \leq i < j < k \leq n.$$ 

Let $I$ denote a subset of $\{1, \ldots, n\}$ with $|I| \geq 3$ and let $\alpha$ be an integer with $1 \leq \alpha \leq |I| - 2$. It is well-known that the following so-called clique inequalities

$$\alpha \sum_{i \in I} x_i - \sum_{i,j \in I, i<j} X_{ij} \leq \alpha(\alpha + 1)$$

are facet-defining for the Boolean quadric polytope [7]. Since the coefficients of $X_{ij}$ are nonpositive for all $1 \leq i < j \leq n$, it follows the clique inequalities define facets of $\text{conv}(Q^b)$ as well. Now suppose that $n$ is an odd number and $n \geq 3$, implying that $(n-1)/2$ is an integer and $(n-1)/2 \leq n - 2$. Letting $\alpha = (n-1)/2$, in (10) yields

$$\frac{(n-1)}{2} \sum_{i=1}^{n} x_i - \sum_{i,j \in I, i<j} X_{ij} \leq \frac{n(n-1)}{8}.$$ 

Since the objective function of Problem (MTx) is parallel to a facet of $\text{conv}(Q^b)$ defined by (11), it follows that an upper bound on the optimal value of this problem is given by $\bar{\gamma} = 1 + \frac{1}{n}$. Now, let $n \geq 4$ be an even number, and let $I$ denote a subset of $\{1, \ldots, n\}$ of cardinality $n - 1$. By summing up over $x_i - 2X_{ij} + x_j = \frac{\gamma}{2}$ for all $i, j \in I$ with $i < j$ and following a similar line of arguments, we obtain that for an even $n$, an upper bound on Problem (MTx) is given by $\bar{\gamma} = 1 + \frac{1}{n-1}$.

It is well-understood that the Boolean quadric polytope has a very complex structure. In fact, an explicit description for BQP is only available for $n \leq 6$ [4], implying that a closed-form description of $\text{conv}(Q^b)$, $n \geq 6$ is not available either. In the following, we first construct a relaxation of $\text{conv}(Q^b)$ and subsequently show that the upper bound $\bar{\gamma}$ defined above is sharp for this relaxation. Denote by $C_x$ the polytope defined by all inequalities of the form

$$\alpha \sum_{i=1}^{m} x_i - \sum_{1 \leq i < j \leq m} X_{ij} \leq \frac{\alpha(\alpha + 1)}{2}, \quad \forall m \in \{2, \ldots, n\}, \forall 1 \leq \alpha \leq \max\{m-2, 1\}$$

(12)

It is well-known that the above inequalities induce facets of the Boolean quadric polytope and hence are facet-defining for $\text{conv}(Q^b)$. In addition, these inequalities constitute all pure hypermetric-correlation inequalities that are facet-defining for $\text{conv}(Q^b)$ [4]. We should remark that $\text{conv}(Q^b) = C_x$ for $n \leq 4$ while $\text{conv}(Q^b) \subset C_x$ for $n \geq 5$. Consider the following relaxation of Problem (MT):

$$(\text{MT}_{\text{clique}}) \quad \text{maximize} \quad \gamma$$

subject to

$$(x, X) \in C_x$$

$$(y, Y) \in C_y$$

$X_{ii} \leq x_i, Y_{ii} \leq y_i, 1 \leq i \leq n.$$
Clearly, \( \tilde{\gamma} \) is valid upper bound on the optimal value of Problem \((\text{MT}^{\text{clique}})\) as well. Now suppose that \( n \) is an odd number and consider the point

\[
\tilde{x}_i = \tilde{y}_i = \frac{1}{2}(1 + \frac{1}{n}), \quad \forall \ i = 1, \ldots, n,
\]

\[
\tilde{X}_{ii} = \tilde{x}_i, \quad \forall \ i = 1, \ldots, n,
\]

\[
\tilde{Y}_{ii} = \tilde{y}_i, \quad \forall \ i = 1, \ldots, n,
\]

\[
\tilde{X}_{ij} = \tilde{Y}_{ij} = \frac{1}{2}(1 + \frac{1}{n}), \quad \forall \ 1 \leq i < j \leq n.
\]

Clearly, \( \tilde{x}_i - 2\tilde{X}_{ij} + \tilde{x}_j = \tilde{y}_i - 2\tilde{Y}_{ij} + \tilde{y}_j = \frac{\tilde{\gamma}}{2} = \frac{1}{2}(1 + \frac{1}{n}) \) for all \( 1 \leq i < j \leq n \). Thus, to prove the feasibility of \((\tilde{x}, \tilde{y}, \tilde{X}, \tilde{Y}, \tilde{\gamma})\) for Problem \((\text{MT}^{\text{clique}})\), we need to show that \((\tilde{x}, \tilde{X}) \in C_x tangled\) (or equivalently \((\tilde{y}, \tilde{Y}) \in C_y)\). To do so, it suffices to show that the optimal value of the following bivariate integer quadratic program is equal to zero:

\[
\begin{align*}
\text{maximize} & \quad -\frac{1}{8}(1 + \frac{1}{n})m^2 + \frac{1}{2}(1 + \frac{1}{n})\alpha m - \frac{1}{2}\alpha^2 + \frac{1}{8}(1 + \frac{1}{n})m - \frac{\alpha}{2} \\
\text{subject to} & \quad 1 \leq \alpha \leq m - 2 \\
& \quad 3 \leq m \leq n \\
& \quad \alpha, \ m, \ \text{integer}.
\end{align*}
\]

It is simple to check that the Hessian of the objective function of the above problem is indefinite inside feasible region while the restriction of the quadratic function to each edge of the triangular domain is concave. By examining the corresponding concave univariate function over each edge of the region, we find that the maximum of the above problem is either attained along edge \( m = n \) at \( \alpha = \frac{n+1}{2} \) or \( \alpha = \frac{n-1}{2} \), or is attained along the edge \( \alpha = 1 \) at \( m = 3 \) and is equal to zero. For an even \( n \), we can use a similar line of arguments by considering the point \( \tilde{x}_i = \frac{1}{2}(1 + \frac{1}{n}) \) for \( i = 1, \ldots, n \), and \( \tilde{X}_{ij} = \frac{1}{2}(1 + \frac{1}{n}) \) for \( 1 \leq i < j \leq n \). Thus we conclude that the optimal value Problem \((\text{MT}^{\text{clique}})\) is given by

\[
\gamma^* = 1 + \frac{1}{n},
\]

if \( n \) is odd, and is given by

\[
\gamma^* = 1 + \frac{1}{n-1},
\]

if \( n \) is even.

**Tight variable bounds.** In the following, we derive a better upper bound for the Circle packing problem by incorporating tighter bounds on \( x \) and \( y \) variables to construct a Multi-row polyhedral relaxation of Problem \((\text{CP})\); that is, by letting \( 0 \leq x_i \leq \frac{1}{2}, \) for \( i = 1, \ldots, n_x = \lfloor n/2 \rfloor \) and \( 0 \leq y_i \leq \frac{1}{3}, \) for \( i = 1, \ldots, n_y = \lfloor n_x/2 \rfloor \), we obtain the following relaxation of Problem \((\text{CP})\):

\[
\begin{align*}
\text{(MTbnd) maximize } & \quad \gamma \\
\text{subject to } & \quad X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \ 1 \leq i < j \leq n \\
& \quad (x, X) \in \text{conv}(Q^b_{x_{\text{bnd}}}) \\
& \quad (y, Y) \in \text{conv}(Q^b_{y_{\text{bnd}}}) \\
& \quad X_{ii} \leq \frac{x_i}{2}, \quad 1 \leq i \leq n_x \\
& \quad X_{ii} \leq x_i, \quad n_x + 1 \leq i \leq n \\
& \quad Y_{ii} \leq \frac{y_i}{2}, \quad 1 \leq i \leq n_y, \\
& \quad Y_{ii} \leq y_i, \quad n_y + 1 \leq i \leq n,
\end{align*}
\]

where \( Q^b_{x_{\text{bnd}}} = \{(x, X) : X_{ij} \geq x_ix_j, 1 \leq i < j \leq n, x_i \in [0, 1], \ 1 \leq i \leq n_x, \ x_i \in [0, 1], \ n_x + 1 \leq i \leq n \} \) and \( Q^b_{y_{\text{bnd}}} = \{(y, Y) : Y_{ij} \geq y_iy_j, 1 \leq i < j \leq n, y_i \in [0, 1], \ 1 \leq i \leq n_y, \ y_i \in [0, 1], \ n_y + 1 \leq i \leq n \} \).
The polyhedron \( \text{conv}(\mathcal{Q}_{x,\text{bnd}}^b(x, X)) \) can be obtained from \( \text{conv}(\mathcal{Q}_{x}^b(\hat{x}, \hat{X})) \) defined before, via the one-to-one linear mapping:

\[
\begin{align*}
    x_i &= \frac{\hat{x}_i}{2}, \quad \forall \ 1 \leq i \leq n_x \\
    x_i &= \hat{x}_i, \quad \forall \ n_x + 1 \leq i \leq n \\
    X_{ij} &= \frac{X_{ij}}{2}, \quad \forall \ 1 \leq i < j \leq n_x \\
    X_{ij} &= \frac{X_{ij}}{2}, \quad \forall \ 1 \leq i \leq n_x < j \leq n \\
    X_{ij} &= \frac{X_{ij}}{2}, \quad \forall \ n_x < i < j \leq n.
\end{align*}
\]

Similarly, \( \text{conv}(\mathcal{Q}_{y,\text{bnd}}^b) \) can be obtained from \( \text{conv}(\mathcal{Q}_{y}^b) \) using a one-to-one linear mapping. As in the previous case, we first infer an upper bound on the optimal value of Problem (MTbnd) and subsequently present a relaxation of this problem for which the proposed upper bound is tight. Suppose that \( n \geq 5 \), so that \( n_y \geq 2 \). Consider the following subset of constraints of Problem (MTbnd)

\[
\begin{align*}
    X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} &\geq \gamma, \quad 1 \leq i < j \leq n_y \\
    (x, X) &\in \text{conv}(\mathcal{Q}_{x}^b) \\
    (y, Y) &\in \text{conv}(\mathcal{Q}_{y}^b) \\
    X_{ii} &\leq \frac{\hat{y}_i}{2}, \quad 1 \leq i \leq n_y \\
    Y_{ii} &\leq \frac{\hat{x}_i}{2}, \quad 1 \leq i \leq n_y,
\end{align*}
\]

where \( \mathcal{Q}_{x}^b = \{(x, X) : X_{ij} \geq x_i x_j, 1 \leq i < j \leq n_y, x \in [0, \frac{1}{2}]^{n_x}\} \) and \( \mathcal{Q}_{y}^b = \{(y, Y) : Y_{ij} \geq y_i y_j, 1 \leq i < j \leq n_y, y_i \in [0, \frac{1}{2}]^{n_y}\} \). Over the relaxed feasible region defined by (15), consider the set of points at which the maximum value of \( \gamma \) is attained. As this constraint set is symmetric in \((x, X)\) and \((y, Y)\), there exist points satisfying \( \frac{n_y}{2} - 2X_{ij} + \frac{\hat{y}_i}{2} = \frac{n_y}{2} - 2Y_{ij} + \frac{\hat{x}_i}{2} = \frac{\gamma}{2} \) for all \( 1 \leq i < j \leq n_y \), implying:

\[
(n_y - 1) \sum_{i=1}^{n_y} x_i - 4 \sum_{1 \leq i < j \leq n_y} X_{ij} = \frac{n_y(n_y - 1)}{2} \gamma.
\]

Suppose that \( n_y \) is an odd number. Since \((x, X) \in \text{conv}(\mathcal{Q}_{x}^b)\) and the following clique inequality

\[
2\alpha \sum_{i=1}^{n_y} x_i - 4 \sum_{1 \leq i < j \leq n_y} X_{ij} \leq \frac{\alpha(\alpha + 1)}{2}
\]

is facet defining for \( \text{conv}(\mathcal{Q}_{x}^b) \), for any integer \( \alpha \) smaller than \( n_y - 1 \), by letting \( \alpha = (n_y - 1)/2 \) in the above inequality, we conclude that an upper bound on the maximum of \( \gamma \) over the polyhedron defined by (15) is given by \( \tilde{\gamma} = \frac{1}{2}(1 + \frac{1}{n_y}) \). This in turn implies that \( \tilde{\gamma} \) is an upper bound on the optimal value of Problem (MTbnd) as well. For an even \( n \), employing a similar line of arguments, we obtain that an upper bound on the optimal value that (MTbnd) is given by \( \tilde{\gamma} = \frac{1}{2}(1 + \frac{1}{n_y - 1}) \).

Consider the polyhedron \( C_x \) defined by inequalities (12). Denote by \( C_{x,\text{bnd}} \) the image of \( C_x \) under the linear mapping defined by (14). The polyhedron \( C_{y,\text{bnd}} \) is similarly defined. We now construct a relaxation of Problem (MTbnd) by replacing the constraints \((x, X) \in \text{conv}(\mathcal{Q}_{x,\text{bnd}}^b)\) and \((y, Y) \in \text{conv}(\mathcal{Q}_{y,\text{bnd}}^b)\) with the constraints \((x, X) \in C_{x,\text{bnd}}\) and \((y, Y) \in C_{y,\text{bnd}}\), respectively. We refer to the resulting LP as (MTbnd_{\text{clique}}). Next we present a feasible point of Problem (MTbnd_{\text{clique}}) whose objective value is equal to \( \tilde{\gamma} \) defined above. Consider the point

\[
\begin{align*}
    \hat{x}_i &= \hat{y}_i = \frac{1}{2}(1 + \frac{1}{n_y}), \quad i = 1, \ldots, n_y, \\
    \hat{x}_i &= \hat{y}_i = \frac{1}{2}, \quad i = n_y + 1, \ldots, n, \\
    \hat{X}_{ii} &= \hat{X}_{ii} = \frac{1}{2}, \quad i = 1, \ldots, n_x, \\
    \hat{X}_{ii} &= \hat{X}_{ii} = \frac{1}{2}, \quad i = n_x + 1, \ldots, n, \\
    \hat{Y}_{ii} &= \hat{Y}_{ii} = \frac{1}{2}, \quad i = 1, \ldots, n_y, \\
    \hat{Y}_{ii} &= \hat{Y}_{ii} = \frac{1}{2}, \quad i = n_y + 1, \ldots, n, \\
    \hat{X}_{ij} &= \hat{Y}_{ij} = \frac{1}{16}(1 + \frac{1}{n_y}), \quad 1 \leq i < j \leq n_y, \\
    \hat{X}_{ij} &= \hat{Y}_{ij} = \frac{1}{8}(1 + \frac{1}{n_y}), \quad 1 \leq i \leq n_y < j \leq n, \\
    \hat{X}_{ij} &= \hat{Y}_{ij} = \frac{1}{4}, \quad n_y < i < j \leq n.
\end{align*}
\]
It can be checked that \((\tilde{x}, \tilde{y}, \tilde{X}, \tilde{Y})\) satisfies \(\tilde{X}_{ij} - 2\tilde{X}_{ij} + \tilde{X}_{jj} + \tilde{Y}_{ii} - 2\tilde{Y}_{ij} + \tilde{Y}_{jj} = \tilde{\gamma} = \frac{1}{4} (1 + \frac{1}{n_y})\) for all \(1 \leq i < j \leq n_y\), while \(\tilde{X}_{ii} - 2\tilde{X}_{ij} + \tilde{X}_{jj} + \tilde{Y}_{ii} - 2\tilde{Y}_{ij} + \tilde{Y}_{jj} > \tilde{\gamma}\), otherwise. In addition, we have \(\tilde{X}_{ij} = \tilde{x}_i \tilde{x}_j\) and \(\tilde{Y}_{ij} = \tilde{y}_i \tilde{y}_j\) for all \(1 \leq i < j \leq n\) with \(j > n_y\). Let \((\tilde{x}, \tilde{X})_{n_y}\) (resp. \((\tilde{y}, \tilde{Y})_{n_y}\)) contain the components \(\tilde{x}_i\) (resp. \(\tilde{y}_i\)) with \(i \leq n_y\) and \(\tilde{X}_{ij}\) (resp. \(\tilde{Y}_{ij}\)) with \(1 \leq i < j \leq n_y\). To prove feasibility of \((\tilde{x}, \tilde{y}, \tilde{X}, \tilde{Y})\) for Problem (MTbndclique), it suffices to show that \((\tilde{x}, \tilde{X})_{n_y} \in \tilde{C}_x\) (or equivalently \((\tilde{y}, \tilde{Y})_{n_y} \in \tilde{C}_y\)), where \(\tilde{C}_x\) denotes the polytope defined by all clique inequalities in the space of \(X_{ij} = x_i x_j, 1 \leq i < j \leq n_y, \ x \in [0, 0.5]^{n_y}\). The polytope \(\tilde{C}_y\) is similarly defined. As the point defined by (13) belongs to \(\tilde{C}_y\) and \((\tilde{x}, \tilde{X})_{n_y}\) are the image of \(C_x\) and point (13) under the same linear mapping, respectively, it follows that \((\tilde{x}, \tilde{X})_{n_y} \in \tilde{C}_x\). Similarly, we conclude that \((\tilde{y}, \tilde{Y})_{n_y} \in \tilde{C}_y\). It then follows that the point defined by (16) is feasible for Problem (MTbndclique), implying that the optimal value of this problem is

\[
\gamma^* = \frac{1}{4} (1 + \frac{1}{n_y}),
\]

if \(n\) is odd. Using a similar line of arguments, it follows that, for an even \(n\) with \(n \geq 4\), the optimal value of (MTbndclique) is given by:

\[
\gamma^* = \frac{1}{4} (1 + \frac{1}{n_y - 1}).
\]

**Order constraints.** Next, we obtain a multi-row polyhedral relaxation of Problem (MT) by incorporating the order constraints (4) on \(x\) variables. More precisely, we characterize the convex hull of the following set:

\[
P_{\text{ord}} = \{(x, y, \beta, \gamma) : (x_j - x_i)^2 + (y_j - y_i)^2 \geq \gamma_{ij}, 1 \leq i < j \leq n, \\
0 \leq x_1 \leq \ldots \leq x_n \leq 1, \ y \in [0, 1]^n\}. \]

To do so, it suffices to characterize the convex hull of the set:

\[
Q_{\text{ord}} = \{(x, \zeta) : (x_j - x_i)^2 \geq \zeta_{ij}, 1 \leq i < j \leq n, \ 0 \leq x_1 \leq \ldots \leq x_n \leq 1\},
\]

as \(\text{conv}(P_{\text{ord}})\) is the image of \(\text{conv}(Q_{\text{ord}}) \times \text{conv}(Q_y)\) under a linear mapping, where as before we define \(Q_y = \{(y, Y) : y_i^2 \geq Y_{ii}, \ \forall 1 \leq i \leq n, \ Y_{ij} \geq y_i y_j, \ \forall 1 \leq i < j \leq n, \ y \in [0, 1]^n\}\). We claim that

\[
\text{conv}(Q_{\text{ord}}) = \{(x, \zeta) : x_j - x_i \geq \zeta_{ij}, 1 \leq i < j \leq n, \ 0 \leq x_1 \leq \ldots \leq x_n \leq 1\}. \tag{17}
\]

First note that the polyhedra defined by (17) is a valid relaxation of the set \(Q_{\text{ord}}\) as it is obtained by replacing each convex function \((x_j - x_i)^2\) by its concave envelope over \(0 \leq x_i \leq x_j \leq 1\). In addition, this relaxation coincides with \(\text{conv}(Q_{\text{ord}})\), as the projection of each point in the convex hull of \(\{(x_i, x_j, \zeta_{ij}) : (x_j - x_i)^2 \geq \zeta_{ij}, 0 \leq x_i \leq x_j \leq 1\}\) onto the \((x_i, x_j)\) space can be uniquely determined as a convex combination of the vertices of the simplex \(0 \leq x_i \leq x_j \leq 1\). Hence, the following relaxation of Problem (CPr)

\[
\text{maximize} \quad \gamma \\
\text{subject to} \quad (x, y, \beta, \gamma) \in \text{conv}(P_{\text{ord}}) \cap K
\]

can be equivalently written as

\[
\text{(MTord) maximize} \quad \gamma \\
\text{subject to} \quad x_j - x_i + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, 1 \leq i < j \leq n \\
(y, Y) \in \text{conv}(Q_{\text{ord}}) \\
Y_{ii} \geq y_i, \ \forall 1 \leq i \leq n.
\]

We now analyze the quality of the upper bound given by Problem (MTord). As in previous cases, we can argue that there exist optimal solutions at which \(Y_{ii} = y_i\) for all \(1 \leq i \leq n\), and

\[
x_j - x_i + y_i - 2Y_{ij} + y_j = \gamma, \ \forall 1 \leq i < j \leq n.
\]
Summing up over any three of above equalities, it follows that there exist optimal solutions at which we have
\[
\gamma = \frac{2}{3} \left( x_k - x_i + y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk} \right), \quad 1 \leq i < j < k \leq n
\]
Since \( x_i \leq x_j \leq x_k \), for all \( 1 \leq i < j < k \leq n \), the expression \( x_k - x_i \) attains its smallest value when \( j = i + 1 \) and \( k = j + 1 \). Furthermore, as we mentioned before, the following clique inequalities are facet defining for \( \text{conv}(Q^b_{Y}) \):
\[
y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk} \leq 1.
\]
Consequently, at an optimal solution we have \( \gamma \leq \frac{2}{3}(x_{i+2} - x_i + 1) \) for all \( i \in \{1, \ldots, n - 2\} \). It then follows that the optimal value of the following problem provides an upper bound on the optimal value of Problem (MTord):
\[
\begin{align*}
\text{maximize} & \quad \frac{2}{3}(1 + \Delta x) \\
\text{subject to} & \quad x_{i+2} - x_i \geq \Delta x, \quad 1 \leq i \leq n - 2.
\end{align*}
\]
It is simple to verify that the optimal value of the above problem is attained at \( \Delta x = 1/\lfloor (n - 1)/2 \rfloor \) and is equal to
\[
\hat{\gamma} = \frac{2}{3} \left( 1 + \frac{1}{\lfloor (n - 1)/2 \rfloor} \right).
\]
As in the previous case, we now construct a relaxation of Problem (MTord) by replacing the constraint \((y, Y) \in \text{conv}(Q^b_{Y})\) with the constraint \((y, Y) \in C_y\) to obtain the following relaxation:
\[
\begin{align*}
\text{(MTord}^{\text{clique}}) \quad \text{maximize} & \quad \gamma \\
\text{subject to} & \quad x_j - x_i + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \quad 1 \leq i < j \leq n \\
& \quad (y, Y) \in C_y \\
& \quad Y_{ii} \leq y_i, \ \forall 1 \leq i \leq n.
\end{align*}
\]
Our numerical experimentations show that the optimal value of MTord^{clique} is equal to \( \gamma \) given by (19) for \( n < 13 \). Indeed for \( n = 13 \), the optimal value of the above problem is \( \gamma^* = 0.7742 \) while \( \hat{\gamma} = 0.7778 \). However, our numerical experiments reveal that the relative gap \( (\hat{\gamma} - \gamma^*)/\gamma^* \times 100 \% \) remain below five percent for \( 13 \leq n \leq 30 \). Hence, we argue that \( \hat{\gamma} \) defined by (19) is a reasonable measure for the quality of the bound given by Problem (MTord^{clique}). In fact, the optimal value of the following relaxation of (MTord^{clique}) is equal to \( \hat{\gamma} \):
\[
\begin{align*}
\text{(MTord}^{\text{tri}}) \quad \text{maximize} & \quad \gamma \\
\text{subject to} & \quad x_j - x_i + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \quad 1 \leq i < j \leq n \\
& \quad y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk} \leq 1, \quad 1 \leq i < j < k \leq n \\
& \quad Y_{ii} \leq y_i, \ \forall 1 \leq i \leq n.
\end{align*}
\]
First, we establish that \( \hat{\gamma} \) is a valid upper bound for Problem (MTord^{clique}) via the exact line of arguments we used to prove that \( \tilde{\gamma} \) is an upper bound for (MTord^{clique}). Now consider the point:
\[
\begin{align*}
\tilde{x}_i = \frac{i}{3} \Delta x, & \quad i = 1, \ldots, n, \\
\tilde{y}_i = \frac{1 + \Delta x}{3}, & \quad i = 1, \ldots, n, \\
\tilde{Y}_{ij} = \frac{i - j}{3} \Delta x, & \quad 1 \leq i < j \leq n.
\end{align*}
\]
where as before \( \Delta x = 1/\lfloor (n - 1)/2 \rfloor \). It can be checked that \( \tilde{x}_j - \tilde{x}_i + \tilde{Y}_{ii} - 2\tilde{Y}_{ij} + \tilde{Y}_{jj} = \frac{2}{3}(1 + \Delta x) = \hat{\gamma} \) for all \( 1 \leq i < j \leq n \). Moreover, we have \( \tilde{y}_i + \tilde{y}_j + \tilde{y}_k - \tilde{Y}_{ij} - \tilde{Y}_{jk} - \tilde{Y}_{ik} = 1 + (1 - \frac{k - i}{2})\Delta x \leq 1 \), where the last inequality is valid since \( k - i \geq 2 \). Hence, the point defined by (22) is feasible for Problem (MTord^{tri}), implying that its optimal value is given by (19). This observation has important computational implications, as Problem (MTord^{tri}) can be solved significantly faster than Problem (MTord^{clique}), which is particularly beneficial when these relaxations are embedded in branch-and-cut global solvers.
**Best Multi-row polyhedral relaxations.** Finally, consider the Multi-row polyhedral relaxation of the Circle packing problem obtained by combining the order constraints on $x$ variables and tighter upper bounds on $x$ and $y$ variables. We replace each bivariate quadratic $(x_j - x_i)^2$ by its concave envelope over the triangular, rectangular, or trapezoidal domain, let $(y, Y) \in \text{conv}(Q_{\text{bnd}})$ and refer to the resulting LP as (MTcomb). Subsequently, we construct a relaxation of Problem (MTcomb), denoted by (MTcombclique) by replacing the constraint $(y, Y) \in \text{conv}(Q_{\text{bnd}})$ with the constraint $(y, Y) \in C_{\text{bnd}}$. We now obtain an upper bound on the optimal value of Problem (MTcombclique). Suppose that $n \geq 9$, so that $n_y \geq 3$. Consider the following inequalities present the constraint set of (MTcombclique):

$$\frac{x_j - x_i}{2} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \quad 1 \leq i < j \leq n_y.$$ 

Summing up over any three such inequalities and using the fact that there exist optimal solutions of Problem (MTcombclique) at which $Y_{ii} = \frac{y_i}{2}$ for all $1 \leq i \leq n_y$, we obtain

$$\gamma^* \leq \frac{1}{3}(x_k - x_i + y_i + y_j + y_k - 2Y_{ij} - 2Y_{ik} - 2Y_{jk}).$$

As we detailed before, the inequality $2y_i + 2y_j + 2y_k - 4Y_{ij} - 4Y_{ik} - 4Y_{jk} \leq 1$ is facet-defining for the polyhedron $C_{\text{bnd}}$. Moreover, as $x_i \leq x_{i+1}$ for all $1 \leq i \leq n$, a minimum value of $x_k - x_i$ is attained when $k = i + 2$. Finally, the maximum value of $x_{i+2} - x_i$, $x_i \in [0, 0.5]$ for all $1 \leq i \leq n_y$ is equal to $\frac{1}{2(n_y - 1)/2}$.

Hence, we conclude that an upper bound on the optimal value of (MTcombclique) is given by:

$$\bar{\gamma} = \frac{1}{6}(1 + \frac{1}{\lfloor (n_y - 1)/2 \rfloor}) \quad (21)$$

Our numerical experiments show that for $5 \leq n \leq 30$, the relative gap between the optimal value of Problem (MTcombclique) and $\bar{\gamma}$ remain below five percent and thus we argue that (21) is a reasonable measure of the quality of the bound given by Problem (MTcombclique). Now, consider a relaxation of the Problem (MTcombclique), denoted by (MTcombtri), in which the constraint set $(y, Y) \in C_{\text{bnd}}$ is replaced with the following set of clique inequalities:

$$\begin{align*}
2y_i + 2y_j + 2y_k - 4Y_{ij} - 4Y_{ik} - 4Y_{jk} &\leq 1, \quad 1 \leq i < j < k \leq n_y \\
2y_i + 2y_j + y_k - 4Y_{ij} - 2Y_{ik} - 2Y_{jk} &\leq 1, \quad 1 \leq i < j \leq n_y < k \leq n \\
2y_i + y_j + y_k - 2Y_{ij} - 2Y_{ik} - Y_{jk} &\leq 1, \quad 1 \leq i \leq n_y < j < k \leq n \\
y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk} &\leq 1, \quad n_y < i < j < k \leq n.
\end{align*}$$

It can be checked that the optimal value of Problem (MTcombtri) is given by (21), and this optimal value is attained at:

$$\begin{align*}
\bar{x}_i &= \frac{1}{4}x_i, \quad i = 1, \ldots, n_y, \\
\bar{y}_i &= \frac{1}{8}\Delta x, \quad i = 1, \ldots, n_y, \\
\bar{x}_i &= \bar{y}_i = \frac{1}{2}, \quad i = n_y + 1, \ldots, n, \\
\bar{Y}_{ii} &= \bar{y}_i, \quad i = 1, \ldots, n_y \\
\bar{Y}_{ii} &= \bar{y}_i, \quad i = n_y + 1, \ldots, n \\
\bar{Y}_{ij} &= \frac{i}{2}\Delta x, \quad 1 \leq i < j \leq n_y \\
\bar{Y}_{ij} &= \frac{i}{2}\Delta x, \quad 1 \leq i \leq n_y < j \leq n \\
\bar{Y}_{ij} &= \frac{1}{4}, \quad n_y < i < j \leq n,
\end{align*}$$

where $\Delta x = \frac{1}{2\lfloor (n_y - 1)/2 \rfloor}$.

The following theorem summarizes our results.

**Theorem 2.** Consider the multi-row polyhedral relaxations of the Circle packing problem defined above:
(i) Let \( n \geq 3 \). Then the optimal value of Problem \((MT^{\text{clique}})\) is equal to

\[
\gamma^* = 1 + \frac{1}{n},
\]

if \( n \) is odd and is equal to

\[
\gamma^* = 1 + \frac{1}{n-1},
\]

if \( n \) is even.

(ii) Let \( n \geq 5 \) and let \( n_y = \lceil n/4 \rceil \). Then the optimal value of Problem \((MT^{\text{bnd\,clique}})\) is equal to

\[
\gamma^* = \frac{1}{4} \left( 1 + \frac{1}{n_y} \right),
\]

if \( n_y \) is odd, and is equal to

\[
\gamma^* = \frac{1}{4} \left( 1 + \frac{1}{n_y - 1} \right),
\]

if \( n_y \) is even.

(iii) Let \( n \geq 3 \). Then the optimal value of Problem \((MT^{\text{ord\,tri}})\) is

\[
\gamma^* = \frac{2}{3} \left( 1 + \frac{1}{\lceil (n-1)/2 \rceil} \right).
\]

(iv) Let \( n \geq 5 \) and let \( n_y = \lceil n/4 \rceil \). Then the optimal value of Problem \((MT^{\text{comb\,tri}})\) is given by \( \gamma^* = \frac{1}{2} \) for \( n \leq 8 \) (i.e., for \( n_y = 2 \)) and is given by

\[
\gamma^* = \frac{1}{6} \left( 1 + \frac{1}{\lceil (n_y-1)/2 \rceil} \right),
\]

for \( n \geq 9 \) (i.e., for \( n_y \geq 3 \)).

4 Semidefinite relaxations

The basic approach. Semidefinite relaxations are among the most popular techniques for bounding nonconvex QCQPs [12]. The basic idea is to lift the problem to a higher dimensional space by introducing new variables of the form \( X_{ij} = x_i x_j \) (resp. \( Y_{ij} = y_i y_j \)), for all \( 1 \leq i \leq j \leq n \), and subsequently replace the nonconvex set \( \{(x,X) : X = xx^T\} \) (resp. \( \{(y,Y) : Y = yy^T\} \)) by its semi-definite relaxation \( \{(x,X) : X \succeq xx^T\} \) (resp. \( \{(y,Y) : Y \succeq yy^T\} \)). Such a relaxation can be further strengthened by including constraints of the form

\[
X_{ii} \leq x_i, \quad Y_{ii} \leq y_i, \quad \forall i \in \{1, \ldots, n\},
\]

on the diagonal entries of matrices \( X \) and \( Y \). It follows that, the following SDP provides an upper bound on the optimal value of the Circle packing problem:

\[
(\text{SDP1}) \quad \text{maximize} \quad \gamma \\
\text{subject to} \quad X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \quad 1 \leq i < j \leq n \\
X \succeq xx^T, \quad Y \succeq yy^T \\
X_{ii} \leq x_i, \quad Y_{ii} \leq y_i, \quad 1 \leq i \leq n \\
0 \leq x \leq 1, \quad 0 \leq y \leq 1.
\]

First, note that the above problem is symmetric in \((x,X)\) and \((y,Y)\). Since the feasible region of \((\text{SDP1})\) is convex, it follows that there exists an optimal solution with \( x = y = X = Y \). Now consider \( X_{ii} \leq x_i \),
Clearly, at an optimal solution, at least one of these inequalities is active, since otherwise it is possible to improve the objective value by increasing one of the diagonal entries of $X$. We argue that at an optimal solution, all these inequalities are binding. Suppose not. Denote by $l$ the index of the inactive inequality constraint. Since the problem is symmetric in $(x_i, X_{ii})$, $i = 1, \ldots, n$, it follows that there exists an optimal solution with $X_{ii} < x_l$ for any $l \in \{1, \ldots, n\}$. Hence, by taking the average over all such solutions, we obtain an optimal solution of (SDP1) for which $X_{ii} < x_l$ for all $i = 1, \ldots, n$. Thus, at an optimal solution $X_{ii} = x_l$, for all $i \in \{1, \ldots, n\}$. Using a similar symmetry argument, we conclude that at an optimal solution

$$X_{ii} - 2X_{ij} + X_{jj} = \frac{\gamma}{2}$$

for all $1 \leq i < j \leq n$. Thus, (SDP1) simplifies to the following problem:

$$\begin{align*}
\text{maximize} & \quad \gamma \\
\text{subject to} & \quad x_i - 2X_{ij} + x_j = \frac{\gamma}{2}, \quad 1 \leq i < j \leq n \\
& \quad X \succeq xx^T \\
& \quad 0 \leq x \leq 1.
\end{align*}$$

(24)

To further simplify the above problem, we eliminate $X_{ij}$, $1 \leq i < j \leq n$ using the equality constraints, and write this SDP in terms of $x$ variables. Define $\bar{X} = \begin{pmatrix} 1 & x^T \\ x & \bar{X} \end{pmatrix}$, where $\bar{X}_{ii} = x_i$ for all $i = 1, \ldots, n$ and $\bar{X}_{ij} = \frac{1}{2}(x_i + x_j - \frac{\gamma}{2})$, $1 \leq i < j \leq n$. It then follows that Problem (24) can be equivalently written as:

$$\begin{align*}
\text{maximize} & \quad \gamma \\
\text{subject to} & \quad \bar{X} \succeq 0 \\
& \quad 0 \leq x \leq 1.
\end{align*}$$

(25)

Now consider a feasible solution of the above problem denoted by $(\bar{x}, \bar{\gamma})$. Clearly, any permutation of $\bar{x}$, denoted by $\bar{x}_\pi$ results in a feasible solution of the form $(\bar{x}_\pi, \bar{\gamma})$. Since, the feasible set of (25) is convex, by taking the average of all such feasible points, we obtain a feasible solution of the form $(\bar{x}, \bar{\gamma})$, where $\bar{x}_1 = \bar{x}_2 = \ldots = \bar{x}_n$. Let $\bar{x}_i = t$ and let $\bar{X}_{ij} = z$. Then Problem (25) simplifies to a bivariate SDP:

$$\begin{align*}
\text{maximize} & \quad 4(t - z) \\
\text{subject to} & \quad \begin{pmatrix} 1 & t & t & \ldots & t \\ t & t & z & \ldots & z \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t & z & z & \ldots & t \end{pmatrix} \succeq 0 \\
& \quad 0 \leq t \leq 1, 0 \leq z \leq 1.
\end{align*}$$

(26)

To further characterize the feasible region of Problem (26), equivalently, we examine the positive semi-definiteness of the following matrix:

$$A = \begin{pmatrix} t - t^2 & z - t^2 & \ldots & z - t^2 \\ z - t^2 & t - t^2 & \ldots & z - t^2 \\ \vdots & \vdots & \ddots & \vdots \\ z - t^2 & z - t^2 & \ldots & t - t^2 \end{pmatrix}.$$ 

By direct calculation, it can be shown that the $m$th order principal minor of $A$ is given by:

$$M_m = (t - z)^{m-1}(t + (m - 1)z - mt^2), \quad 2 \leq m \leq n.$$ 

Since the objective of (26) is to maximize $(t - z)$, we can assume that at an optimal solution $t - z > 0$. Thus, $M_m \geq 0$ if and only if $t + (m - 1)z - mt^2 \geq 0$, or equivalently, $z \geq (mt^2 - t)/(m - 1)$. In addition, the right-hand side of this inequality is increasing in $m$ for any $t \in [0, 1]$. Thus, for a given $t \in [0, 1]$, the matrix $A$ is positive semidefinite if, $z \geq \frac{mt^2 - t}{m - 1}$ and at the optimal solution we have $z = \frac{mt^2 - t}{n - 1}$. Thus, problem (26) simplifies to the following univariate optimization problem:

$$\max_{0 \leq t \leq 1} \frac{4n}{n - 1}(t - t^2).$$
It is simple to verify that the optimal value of the above problem is attained at \( t = \frac{1}{2} \) and is equal to 
\[ 1 + \frac{1}{n-1}. \]
Accordingly, an optimal solution of (SDP1) is attained at:
\[
\begin{align*}
  x_i^* &= y_i^* = X_{ii}^* = Y_{ii}^* = \frac{1}{2}, & 1 \leq i \leq n \\
  X_{ij}^* &= Y_{ij}^* = \frac{n-2}{4(n-1)}, & 1 \leq i < j \leq n \\
  \gamma^* &= 1 + \frac{1}{n-1}.
\end{align*}
\]  

(27)

**Remark 6.** Consider the first-level RLT constraints of the Circle packing problem as defined in Remark 1. It is simple to verify that the point defined by (27) satisfies these constraints, implying that the addition of RLT constraints to (SDP1) does not strengthen the relaxation.

**Tighter variable bounds** The optimal solution of Problem (SDP1) given by (27) satisfies the tighter bound requirements on \( x \) and \( y \) variables, as defined by (2) and (3), respectively. Thus, the simple addition of these constraints to (SDP1) does not improve the value of the upper bound. However, relations (2) and (3) can be utilized to strengthen (SDP1) as follows. We replace the linear constraints defined by (23) by the following inequalities:
\[
\begin{align*}
  X_{ii} &\leq \frac{x_i}{2}, & 1 \leq i \leq n_x \\
  X_{ii} &\leq x_i, & n_x + 1 \leq i \leq n \\
  Y_{ii} &\leq \frac{y_i}{2}, & 1 \leq i \leq n_y \\
  Y_{ii} &\leq y_i, & n_y + 1 \leq i \leq n.
\end{align*}
\]
We refer to the resulting relaxation as (SDP2). As before, we first provide an upper bound on the optimal solution of this SDP by considering a specific subset of the constraints. Subsequently, we provide a feasible solution of (SDP2) that attains this bound. Consider the following relaxation of (SDP2) which only contains the points in lower left quadrant of the unit square:
\[
\text{(SDPr)} \quad \begin{array}{ll}
  \text{maximize} & \gamma \\
  \text{subject to} & X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, & 1 \leq i < j \leq n_y \\
  & X_{ii} \leq \frac{x_i}{2}, & 1 \leq i \leq n_x \\
  & Y_{ii} \leq \frac{y_i}{2}, & 1 \leq i \leq n_y \\
  & X \succeq xx^T, & Y \succeq yy^T \\
  & 0 \leq x_i \leq \frac{1}{2}, & 0 \leq y_i \leq \frac{1}{2}, & 1 \leq i \leq n_y.
\end{array}
\]
Note that in the above problem, \( X \) and \( Y \) are \( n_y \times n_y \) matrices. Clearly, the optimal solution of the above problem provides an upper bound on the optimal solution of (SDP2). The important property of Problem (SDPr), however, is its symmetry in \( x \) and \( y \) variables. Thus, we can employ a similar line of arguments as for (SDP1), to conclude that there exists an optimal solution of (SDPr) with (i) \( x = y \) and \( X = Y \), (ii) \( X_{ii} = \frac{x_i}{2}, Y_{ii} = \frac{y_i}{2}, i = 1, \ldots, n_y \), and (iii) \( X_{ii} - 2X_{ij} + X_{jj} = \frac{t}{2} \) for all \( 1 \leq i < j \leq n_y \). Let \( t = x_i, z = X_{ij} \), and
\[
\bar{X} = \begin{pmatrix}
  t/2 - t^2 & z - t^2 & \ldots & z - t^2 \\
  z - t^2 & t/2 - t^2 & \ldots & z - t^2 \\
  \vdots & \vdots & \ddots & \vdots \\
  z - t^2 & z - t^2 & \ldots & t/2 - t^2
\end{pmatrix}
\]
It follows that (SDPr) simplifies to the following problem:
\[
\begin{array}{ll}
  \text{maximize} & 2(t - 2z) \\
  \text{subject to} & \bar{X} \succeq 0 \\
  & 0 \leq t \leq \frac{1}{2}
\end{array}
\]
(28)
By direct calculation, it can be shown that the \( m \)th order principal minor of \( \bar{X} \) is given by:
\[
M_m = \left( \frac{1}{2} \right)^m (t - 2z)^{m-1}(t + 2(m-1)z - 2mt^2).
\]
Since the objective of (28) is to maximize $t - 2z$, it follows that $\tilde{X}$ is positive semidefinite, if $t + 2(n_y - 1)z - 2n_yz^2 \geq 0$, and at an optimal solution we have $z = \frac{2n_y t - t \gamma}{2(n_y - 1)}$. Therefore, the optimal solution of (28) is attained at $t^* = \frac{1}{4}$, $z^* = \frac{n_y - 2}{16(n_y - 1)}$ and is equal to $f^* = \frac{1}{4}(1 + \frac{1}{n_y - 1})$. We now construct a feasible point of (SDP2) whose objective value is equal to $f^*$. Consider

\[
\begin{align*}
\tilde{x}_i &= \tilde{y}_i = \frac{1}{4}, \quad \forall i = 1, \ldots, n_y, \\
\hat{x}_i &= \hat{y}_i = \frac{1}{2}, \quad \forall i = n_y + 1, \ldots, n, \\
\tilde{X}_{ii} &= \frac{\hat{X}_{ii}}{2}, \quad \forall i = 1, \ldots, n_x, \\
\hat{X}_{ii} &= \hat{x}_i, \quad \forall i = n_x + 1, \ldots, n, \\
\tilde{Y}_{ii} &= \frac{\hat{Y}_{ii}}{2}, \quad \forall i = 1, \ldots, n_y, \\
\hat{Y}_{ii} &= \hat{y}_i, \quad \forall i = n_y + 1, \ldots, n, \\
\tilde{X}_{ij} &= \tilde{Y}_{ij} = \frac{n_y^2 - 2}{16(n_y - 1)}, \quad \forall 1 \leq i < j \leq n_y, \\
\hat{X}_{ij} &= \hat{Y}_{ij} = \frac{1}{n_y^2}, \quad \forall 1 \leq i \leq n_y, n_y + 1 \leq j \leq n, \\
\tilde{X}_{ij} &= \tilde{Y}_{ij} = \frac{1}{4}, \quad \forall n_y + 1 \leq i < j \leq n.
\end{align*}
\]

(29)

It is simple to verify that $\tilde{X}_{ii} - 2\tilde{X}_{ij} + \tilde{X}_{jj} + \tilde{Y}_{ii} - 2\tilde{Y}_{ij} + \tilde{Y}_{jj} \geq \tilde{\gamma} = \frac{1}{4}(1 + \frac{1}{n_y - 1})$ for all $1 \leq i < j \leq n$. Thus to prove feasibility of (29), it suffices show that $\tilde{X} - \tilde{x}\tilde{x}^T \succeq 0$ and $\tilde{Y} - \tilde{y}\tilde{y}^T \succeq 0$. Let $\tilde{X} = (\tilde{x}_i \tilde{X}_{ij})$ and $\tilde{Y} = (\tilde{y}_i \tilde{Y}_{ij})$. To show $\tilde{X} \succeq 0$ at $(\tilde{x}, \tilde{X})$ (resp. $\tilde{Y} \succeq 0$ at $(\tilde{y}, \tilde{Y})$), it suffices to factorize $\tilde{X}$ as $\tilde{X} = L_xD_xL_x^T$ (resp. $\tilde{Y}$ as $\tilde{Y} = L_yD_yL_y^T$), where $L_x$ (resp. $L_y$) is a lower triangular matrix with ones in the diagonal and $D_x = \text{diag}(d_x^T)$, $d_x \in \mathbb{R}^n$ (resp. $D_y = \text{diag}(d_y^T)$, $d_y \in \mathbb{R}^n$) is a nonnegative diagonal matrix. Define $d_x^* = 1$ and

\[
d_x^T = \begin{cases} 
\frac{1}{16} \prod_{i=1}^{j-1} \left(1 - \frac{1}{(n_y - 1)^2}\right), & 1 < j \leq n_y + 1 \\
0, & n_y + 1 < j \leq n_x + 1 \\
\frac{1}{4}, & n_x + 1 < j \leq n + 1.
\end{cases}
\]

Let

\[
L_x(i, j) = \begin{cases} 
1, & \text{if } i = j \\
x_{i-1}, & \text{if } j = 1, 2 \leq i \leq n + 1 \\
\frac{1}{n_y - j + 1}, & \text{if } 2 < j < i \leq n_y + 1 \\
0, & \text{otherwise}.
\end{cases}
\]

Similarly, let $L_y = L_x$ and $d_y^T = d_x^T$ for $i = 1, \ldots, n_y + 1$, and $d_i^T = \frac{1}{4}$, for $i = n_y + 2, \ldots, n + 1$. Hence, we have shown that the point defined by (29) is a feasible solution of Problem (SDP2) implying that the optimal value of this problem is given by

\[
\gamma^* = \frac{1}{4}(1 + \frac{1}{n_y - 1}).
\]

**Remark 7.** Consider the first-level RLT constraints of the Circle packing problem corresponding to the tightened variable bounds as defined in Remark 2. It is simple to verify that the optimal solution of Problem (SDP2) defined by (29), satisfies these constraints. Hence, adding first-level RLT constraints to (SDP2) does not strengthen the SDP relaxation.

The following theorem summarizes our results in this section. The bounds given in this theorem were conjectured and numerically verified by Anstreicher [1].

**Theorem 3.** Consider the SDP relaxations of the Circle packing problem defined above:

(i) Let $n \geq 2$. Then, the optimal value of Problem (SDP1) is

\[
\gamma^* = 1 + \frac{1}{n - 1}
\]

and is attained at $x_i^* = y_i^* = X_{ii}^* = Y_{ii}^* = \frac{1}{2}$, for $1 \leq i \leq n$, and $X_{ij}^* = \frac{n - 2}{4(n - 1)}$, for $1 \leq i < j \leq n$. 


(ii) Let $n \geq 5$. Then, the optimal value of Problem (SDP2) is

\[ \gamma^* = \frac{1}{4} \left( 1 + \frac{1}{\lfloor (n-1)/4 \rfloor} \right) \]

and is attained at $x_i^* = y_i^* = \frac{1}{4}$, for $i = 1, \ldots, n$, $x_i^* = y_i^* = \frac{1}{8}$, for $i = n_y + 1, \ldots, n$, $X_{ii}^* = \frac{5}{16}$, for $i = 1, \ldots, n_x$, $X_{ii}^* = x_i^*$, for $i = n_x + 1, \ldots, n$, $Y_{ii}^* = \frac{1}{4}$, for $i = 1, \ldots, n_y$, $Y_{ii}^* = y_i$, for $i = n_y + 1, \ldots, n$, $X_{ij}^* = Y_{ij}^* = \frac{1}{4}$, for $1 \leq i < j \leq n$, $X_{ij}^* = \frac{1}{4}$, for $n_y + 1 \leq i < j \leq n$.

Furthermore, addition of first-level RLT constraints do not improve the bounds given by (SDP1) and (SDP2).

Order constraints. Consider the RLT-type inequalities (7) obtained utilizing the order constraints (4).

Clearly, Problem (SDP1ord) can be further simplified by noting that there exist optimal solutions with order constraints.

Order constraints.

Consider the RLT-type inequalities (7) obtained utilizing the order constraints (4).

Order constraints.

Consider the set

\[ \mathcal{S} = \{(x, X, \zeta) : X_{ii} - 2X_{ij} + X_{jj} \geq \zeta_{ij}, \quad X_{ii} \leq X_{ij}, \quad x_i - x_j \leq x_{ij}, \quad 1 \leq i < j \leq n, \quad X_{ii} \leq x_i, \quad 1 \leq i \leq n \} \]

It can be shown that the projection of the above set onto $(x, \zeta)$ is given by \{(x, \zeta) : x_j - x_i \geq \zeta_{ij}, \quad 1 \leq i < j \leq n\}, and as detailed in the previous section, this set is the convex hull of \{(x, \zeta) : (x_j - x_i)^2 \geq \zeta_{ij}, \quad 1 \leq i < j \leq n, \quad 0 \leq x_1 \leq \ldots \leq x_n \leq 1\}. This in turn implies that the constraint $X \succeq xx^T$ in the description of Problem (SDP1ord) is redundant and this problem can be equivalently written as:

\[(\text{SDPord}) \quad \text{maximize} \quad \gamma \]

subject to

\[
\begin{align*}
x_j - x_i + Y_{ii} - 2Y_{jj} + y_{jj} &\geq \gamma, \quad 1 \leq i < j \leq n \\
y_{ii} &\leq y_i, \quad 1 \leq i \leq n \\
Y &\succeq yy^T \\
x &\in [0, 1]^n, \quad y \in [0, 1]^n.
\end{align*}
\]

Clearly, Problem (SDPord) can be further simplified by noting that there exist optimal solutions with $y_{ii} = y_i$ for all $i \in \{1, \ldots, n\}$. In Figure 1(a), we compare the the optimal value of Problem (SDPord) with that of Problem (MTord$^{(ii)}$), as given by Part (iii) of Theorem 2, for $3 \leq n \leq 30$: while the SDP bounds are slightly stronger than the polyhedral counterparts for $n > 13$, the relative gap between the two bounds is below five percent for all values of $n$. Moreover, the computational cost of solving Problem (MTord$^{(ii)}$) is significantly lower than that of (SDPord).

Best SDP relaxations. We combine the two types of symmetry-breaking constraints discussed above by adding inequalities (8) to Problem (SDP2) and denote the resulting SDP relaxation by (SDPcomb). In Figure 1(b), we compare the the optimal value of Problem (SDPcomb) with that of Problem (MTcomb$^{(ii)}$), as given by Part (iv) of Theorem 2, for $5 \leq n \leq 30$: while the bounds given by the two relaxations coincide for $5 \leq n \leq 8$, the multi-row polyhedral bounds are stronger than the SDP bounds for all $n \geq 9$.

5 Discussions and future directions

In previous sections, we conducted a theoretical assessment of several convexification techniques for the Circle packing problem: single-row polyhedral relaxations, multi-row polyhedral relaxations, and semidefinite relaxations. Our main findings are stated in Theorems 1-3: from Theorem 1 and Theorem 3 it follows that (i) the bound given by the basic SDP relaxation is identical to that of the single-row polyhedral relaxation with order constraints, (ii) the bound given by the SDP relaxation with tightened variable bounds is identical to that of the best single-row polyhedral relaxation. In addition, via numerical experimentations (see
Figure 1: Comparison of the upper bounds for the Circle packing problems obtained by SDP relaxations versus the LP counterparts. In Figure 1(a) the optimal value of Problem (SDPord) is compared with that of Problem (MTord\text{tri}). In Figure 1(b) the optimal value of Problem (SDPcomb) is compared with that of Problem (MTcomb\text{tri}).

In Figure 1(b), we discovered that the upper bound given by the best multi-row polyhedral relaxation is better than that of the best SDP relaxation. As the computational cost of solving aforementioned polyhedral relaxations is significantly lower than SDP relaxations, we conclude that for Circle packing problem, polyhedral relaxations are superior to SDP relaxations.

From Theorem 1 and Theorem 2 it follows that the proposed multi-row polyhedral relaxations are considerably better than single-row polyhedral relaxations. That is, by utilizing certain facets of the Boolean quadric polytope, we are able to improve the quality of the upper bound on Problem (CP) by about 30\% for large \(n\) values. In Figure 2, we plot the upper bounds given by the best single-row and multi-row polyhedral relaxations along with the optimal value of Problem (CP) for \(5 \leq n \leq 50\). The exact solutions of the Circle packing problem are taken from www.packomania.com. As can be seen from Figure 2, by increasing the value of \(n\), the quality of the multi-row polyhedral bounds deteriorates quickly.

We further demonstrate the above fact by incorporating our best multi-row polyhedral relaxations in the global solver BARON [9]. We employ two upper bounding schemes to solve Problem (CP) to global optimality: the basic single-row polyhedral relaxation (TW) and the best multi-row polyhedral relaxation (MTcomb\text{tri}). These relaxations are constructed at every node in the branch-and-bound tree of the global solver. For each upper bounding scheme, we solve the Circle packing problem for all \(3 \leq n \leq 20\). All problems are solved with relative/absolute optimality tolerance of \(10^{-6}\), and a CPU time limit of 1200 seconds. Other algorithmic parameters are set to the default settings of the GAMS/BARON distribution.

Results are listed in Table 1; for each run, we present five quantities: CPU time in seconds (\(T\)), total number of nodes in the branch-and-bound tree (\(N\)), upper bound on the optimal solution upon termination (\(UB\)), lower bound on the optimal solution upon termination (\(LB\)), and the percentage of relative optimality gap upon termination \(\delta = (UB - LB)/UB \times 100\%\). As can be seen from this table, for \(n < 9\), utilizing multi-row relaxations results in significant speed ups. However, for \(n \geq 10\), BARON is not able solve the Circle packing problem to global optimality within the time limit. For all these problems, the proposed multi-row relaxations result in a 30\% reduction in relative optimality gap.

Recall that to construct the proposed multi-row polyhedral relaxations, we considered a reformulation of the Circle packing problem; namely, Problem (CPr), and argued that the polyhedron \(\text{conv}(P) \cap K\) could serve as a good relaxation of \(\text{conv}(P \cap K)\). It can be shown that the set \(\text{conv}(P \cap K)\) is polyhedral as well. In addition, it can be shown that even for \(n = 3\), the polyhedron \(\text{conv}(P \cap K)\) is strictly contained in \(\text{conv}(P) \cap K\). In fact, the clique inequality \(x_1 + x_2 + x_3 - X_{12} - X_{13} - X_{23} \leq 1\) (or \(y_1 + y_2 + y_3 - Y_{12} - Y_{13} - Y_{23} \leq 1\)) is not facet-defining for \(\text{conv}(P \cap K)\). Therefore, an interesting future research direction is to study the facial structure of \(\text{conv}(P \cap K)\) directly, possibly by using ideas from reverse convex programming [5].
Figure 2: Comparison of the upper bounds for the Circle packing problem obtained by the best single-row (TWcomb) and the best multi-row (MTcomb\textsuperscript{tri}) polyhedral relaxations versus the exact optimal solution (exact).

References


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Table 1: Effect of the basic single-row (TW) and the best multi-row (MTcomb^{tri}) upper bounding schemes on the performance of BARON for Circle packing problems with $3 \leq n \leq 20$. The two algorithms are compared with respect to CPU time ($T$), total number of nodes in the branch-and-bound tree ($N_t$), final upper bound ($UB$), final lower bound ($LB$), and final relative optimality gap ($\delta\%$).