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. The nonconvexity stems from a collection of pairwise non-overlapping constraints, a structure that appears in many important applications such as metal cutting, communication networks, and distance geometry. We study several existing and new 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 a branch-and-cut based global solver, 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:

\[
\text{Locate } n \text{ points in a unit square, such that the minimum distance between any two points is maximal.}
\]

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:

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

where \( \gamma \) denotes the minimum squared pair-wise distance of the points in the unit square and \( n \geq 2 \). The corresponding radius \( r \) for \( n \) circles that can be packed into the unit square is then given by \( r = \frac{\sqrt{\gamma}}{2(1 + \sqrt{\gamma})} \).

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 non-overlapping constraints defined by (1). In fact, non-overlapping constraints appear in a variety of applications including circular cutting, communication networks, facility layout problems, and distance geometry applications (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 (see [12] 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

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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. Indeed, current global solvers exhibit very slow convergence rates for optimization problems containing non-overlapping constraints.

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. To this end, we consider the Circle packing problem as our prototypical example in that its simple formulation makes it amenable to a theoretical study, yet it demonstrates the limitations of existing convexification schemes. We consider various widely-used 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. We should emphasize that the purpose of this paper is not to identify the most efficient customized optimization algorithm for the Circle packing problem but to examine the applicability of the most widely-used convexification schemes for non-overlapping 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 multi-row polyhedral relaxations. Finally, in Section 5, we incorporate our best multi-row polyhedral relaxations in the global solver BARON [9] 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 convex 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 function of the form $f(u) = (u_1 - u_2)^2$ over the box $\mathcal{H} = [0, 1]^2$ is given by $\text{conc}_\mathcal{H} f(u) = \min\{u_1 + u_2, 2 - u_1 - u_2\}$. Since non-overlapping constraints are separable in $x$ and $y$ variables, we have

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

$$\{(x_i, x_j, y_i, y_j, \gamma) : \text{conc}_\mathcal{H} f(x) + \text{conc}_\mathcal{H} f(y) \geq \gamma, \ x \in [0, 1]^2, y \in [0, 1]^2\}$$

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

\[
\begin{align*}
\text{(TW)} & \quad \text{maximize} & & \gamma \\
& \quad \text{subject to} & & x_i + x_j + y_i + y_j \geq \gamma \\
& & & -x_i - x_j + y_i + y_j + 2 \geq \gamma \\
& & & x_i + x_j - y_i - y_j + 2 \geq \gamma \\
& & & -x_i - x_j - y_i - y_j + 4 \geq \gamma \\
& & & 0 \leq x \leq 1, 0 \leq y \leq 1.
\end{align*}
\]
Claim 1. The optimal value of Problem (TW) is $\gamma^* = 2$ for all $n \geq 2$.

Proof. Denote by $(\tilde{x}, \tilde{y})$ a point at which $\gamma^*$ is attained. By symmetry, $\gamma^*$ is also attained at the following points: $(1 - \tilde{x}, \tilde{y})$, $(\tilde{x}, 1 - \tilde{y})$, and $(1 - \tilde{x}, 1 - \tilde{y})$. Hence, by convexity of the feasible region, $\gamma^*$ is also attained at the point obtained by taking the average over the above four points; i.e., $x_i = y_i = \frac{1}{2}$ for $i = 1, \ldots, n$. It then follows that $\gamma^* = 2$ for all $n \geq 2$. □

Remark 1. Define $X_{ij} = x_ix_j$ and $Y_{ij} = y_iy_j$, for all $1 \leq i \leq j \leq n$. Then the feasible region of Problem (CP) can be equivalently written as $\mathcal{P} = \{(x, y, X, Y, \gamma) : X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \forall 1 \leq i < j \leq n, X_{ij} = x_ix_j, Y_{ij} = y_iy_j, \forall 1 \leq i \leq j \leq n\}$. 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 $1 \leq i < j \leq n$. Moreover, 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 $\mathcal{P}$:

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

It is simple to verify that the projection of $\mathcal{S}$ 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 [11] 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 stronger polyhedral relaxations for Problem (CP) by utilizing a couple of simple symmetry-breaking type constraints.

Tighter 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 function in (1) by its concave envelope over the corresponding box, we obtain the following relaxation of Problem (CP):

\[
\begin{align*}
\text{(TWbnd) } & \quad \text{maximize } \gamma \\
& \quad \text{subject to } \\
& \quad \begin{align*}
& x_i + x_j + y_i + y_j \geq 2\gamma, \\
& x_i + x_j - y_i - y_j + 1 \geq 2\gamma, \\
& -x_i - x_j + y_i + y_j + 1 \geq 2\gamma, \\
& -3x_i - x_j - y_i - y_j + 2 \geq 2\gamma, \\
& x_i + x_j + y_i + 2y_j \geq 2\gamma, \\
& x_i + x_j - 3y_i + 2 \geq 2\gamma, \\
& -x_i - x_j + y_i + 2y_j + 1 \geq 2\gamma, \\
& -x_i - x_j - 3y_i + 3 \geq 2\gamma, \\
& x_i + 2x_j + y_i + 2y_j \geq 2\gamma, \\
& x_i + 2x_j - 3y_i + 2 \geq 2\gamma, \\
& -3x_i + y_i + 2y_j + 2 \geq 2\gamma, \\
& -3x_i - 3y_i + 4 \geq 2\gamma, \\
& x_i + x_j + 2y_i + 2y_j \geq 2\gamma, \\
& x_i + x_j - 2y_i - 2y_j + 4 \geq 2\gamma, \\
& -x_i - x_j + 2y_i + 2y_j + 1 \geq 2\gamma, \\
& -x_i - x_j - 2y_i - 2y_j + 5 \geq 2\gamma, \\
& x_i + 2x_j + 2y_i + 2y_j \geq 2\gamma, \\
& x_i + 2x_j - 2y_i - 2y_j + 4 \geq 2\gamma, \\
& -3x_i + 2y_i + 2y_j + 2 \geq 2\gamma, \\
& -3x_i - 2y_i - 2y_j + 6 \geq 2\gamma, \\
& x_i + x_j + y_i + y_j \geq \gamma, \\
& x_i + x_j - y_i - y_j + 2 \geq \gamma, \\
& -x_i - x_j + y_i + y_j + 2 \geq \gamma, \\
& -x_i - x_j - y_i - y_j + 4 \geq \gamma
\end{align*}
\end{align*}
\]

\(1 \leq i < j \leq n_y\)

\(1 \leq i < n_x < j\)

\(1 \leq i \leq n_y < n_x < j\)

\(1 \leq i \leq n_y < j < n_x\)

\(1 \leq i \leq n_y \leq n_x < j\)

\(1 \leq i \leq n_y < i < j \leq n_x\)

\(1 \leq i < j \leq n_x\)

\(1 \leq i < n_x < j \leq n_y\)

\(1 \leq i < n_x \leq j \leq n_y\)

\(0 \leq x_i \leq \frac{1}{2}, \ i = 1, \ldots, n_x, \ 0 \leq x_i \leq 1, \ i = n_x + 1, \ldots, n\)

\(0 \leq y_i \leq \frac{1}{2}, \ i = 1, \ldots, n_y, \ 0 \leq y_i \leq 1, \ i = n_y + 1, \ldots, n.\)

**Claim 2.** The optimal value of Problem (TWbnd) is \(\gamma^* = \frac{1}{2}\) for all \(n \geq 5\).

**Proof.** If \(n \geq 5\), we have \(n_y \geq 2\); i.e., there exists at least one pair \((i, j)\) satisfying inequalities (4) in the constraint set of (TWbnd). We first obtain an upper bound \(\hat{\gamma}\) on the optimal value of Problem (TWbnd), by finding the maximum value of \(\gamma\) over the the constraint set (4) together with lower and upper bounds on the corresponding \(x\) and \(y\) variables. Subsequently, we show that \(\hat{\gamma}\) is sharp by providing a feasible solution of (TWbnd) that attains this bound. Now consider the constraint set (4); using a similar line of arguments as in the proof of Claim 1, by symmetry, from these inequalities it follows that \(\hat{\gamma} = \frac{1}{2}\). Consider the point \((\tilde{x}, \tilde{y}, \tilde{\gamma})\), where \(\tilde{x}_i = \tilde{y}_i = \frac{1}{4}\) for \(1 \leq i \leq n_y\) and \(\tilde{x}_i = \tilde{y}_i = \frac{1}{2}\) for \(n_y < i \leq n\). It is simple to verify that \((\tilde{x}, \tilde{y}, \tilde{\gamma})\) is a feasible solution of Problem (TWbnd) and this completes the proof. \(\Box\)

**Remark 2.** An equivalent formulation for Problem (TWbnd) 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 $\mathcal{S}_{\text{bnd}}$ 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 (TWbnd).

**Order constraints.** Next, we study the impact of 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

\[
0 \leq x_1 \leq x_2 \leq \cdots \leq x_n \leq 1, \tag{5}
\]

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

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

**Claim 3.** The optimal value of Problem (TWord) is $\gamma^* = 1 + \frac{1}{n-1}$ for all $n \geq 2$.

**Proof.** Consider the following constraints of Problem (TWord):

\[
\begin{align*}
x_{i+1} - x_i + y_i + y_{i+1} \geq \gamma \\
x_{i+1} - x_i - y_i - y_{i+1} + 2 \geq \gamma 
\end{align*}, \quad 1 \leq i < n. \tag{6}
\]

We now 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 an optimal solution of this auxiliary LP. By symmetry $(\tilde{x}, 1 - \tilde{y}, \tilde{\gamma})$ is also an optimal solution. Hence, by convexity of the feasible region, there exists an optimal solution of the form $(\tilde{x}, \tilde{y}, \tilde{\gamma})$, where $\tilde{y}_i = \frac{1}{2}$ for $i \in \{1, \ldots, n\}$. It then follows that $\tilde{\gamma}$ is equal to the optimal value of the following problem:

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

It can be shown that the optimal value of the above problem is attained at $x_i = \frac{i-1}{n-1}$, $i = 1, \ldots, n$ and is equal to $\tilde{\gamma} = 1 + \frac{1}{n-1}$. Furthermore, it is simple to check that $(\tilde{x}, \tilde{y}, \tilde{\gamma})$ with $\tilde{x}_i = \frac{i-1}{n-1}$, $\tilde{y}_i = \frac{1}{2}$, for all $i = 1, \ldots, n$ is a feasible solution of (TWord) and this completes the proof. \qed
Claim 4. The optimal value of Problem (TWcomb) is $\gamma^* = \frac{1}{4} \left( 1 + \frac{1}{n - 1} \right)$ for all $n \geq 5$.

Proof. If $n \geq 5$, we have $n_y \geq 2$; consider the following inequalities present in constraint set (8) of (TWcomb):

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

Remark 3. Consider the first-level RLT relaxation of the feasible region of Problem (CP) as defined in Remark 1. We can strengthen this relaxation by utilizing the order constraints given by (5) to generate the following RLT-type constraints:

$$
\begin{align*}
X_{ij} - X_{ij} & \leq x_j - X_{ij} \\
X_{ij} & \leq x_i - X_{ij}
\end{align*}
$$

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 (TWcomb). Using inequalities (5) 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 upper bound obtained from 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 $n_y \geq 2$. If we impose tighter bounds on $x$ and $y$ variables as given by (2) and (3), then $x_{n_y} \leq x_{n_y+1}$ is no longer valid. Thus, we impose the order constraints as follows

$$
\begin{align*}
& x_i \leq x_{i+1}, \quad \forall i \in \{1, \ldots, n-1\} \setminus \{n_y\}.
\end{align*}
$$

Subsequently, we replace each quadratic term by its concave envelope over the corresponding rectangular, triangular or trapezoidal domain to obtain the following relaxation:

$$(TWcomb) \quad \text{maximize} \quad \gamma$$

subject to

$$
\begin{align*}
& x_j - x_i + y_i + y_j \geq 2\gamma \\
& x_j - x_i - y_i - y_j + 1 \geq 2\gamma \\
& x_i + x_j + y_i + 2y_j \geq 2\gamma \\
& x_i + x_j - 3y_i + 2 \geq 2\gamma \\
& -x_i - x_j + y_i + 2y_j + 1 \geq 2\gamma \\
& -x_i - x_j - 3y_i + 3 \geq 2\gamma \\
& x_i + 2x_j + y_i + 2y_j \geq 2\gamma \\
& x_i + 2x_j - 3y_i + 2 \geq 2\gamma \\
& -3x_i + y_i + 2y_j + 2 \geq 2\gamma \\
& -3x_i - 3y_i + 4 \geq 2\gamma \\
& x_j - x_i + 2y_i + 2y_j \geq 2\gamma \\
& x_j - x_i - 2y_i - 2y_j + 4 \geq 2\gamma \\
& x_j - x_i + 2y_i + 2y_j \geq 2\gamma \\
& x_j - x_i - 2y_i - 2y_j + 4 \geq 2\gamma \\
& 2x_j - 3x_i + 2y_i + 2y_j \geq 2\gamma \\
& 2x_j - 3x_i - 2y_i - 2y_j + 4 \geq 2\gamma \\
& x_j - x_i + y_i + y_j \geq \gamma \\
& x_j - x_i - y_i - y_j + 2 \geq \gamma \\
& 0 \leq x_i \leq \frac{1}{2}, \quad i = 1, \ldots, n_x, \\
& 0 \leq x_i \leq 1, \quad i = n_x + 1, \ldots, n \\
& 0 \leq y_i \leq \frac{1}{2}, \quad i = 1, \ldots, n_y, \\
& 0 \leq y_i \leq 1, \quad i = n_y + 1, \ldots, n.
\end{align*}
$$

Claim 4. The optimal value of Problem (TWcomb) is $\gamma^* = \frac{1}{4} \left( 1 + \frac{1}{n - 1} \right)$ for all $n \geq 5$.

Proof. If $n \geq 5$, we have $n_y \geq 2$; consider the following inequalities present in constraint set (8) of (TWcomb):
and denote by \( \hat{\gamma} \) the maximum value of \( \gamma \) over the region defined by the above inequalities together with lower and upper bounds on \( x \) and \( y \) variables. Using a similar line of arguments as in the proof of Claim 3, it follows that \( \gamma \leq \frac{1}{2}(1 + \frac{1}{n_y - 1}) \), and this upper bound is attained at \( x_{i+1} = x_i = \frac{1}{2(\gamma - 1)} \) and \( y_i = \frac{1}{2} \) for all \( 1 \leq i < n_y \). Now, consider the point \((\bar{x}, \bar{y}, \hat{\gamma})\) where \( \bar{x}_i = \frac{\gamma - 1}{2(\gamma - 1)} \), \( \bar{y}_i = \frac{1}{2} \) for \( i = 1, \ldots, n_y \), and \( \bar{x}_i = \bar{y}_i = \frac{1}{2} \) for \( i = n_y + 1, \ldots, n \). It is simple to verify that \((\bar{x}, \bar{y}, \hat{\gamma})\) is a feasible solution of (TWcomb) implying \( \gamma^* = \hat{\gamma} \). \( \square \)

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

\[
X_{ii} \leq X_{ij}, \quad \forall (i, j) \in I
\]

\[
\frac{x_i}{2} - X_{ij} \leq \frac{x_j}{2} - X_{jj}, \quad \forall (i, j) \in I \text{ with } j \leq n_x
\]

\[
x_i - X_{ij} \leq x_j - X_{jj}, \quad \forall (i, j) \in I \text{ with } j > n_x
\]

**Remark 5.** To combine the order constraints (5) with the tighter variables bounds (2) and (3), we eliminated the order constraint \( x_{n_y} \leq x_{n_y + 1} \), 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 (5) 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 function with its concave envelope over the corresponding domain. It can be shown that the optimal value of this relaxation is \( \gamma^* = 1 + \frac{1}{4(n_2 - 1)} \), 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 \( x_i^* = y_i^* = \frac{1}{2} \), for all \( i = 1, \ldots, n \), 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 value of Problem (TWbnd) is attained at \( x_i^* = y_i^* = \frac{1}{2} \) for all \( 1 \leq i \leq n_y \), \( x_i^* = y_i^* = \frac{1}{2} \) for all \( n_y + 1 \leq i \leq n \), and is equal to

\[ \gamma^* = \frac{1}{2}. \]

(iv) Let \( n \geq 5 \). Then the optimal value of Problem (TWcomb) is is attained at \( x_i^* = \frac{i-1}{2(n_2 - 1)}, \ y_i^* = \frac{1}{2} \), for all \( 1 \leq i \leq n_y \), \( x_i^* = y_i^* = \frac{1}{2} \) for all \( n_y + 1 \leq i \leq n \), and is equal to

\[ \gamma^* = \frac{1}{4} \left( 1 + \frac{1}{[(n-1)/4]} \right). \]
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 Section 2, where the feasible region defined by a single constraint was replaced by its convex hull over rectangular or triangular domains. Throughout this section, we assume \( n \geq 3 \) so that the constraint set of (CP) contains multiple non-overlapping constraints. We start by introducing a reformulation of Problem (CP) which will be important for our later developments:

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

Denote by \( \mathcal{X} \) the feasible region of Problem (CPr) and define the sets

\[
\mathcal{P} = \left\{ (x, y, \beta, \gamma) : (x_j - x_i)^2 + (y_j - y_i)^2 \geq \beta_{ij}, \forall 1 \leq i < j \leq n, \, x, y \in [0, 1]^n, \, \beta \in \mathbb{R}^{\frac{n(n-1)}{2}}, \, \gamma \in \mathbb{R} \right\}
\]

and

\[
\mathcal{K} = \left\{ (x, y, \beta, \gamma) : \beta_{ij} \geq \gamma, \forall 1 \leq i < j \leq n, \, x, y \in \mathbb{R}^n, \, \beta \in \mathbb{R}^{\frac{n(n-1)}{2}}, \, \gamma \in \mathbb{R} \right\}.
\]

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

\[
\mathcal{Q} = \left\{ (x, y, X, Y) : x_i^2 \geq X_{ii}, \quad y_i^2 \geq Y_{ii}, \quad \forall 1 \leq i \leq n, \quad X_{ij} \geq x_i x_j, \quad Y_{ij} \geq y_i y_j, \quad \forall 1 \leq i < j \leq n, \, x, y \in [0, 1]^n \right\}
\]

(10)

Denote by \( \bar{\mathcal{P}} \) the projection of \( \mathcal{P} \) onto the space \((x, y, \beta)\). Define the linear mapping \( \mathcal{L} : (x, y, X, Y) \to (x, y, \beta) \), where \( \beta_{ij} = X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \) for all \( 1 \leq i < j \leq n \). It then follows that to characterize \( \text{conv}(\mathcal{P}) \), it suffices to characterize \( \text{conv}(\mathcal{Q}) \), as \( \bar{\mathcal{P}} \) is the image of \( \bar{\mathcal{Q}} \) under the 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 \( \mathcal{Q} \) defined by (10). Denote by \( \bar{\mathcal{Q}}_x \) (resp. \( \bar{\mathcal{Q}}_y \)), the set obtained by dropping the inequalities containing \((y, Y)\) variables (resp. \((x, Y)\) variables) from the description of \( \mathcal{Q} \). It then follows that \( \text{conv}(\mathcal{Q}) = \text{conv}(\bar{\mathcal{Q}}_x) \cap \text{conv}(\bar{\mathcal{Q}}_y) \). Let \( \bar{\mathcal{Q}}_x \) denote the projection of \( \bar{\mathcal{Q}}_x \) onto the \((x, X)\) space; it can be shown that the vertices of \( \text{conv}(\bar{\mathcal{Q}}_x) \) are binary valued by using the fact that there does not exist any function of the form \( f(x) = \sum_{i=1}^{n} \alpha_i x_i + \sum_{i=1}^{n} \omega_i x_i^2 + \sum_{1 \leq i < j \leq n} \omega_{ij} x_i x_j \) for some \( \alpha \in \mathbb{R}^n \), \( \omega_i \geq 0 \) for all \( i \in \{1, \ldots, n\} \) and \( \omega_{ij} \leq 0 \) for all \( 1 \leq i < j \leq n \), whose unique maximizer over the unit hypercube is attained at a non-binary \( x \) (see [13] for more details). Hence, without loss of generality, we can assume that \( x, y \in \{0, 1\}^n \) in (10). Accordingly, define the two sets

\[
\mathcal{Q}^k_\varepsilon = \left\{ (x, X) : x_{ij} \geq x_i x_j, \forall 1 \leq i < j \leq n, \, x \in \{0, 1\}^n \right\}
\]

and

\[
\mathcal{Q}^\varepsilon_* = \left\{ (x, X) : x_i^2 \geq X_{ii}, \forall 1 \leq i \leq n, \, x \in \{0, 1\}^n \right\}.
\]

Claim 5. \( \text{conv}(\mathcal{Q}_x) = \text{conv}(\mathcal{Q}^k_\varepsilon) \cap \text{conv}(\mathcal{Q}^\varepsilon_*) \).

Proof. Let \( I = \{1, \ldots, n\} \) and let \( k \in I \); define \( \mathcal{Q}^k_\varepsilon = \left\{ (x, X) : x_{k:k}^2 \geq X_{k:k}, x_k \in \{0, 1\} \right\} \) and \( \mathcal{Q}^k_\varepsilon = \left\{ (x, X) : x_i^2 \geq X_{ii}, \forall i \in I \setminus \{k\}, \, X_{ij} \geq x_i x_j, \forall 1 \leq i < j \leq n, \, x \in \{0, 1\}^n \right\} \). Consider a point \((\bar{x}, \bar{X}) \in \text{conv}(\mathcal{Q}^k_\varepsilon) \cap \text{conv}(\mathcal{Q}^\varepsilon_*) \). Clearly, \( \bar{x}_k \) can be uniquely written as convex combination of the two points \( \{0, 1\} \); i.e., there exists a unique multiplier \( \lambda \in [0, 1] \) such that \( \bar{x}_k = (1-\lambda)(0) + \lambda(1) = \lambda \). Let \( \mathcal{L}_0 = \{ (x, X) : x_k = 0 \} \) and \( \mathcal{L}_1 = \{ (x, X) : x_k = 1 \} \). Define \( \mathcal{Q}^0 = \mathcal{Q}_x \cap \mathcal{L}_0 \), \( \mathcal{Q}^1 = \mathcal{Q}_x \cap \mathcal{L}_1 \), \( \mathcal{Q}^k_\varepsilon = \mathcal{Q}^k_\varepsilon \cap \mathcal{L}_0 \), \( \mathcal{Q}^k_\varepsilon = \mathcal{Q}^k_\varepsilon \cap \mathcal{L}_1 \), \( \mathcal{Q}^0 = \mathcal{Q}^0 \cap \mathcal{L}_0 \), and \( \mathcal{Q}^1 = \mathcal{Q}^1 \cap \mathcal{L}_1 \).
Clearly, \( \text{conv}(Q_x^*) = \{ (x, X) : X_{ii} \leq x_i, \forall 1 \leq i \leq n, x \in [0, 1]^n \} \). Symmetrically, we obtain a characterization of \( \text{conv}(Q_y) \). Hence, the following relaxation of Problem (CPr)

\[
\begin{align*}
\text{maximize} & \quad \gamma \\
\text{subject to} & \quad (x, y, \beta, \gamma) \in \text{conv}(P) \cap K
\end{align*}
\]

can be equivalently written as

\[
\begin{align*}
\text{(MT)} & \quad \text{maximize} \quad \gamma \\
& \quad \text{subject to} \quad X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \ 1 \leq i < j \leq n \\
& \quad \quad (x, X) \in \text{conv}(Q_x^b) \\
& \quad \quad (y, Y) \in \text{conv}(Q_y^b) \\
& \quad \quad X_{ii} \leq x_i, Y_{ii} \leq y_i, \ 1 \leq i \leq n.
\end{align*}
\]

Now consider \( \text{conv}(Q_x^b) \); this polyhedron is a relaxation of the \textit{Boolean quadratic polytope} [7] defined as

\[
\text{BQP} = \text{conv}\{ (x, X) : X_{ij} = x_i x_j, \forall 1 \leq i < j \leq n, x \in \{0, 1\}^n \}.
\]

While BQP is bounded, \( \text{conv}(Q_x^b) \) is an unbounded polyhedron whose recession cone is given by \( C_\infty = \{ (x, X) : X_{ij} \geq 0, \forall 1 \leq i < j \leq n \} \). Recall that given two sets \( S, T \in \mathbb{R}^n \), their Minkowski sum is defined as \( S \oplus T := \{ s + t : s \in S, t \in T \} \). We have the following characterization of \( \text{conv}(Q_x^b) \).

**Claim 6.** \( \text{conv}(Q_x^b) = \text{BQP} \oplus C_\infty. \)

**Proof.** To prove the statement, it suffices to show that \( \text{conv}(Q_x^b) \) and BQP have the same set of vertices; the result then follows from Minkowski-Weyl theorem (see for example Section 17 of [8]). Let \( \hat{x} \) denote a binary vector in \( \mathbb{R}^n \) and let \( \hat{X}_{ij} = \hat{x}_i \hat{x}_j \) for all \( 1 \leq i < j \leq n \). To show that \( (\hat{x}, \hat{X}) \) is a vertex of \( \text{conv}(Q_x^b) \), it suffices to characterize a linear function \( c^T x + d^T X \) whose maximum over \( \text{conv}(Q_x^b) \) is uniquely attained at \( (\hat{x}, \hat{X}) \). Let \( k = \sum_{i=1}^n \hat{x}_i \). Define \( c_j = -1 \) for all \( j \) such that \( \hat{x}_j = 0 \), \( c_j = k \) for all \( j \) such that \( \hat{x}_j = 1 \), and \( d_{ij} = -1 \) for all \( 1 \leq i < j \leq n \). Using the fact that the function \( f(m) = km - m(m-1)/2 \), where \( 0 \leq m \leq k \) is strictly increasing, we conclude that the unique maximizer of \( c^T x + d^T X \) over \( \text{conv}(Q_x^b) \) is given by \( (\hat{x}, \hat{X}) \). \( \square \)

Claim 6 enables us to characterize several classes of facet-defining inequalities for \( \text{conv}(Q_x^b) \) by leveraging on the existing results for the Boolean quadratic polytope.

**Claim 7.** Suppose that \( ax + bX \leq c \) defines a facet of BQP. Then this inequality is facet-defining for \( \text{conv}(Q_x^b) \) if and only if \( b_{ij} \leq 0 \), for all \( 1 \leq i < j \leq n \).

**Proof.** By Claim 6, a facet-defining inequality \( ax + bX \leq c \) for BQP is valid at all vertices of \( \text{conv}(Q_x^b) \) and is binding at \( n \) affinely independent vertices of this polyhedron. Hence, this inequality defines a facet of \( \text{conv}(Q_x^b) \) if and only if \( ad_x + bd_X \leq 0 \) for all \( (d_x, d_X) \in C_\infty \). By definition of \( C_\infty \) it follows that this statement holds if and only if \( b_{ij} \leq 0 \) for all \( 1 \leq i < j \leq n \). \( \square \)

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

\[
\alpha \sum_{i \in J} x_i - \sum_{i \in J, j \in J, i < j} X_{ij} \leq \frac{\alpha(\alpha + 1)}{2}
\]

are facet-defining for the Boolean quadratc polytope [7]. Since the coefficients of \( X_{ij} \) are nonpositive for all \( 1 \leq i < j \leq n \), by Claim 7, clique inequalities define facets of \( \text{conv}(Q_x^b) \) as well. More generally, any valid
inequality $ax + bX \leq c$ for $\text{conv}(Q^b_x)$ must satisfy $b_{ij} \leq 0$ for all $1 \leq i < j \leq n$. We should remark that the facet-description of $\text{conv}(Q^b_x)$ contains many inequalities that are not present in the description of BQP; the additional inequalities correspond to unbounded facets of $\text{conv}(Q^b_x)$. However, for Problem (MT) such facet-defining inequalities are redundant.

We are now ready to analyze the quality of the upper bound given by Problem (MT).

Claim 8. Let $n \geq 3$. Then the optimal value of Problem (MT) is given by $\gamma^* = 1 + \frac{1}{n}$, if $n$ is an odd number and is given by $\gamma^* = 1 + \frac{1}{n}$, if $n$ is an even number.

Proof. Since Problem (MT) is symmetric in $(x, X)$ and $(y, Y)$ and its feasible region is convex, there exists an optimal solution with $x = y$ and $X = Y$. Consider inequalities (11); at any optimal solution, at least one of these inequalities is active as otherwise, we can obtain a feasible solution with a better objective value by increasing the value of $X$. Thus, at an optimal solution inequalities (11) are all active implying that there exist optimal solutions of (MT) with $X_{kk} \leq x_k$ and $X_{mm} \leq x_m$ are also binding as otherwise it is possible to make the corresponding inequality in (11) inactive by increasing the value of $X_{kk}$ or $X_{mm}$. In fact, we argue that at an optimal solution of (MT), inequalities $X_{ii} \leq x_i$ are binding for all $i \in \{1, \ldots, n\}$. To obtain a contradiction, denote by $l$ the index of an 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 $X_{ij} < x_i$ for any $l \in \{1, \ldots, n\}$. Hence, by taking the average over all such solutions, we obtain an optimal solution of (MT) for which $X_{ii} < x_i$ for all $i = 1, \ldots, n$, which is a contradiction. Thus, at an optimal solution $X_{ii} = x_i$, for all $i \in \{1, \ldots, n\}$. Using a similar symmetry argument, we conclude that at an optimal solution inequalities (11) are all active implying that there exist optimal solutions of (MT) 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:

$$(\text{MTx}) \quad \text{maximize} \quad \frac{8}{n(n-1)} \left(\frac{(n-1)}{2} \sum_{i=1}^{n} x_i - \sum_{1 \leq i < j \leq n} X_{ij}\right)$$
$$\text{subject to} \quad (x, X) \in \text{conv}(Q^b_x)$$
$$x_i - 2X_{ij} + x_j = x_k - 2X_{kl} + x_l, \quad \forall 1 \leq i < j \leq n, \forall 1 \leq k < l \leq n.$$ 

Now suppose that $n$ is an odd number implying that $(n-1)/2$ is an integer. Note that $(n-1)/2 \leq n - 2$ as by assumption $n \geq 3$. Letting $J = \{1, \ldots, n\}$ and $\alpha = (n-1)/2$ in (12) yields

$$\frac{(n-1)}{2} \sum_{i \in J} x_i - \sum_{i \in J, j < j} X_{ij} \leq \frac{(n^2-1)}{8}. \quad (13)$$

By Claim 7, inequality (13) defines a facet of $\text{conv}(Q^b_x)$. Since the objective function of Problem (MTx) is parallel to this facet, it follows that an upper bound on the optimal value of this problem is given by $\tilde{\gamma} = 1 + \frac{1}{\pi}$, if $n$ is an odd number.

Now consider a relaxation of (MTx) denoted by (MTx’), which is obtained by removing the equality constraints from the constraint set of (MTx). Clearly the optimal value of (MTx’) is given by $\tilde{\gamma}$. Denote by $(\tilde{x}, \tilde{X})$ a feasible solution of (MTx’). Let $\tilde{x}_\pi$ denote a permutation of $\tilde{x}$ and let $\tilde{X}_{\Pi(i,j)} = \tilde{X}_{\pi(i),\pi(j)}$ for all $1 \leq i < j \leq n$. It is then simple to verify that $(\tilde{x}_\pi, \tilde{X}_{\Pi})$ is also a feasible solution of (MTx’) with the same objective value. It then follows that by taking the average over the feasible points corresponding
to all possible permutations of \( \tilde{x} \), we obtain a feasible solution \((\tilde{x}, \tilde{X})\) of \((MTx')\) with \(x_1 = \cdots = x_n\) and \(X_{1,2} = \cdots = X_{n-1,n}\) that attains the same objective value as \((\tilde{x}, \tilde{X})\). Hence, we conclude that there exists an optimal solution of \((MTx')\) with \(x_i = t\) for all \(1 \leq i \leq n\) and \(X_{ij} = z\) for all \(1 \leq i < j \leq n\). As such a point clearly satisfies all equality constraints present in \((MTx)\), we conclude that \(\tilde{\gamma}\) is a sharp upper bound for \((MTx)\).

Now, let \(n \geq 4\) be an even number, and let \(J\) 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 \(i, j \in J\) with \(i < j\) and following a similar line of arguments as above, we obtain that for an even \(n\), the optimal value of Problem \((MTx)\) is given by \(\gamma^* = 1 + \frac{1}{n-1}\).

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]. As before let \(I = \{1, \ldots, n\}\) and let \(\alpha\) be an integer. Denote by \(C_x\) the polytope defined by all inequalities of the form

\[
\alpha \sum_{i \in I} x_i - \sum_{(i,j) \in J, i < j} X_{ij} \leq \frac{\alpha(\alpha + 1)}{2}, \quad \forall J \subseteq I, \ J \neq \emptyset, \ \forall \min\{|J| - 2, 1\} \leq \alpha \leq \max\{|J| - 2, 1\}.
\]

(14)

If \(|J| \geq 3\), the above inequalities are clique inequalities defined by (12). If \(|J| = 2\), these inequalities simplify to \(X_{ij} \geq 0\) and \(X_{ij} \geq x_i + x_j - 1\) for all \(1 \leq i < j \leq n\), which are McCormik inequalities and if \(|J| = 1\), they simplify to \(0 \leq x_i \leq 1\) for all \(i \in I\). We should remark that \(\text{conv}(Q_{x}^b) = C_x\) for \(n \leq 4\) while \(\text{conv}(Q_{y}^b) \subset C_x\) for \(n \geq 5\). Consider the following relaxation of Problem \((MT)\):

\[(MT_{\text{clique}}) \quad \text{maximize} \quad \gamma \quad \text{subject to} \quad X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \ 1 \leq i < j \leq n \quad (x, X) \in C_x \quad (y, Y) \in C_y \quad X_{ii} \leq x_i, \ Y_{ii} \leq y_i, \ 1 \leq i \leq n.\]

Claim 9. Let \(n \geq 3\). The optimal value of Problem \((MT_{\text{clique}})\) is given by \(\gamma^* = 1 + \frac{1}{n}\), if \(n\) is an odd number and is given by \(\gamma^* = 1 + \frac{1}{n-1}\), if \(n\) is an even number.

Proof. From the proof of Claim 8 it follows that the bound \(\tilde{\gamma}\) given in this claim is a valid upper bound on the optimal value of Problem \((MT_{\text{clique}})\) as well. The statement then follows from the fact that \((MT_{\text{clique}})\) is a relaxation of \((MT)\).

\[\square\]

Tighter variable bounds. By incorporating tighter bounds on \(x\) and \(y\) variables as defined by (2) and (3), we obtain the following multi-row polyhedral relaxation of Problem \((CP)\):

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

where \(Q_{x_{\text{bnd}}}^b = \{(x, X) : X_{ij} \geq x_i, x_j, \ 1 \leq i < j \leq n, \ x_i \in [0, \frac{1}{2}], \ 1 \leq i \leq n_x, \ x_i \in [0, 1], \ n_x + 1 \leq i \leq n\}\) and \(Q_{y_{\text{bnd}}}^b = \{(y, Y) : Y_{ij} \geq y_i, y_j, \ 1 \leq i < j \leq n, \ y_i \in [0, \frac{1}{2}], \ 1 \leq i \leq n_y, \ y_i \in [0, 1], \ n_y + 1 \leq i \leq n\}.\)
The polyhedron $\text{conv}(\mathcal{Q}^b_{x,\text{bnd}}(x, X))$ can be obtained from $\text{conv}(\mathcal{Q}^b_{x}(\bar{x}, \bar{X}))$ defined before, via the one-to-one linear mapping:

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

(15)

Similarly, $\text{conv}(\mathcal{Q}^b_{y,\text{bnd}})$ can be obtained from $\text{conv}(\mathcal{Q}^b_{y})$ using a one-to-one linear mapping.

Claim 10. Suppose that $n \geq 5$ and let $n_y = \lceil \frac{n}{4} \rceil$. Then the optimal value of Problem (MT\text{bnd}) is given by $\gamma^* = \frac{1}{4}(1 + \frac{1}{n_y})$, if $n_y$ is odd, and is given by $\gamma^* = \frac{1}{4}(1 + \frac{1}{n_y - 1})$, if $n_y$ is even.

Proof. Since $n \geq 5$, we have $n_y \geq 2$. Consider the following subset of constraints of Problem (MT\text{bnd})

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

(16)

where $\mathcal{Q}^b_{x} = \{(x, X) : X_{ij} \geq x_i, x_j, 1 \leq i < j \leq n_y, x \in [0, \frac{1}{2}]^{n_x}\}$ and $\mathcal{Q}^b_{y} = \{(y, Y) : Y_{ij} \geq y_iy_j, 1 \leq i < j \leq \lfloor \frac{n}{4} \rfloor\}$. Over the region defined by constraints (16), consider the set of points at which the maximum value of $\gamma$ is attained. Using a similar argument as in the proof of Claim 8, by symmetry, there exist points satisfying $x_i = y_i$ for all $i \in \{1, \ldots, n_y\}$, $X_{ii} = Y_{ii}$ for all $1 \leq i \leq j \leq n_y$, $X_{ii} = \frac{x_i}{2}$ for all $1 \leq i \leq n_y$, $X_{ij} = \frac{X_{ij}}{2}$ for all $1 \leq i < j \leq n_y$, $Y_{ii} = \frac{y_i}{2}$ for all $1 \leq i \leq n_y$, $Y_{ij} = \frac{Y_{ij}}{2}$ for all $1 \leq i < j \leq n_y$, implying $(n_y - 1)\sum_{i=1}^{n_y} x_i - 4\sum_{1 \leq i < j \leq n_y} X_{ij} = \frac{n_y(n_y-1)}{2}\gamma$. Hence, employing a similar line of arguments as in the proof of Claim 8, we conclude that the maximum value of $\gamma$ over the region defined by (16) is given by $\tilde{\gamma} = \frac{1}{4}(1 + \frac{1}{n_y})$, if $n_y$ is an odd number, and is given by $\tilde{\gamma} = \frac{1}{4}(1 + \frac{1}{n_y - 1})$, if $n_y$ is an even number. Finally, using the linear mapping defined by (15), such an optimal solution can be lifted to a feasible point of Problem (MT\text{bnd}) and this completes the proof.

Consider the polyhedron $\mathcal{C}_x$ defined by inequalities (14). Denote by $\mathcal{C}_{x,\text{bnd}}$ the image of $\mathcal{C}_x$ under the linear mapping defined by (15). The polyhedron $\mathcal{C}_{y,\text{bnd}}$ is similarly defined. We now construct a relaxation of Problem (MT\text{bnd}) by replacing the constraints $(x, X) \in \text{conv}(\mathcal{Q}^b_{x,\text{bnd}})$ and $(y, Y) \in \text{conv}(\mathcal{Q}^b_{y,\text{bnd}})$ with the constraints $(x, X) \in \mathcal{C}_{x,\text{bnd}}$ and $(y, Y) \in \mathcal{C}_{y,\text{bnd}}$, respectively. We refer to the resulting LP as (MT\text{bnd}^{\text{clique}}). It can be shown that the optimal value of (MT\text{bnd}^{\text{clique}}) is equal to the optimal value of (MT\text{bnd}).

Order constraints. Next, we obtain a multi-row polyhedral relaxation of Problem (MT) by incorporating the order constraints (5) on $x$ variables. More precisely, we characterize the convex hull of the following set:

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

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

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

as $\text{conv}(\mathcal{P}_{\text{ord}})$ is the image of $\text{conv}(\mathcal{Q}_{x,\text{ord}}) \times \text{conv}(\mathcal{Q}_y)$ under a linear mapping, where as before we define $\mathcal{Q}_y = \{(y, Y) : y_i^2 \geq Y_{ii}, \forall 1 \leq i \leq n, \ Y_{ij} \geq y_iy_j, \forall 1 \leq i < j \leq n, \ y \in [0, 1]^n\}$.

Claim 11.

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

(17)
Claim 12. Let $Y$ as in the previous proofs, by symmetry, we can argue that at any optimal solution of $(MTord)$ we

$\textbf{Proof.}$ First note that the polyhedra defined by (17) is a valid relaxation of the set $Q_{x,ord}$ 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 $\text{conv}(Q_{x,ord})$, as the projection of each point in the convex hull of $(x_j - x_i)^2 \geq \zeta_{ij}, 0 \leq x_i \leq x_j \leq 1$ 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)

$$\begin{align*}
\text{maximize} & \quad \gamma \\
\text{subject to} & \quad (x, y, \beta, \gamma) \in \text{conv}(P_{ord}) \cap K
\end{align*}$$

can be equivalently written as

$$(MTord) \begin{align*}
\text{maximize} & \quad \gamma \\
\text{subject to} & \quad x_j - x_i + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, 1 \leq i < j \leq n \\
& \quad (y, Y) \in \text{conv}(Q_y) \\
& \quad Y_{ii} \leq y_i, \forall 1 \leq i \leq n.
\end{align*}$$

Claim 12. Let $n \geq 3$. An upper bound on the optimal value of Problem (MTord) is given by

$$\bar{\gamma} = \frac{2}{3}(1 + \frac{1}{\lceil (n - 1)/2 \rceil}).$$

$\textbf{Proof.}$ As in the previous proofs, by symmetry, we can argue that at any optimal solution of (MTord) we have $Y_{ii} = y_i$ for all $1 \leq i \leq n$, and

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

Summing up over three of the above equalities associated with pairs of indices $(i, j)$, $(j, k)$ and $(i, k)$ for some $1 \leq i < j < k \leq n$, it follows that at any optimal solution the following is satisfied

$$\gamma = \frac{2}{3}(x_k - x_i + y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk}), \quad 1 \leq i < j < k \leq n.$$  

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 detailed before, the following clique inequalities are facet defining for $\text{conv}(Q_y)$:

$$y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk} \leq 1, \quad 1 \leq i < j < k \leq n.$$  

Consequently, at an optimal solution we have $\gamma \leq \frac{2}{3}(x_{i+2} - x_i + 1)$ for all $i \in \{1, \ldots, n - 2\}$ implying that the optimal value of the following problem provides an upper bound on the optimal value of Problem (MTord):

$$\begin{align*}
\text{maximize} & \quad \frac{2}{3}(1 + \Delta x) \\
\text{subject to} & \quad x_{i+2} - x_i \geq \Delta x, 1 \leq i \leq n - 2.
\end{align*}$$

It is simple to verify that the optimal value of the above problem is attained at $\Delta x = 1/\lceil (n - 1)/2 \rceil$ and is equal to (18).  

We now construct a relaxation of Problem (MTord) by replacing the constraint $(y, Y) \in \text{conv}(Q_y)$ with the constraint $(y, Y) \in C_y$:

$$(MTord^{\text{clique}}) \begin{align*}
\text{maximize} & \quad \gamma \\
\text{subject to} & \quad x_j - x_i + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, 1 \leq i < j \leq n \\
& \quad (y, Y) \in C_y \\
& \quad Y_{ii} \leq y_i, \forall 1 \leq i \leq n.
\end{align*}$$
Our numerical experimentations show that the optimal value of $\text{MTord}^{\text{clique}}$ is equal to $\tilde{\gamma}$ given by (18) for $n < 13$. Indeed for $n = 13$, the optimal value of the above problem is $\gamma^* = 0.7742$ while $\tilde{\gamma} = 0.7778$. However, our numerical experiments reveal that the relative gap $(\tilde{\gamma} - \gamma^*)/\gamma^* \times 100\%$ remain below five percent for $13 \leq n \leq 30$. Hence, we argue that $\tilde{\gamma}$ defined by (18) is a reasonable measure for the quality of the bound given by Problem $\text{MTord}^{\text{clique}}$. In fact, we have the following sharpness result.

**Claim 13.** Let $n \geq 3$ and consider the following relaxation of Problem $\text{MTord}^{\text{clique}}$:

\[
\begin{align*}
(\text{MTord}^{\text{tri}}) \quad \text{maximize} \quad & \gamma \\
\text{subject to} \quad & x_j - x_i + Y_{ij} - 2Y_{ij} + Y_{jj} \geq \gamma, \quad 1 \leq i < j \leq n \\
& y_i + y_j - y_k - Y_{ij} - Y_{ik} \leq 1, \quad 1 \leq i < j < k \leq n \\
& Y_{ii} \leq y_i, \quad \forall 1 \leq i \leq n.
\end{align*}
\]

The optimal value (MTord\textsuperscript{tri}) is given by $\gamma^* = \frac{2}{3} \left( 1 + \frac{1}{[(n-1)/2]} \right)$. \hfill \Box

**Proof.** First, we establish that $\tilde{\gamma}$ defined by (18) is a valid upper bound for Problem (MTord\textsuperscript{tri}) via the exact line of arguments we used to prove that $\tilde{\gamma}$ is an upper bound for (MTord). Now consider the point:

\[
\begin{align*}
\tilde{x}_i &= \frac{i}{n} \Delta x, \quad i = 1, \ldots, n, \\
\tilde{y}_i &= Y_{ii} = \frac{1}{2} \frac{\Delta x}{\Delta y}, \quad i = 1, \ldots, n, \\
\tilde{Y}_{ij} &= \frac{i - j}{\Delta x}, \quad 1 \leq i < j \leq n, \\
\tilde{\gamma} &= \frac{2}{3} (1 + \Delta x),
\end{align*}
\] (20)

where as before $\Delta x = 1/[(n - 1)/2]$. It can be checked that $\tilde{x}_j - \tilde{x}_i + \tilde{Y}_{ii} - 2\tilde{Y}_{ij} + \tilde{Y}_{jj} = \frac{2}{3} (1 + \Delta x) = \tilde{\gamma}$ for all $1 \leq i < j \leq n$. Moreover, we have $\tilde{y}_i + \tilde{y}_j - \tilde{Y}_{ij} - \tilde{Y}_{ik} - \tilde{Y}_{jk} = 1 + (1 - \frac{k - 1}{2}) \Delta x \leq 1$, where the last inequality is valid since $k - i \geq 2$. Hence, the point defined by (20) is feasible for Problem (MTord\textsuperscript{tri}), implying that its optimal value is given by (18). \hfill \Box

**Best Multi-row polyhedral relaxations.** Finally, consider a 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 as defined by (2) and (3). To construct this relaxation, we replace the set

\[
\mathcal{Q}_{\text{comb}} = \{(x, \zeta) : (x_j - x_i)^2 \geq \zeta_{ij}, \ 1 \leq i < j \leq n, \ x_1 \leq \ldots \leq x_n, \ x_{n+1} \leq \ldots \leq x_n, \\
\quad x_i \in [0, \frac{1}{2}], \ 1 \leq i \leq n, \ x_i \in [0, 1], \ n + 1 \leq i \leq n\},
\]

by its convex hull. Moreover, we let $(y, Y) \in \text{conv}(\mathcal{Q}_{\text{bnd}}^b)$ and refer to the resulting LP as (MTcomb).

**Claim 14.** Let $n \geq 9$. Then an upper bound on the optimal value of Problem (MTcomb) is given by

\[
\tilde{\gamma} = \frac{1}{6} \left( 1 + \frac{1}{[(n_y - 1)/2]} \right)
\] (22)

**Proof.** Since $n \geq 9$, we have $n_y \geq 3$. Consider a pair $(i, j)$ with $1 \leq i < j \leq n_y$ and consider the following inequalities present the constraint set of (MTcomb):

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

Summing up over any three of the above inequalities associated with the pairs of indices $(i, j), (j, k)$ and $(i, k)$ for some $1 \leq i < k \leq n_y$ and using the fact that at any optimal solutions of Problem (MTcomb) we have $Y_{ii} = \frac{1}{2}$ for all $1 \leq i \leq n_y$, we conclude that at an optimal solution we have

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

As we detailed before, the inequality $2y_i + 2y_j + 2y_k - 4Y_{ij} - 4Y_{ik} - 4Y_{jk} \leq 1$ defines a facet of conv($\mathcal{Q}_{\text{bnd}}^b$). Moreover, as $x_i \leq x_{i+1}$ for all $1 \leq i \leq n_y$, a minimum value of $x_k - x_i$ is attained when $k = i + 2$. Finally, the maximum value of $x_{i+1} - x_i$ over $x_i \in [0, \frac{1}{2}]$ 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 (MTcomb) is given by (22). \hfill \Box
Theorem 2. Consider the multi-row polyhedral relaxations of the Circle packing problem defined above:

\[ \text{Claim 15. The optimal value of Problem (MTcomb\textsuperscript{tri}) is given by (22).} \]

Proof. First, employing a similar line of arguments as in the proof of Claim 14, we conclude that \( \tilde{\gamma} \) defined by (22) is an upper bound on the optimal value of Problem (MTcomb\textsuperscript{tri}). Moreover, it can be checked that the point \((\tilde{x}, \tilde{X}, \tilde{y}, \tilde{Y}, \tilde{\gamma})\) with

\[
\begin{align*}
\tilde{x}_i &= \frac{i}{2} \Delta x, & i = 1, \ldots, n_y, \\
\tilde{y}_i &= \frac{i + 2}{6} \Delta x, & i = 1, \ldots, n_y, \\
\tilde{x}_i &= \tilde{y}_i = \frac{1}{2}, & i = n_y + 1, \ldots, n \\
\tilde{Y}_{ii} &= \frac{n_y}{2}, & i = 1, \ldots, n_y \\
\tilde{Y}_{ii} &= \tilde{y}_i, & i = n_y + 1, \ldots, n \\
\tilde{Y}_{ij} &= \frac{i + j}{2} \Delta x, & 1 \leq i < j \leq n_y \\
\tilde{Y}_{ij} &= \frac{i + j}{2} \Delta x, & 1 \leq i \leq n_y < j \leq n \\
\tilde{Y}_{ij} &= \frac{1}{4}, & n_y < i < j \leq n,
\end{align*}
\]

where \( \Delta x = \frac{1}{2[(n_y - 1)/2]} \), is feasible for (MTcomb\textsuperscript{tri}). \( \square \)

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) 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 (MTbnd) 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 (MTord\textsuperscript{tri}) is

\[ \gamma^* = \frac{2}{3} \left( 1 + \frac{1}{\lceil (n - 1)/2 \rceil} \right). \]
Let \( n \geq 5 \) and let \( n_y = \lceil n/4 \rceil \). Then the optimal value of Problem (MTcomb) 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 [14]. 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
\[
X_{ii} - 2X_{ij} + X_{jj} \geq \gamma, \quad 1 \leq i < j \leq n
\]
on the diagonal entries of matrices \( X \) and \( Y \). Hence, the following SDP provides an upper bound on the optimal value of the Circle packing problem:

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

Claim 16. The optimal value of Problem (SDP1) is given by \( \gamma^* = 1 + \frac{1}{n - 1} \) for all \( n \geq 2 \).

Proof. As in the proof of Claim 8, by symmetry, there exist optimal solutions of (SDP1) at which we have \( x = y, \quad X = Y, \quad X_{ii} = x_i \) for all \( i \in \{1, \ldots, n\} \), and \( X_{ii} - 2X_{ij} + X_{jj} = \gamma/2 \) for all \( 1 \leq i < j \leq n \). Thus, (SDP1) simplifies to the following problem:

\[
\text{(25)} \quad \text{maximize} \quad \gamma
\]
subject to
\[
x_i - 2X_{ij} + x_j = \frac{\gamma}{2}, \quad 1 \leq i < j \leq n
\]
\[
X \succeq xx^T
\]
\[
0 \leq x \leq 1.
\]

To further simplify the above problem, we eliminate \( X_{ij}, \quad 1 \leq i < j \leq n \) using the equality constraints, and write this SDP in terms of \( x \) variables. Define \( \hat{X} = \left( \frac{1}{x} x^T X \right) \), where \( \hat{X}_{ii} = x_i \) for all \( i = 1, \ldots, n \) and \( \hat{X}_{ij} = \frac{1}{2}(x_i + x_j - \gamma/2) \), \( 1 \leq i < j \leq n \). It then follows that Problem (25) can be equivalently written as:

\[
\text{(26)} \quad \text{maximize} \quad \gamma
\]
subject to
\[
\hat{X} \succeq 0
\]
\[
0 \leq x \leq 1.
\]

Now consider a feasible solution of the above problem denoted by \( (\hat{x}, \hat{\gamma}) \). Clearly, any permutation of \( \hat{x} \), denoted by \( \hat{x}_\pi \) results in a feasible solution of the form \( (\hat{x}_\pi, \hat{\gamma}) \). Since, the feasible set of (26) 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 (26) simplifies to a bivariate SDP:

\[
\begin{align*}
\text{maximize} & \quad 4(t - z) \\
\text{subject to} & \quad 0 \leq t \leq 1, 0 \leq z \leq 1.
\end{align*}
\]

To further characterize the feasible region of Problem (27), equivalently, we examine the positive semidefiniteness of the following matrix:

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

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 (27) 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 \(z \geq \frac{mt^2 - t}{n-1}\) and at the optimal solution we have \(z = \frac{mt^2 - t}{n-1}\). Thus, problem (27) 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 \(1 + 1/(n - 1)\). Accordingly, an optimal solution of (SDP1) is attained at:

\[
\begin{align*}
x_i^* &= y_i^* = X_{ii}^* = Y_{ii}^* = \frac{1}{2}, \quad 1 \leq i \leq n \\
X_{ij}^* &= Y_{ij}^* = \frac{n-1}{4(n-1)}, \quad 1 \leq i < j \leq n \\
\gamma^* &= 1 + \frac{1}{n-1}
\end{align*}
\]  

(28)

\textbf{Remark 6.} \textit{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 (28) satisfies these constraints, implying that the addition of RLT constraints to (SDP1) does not strengthen the relaxation.}

\textbf{Tighter variable bounds}  The optimal solution of Problem (SDP1) given by (28) 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 (24) by the following inequalities:

\[
\begin{align*}
X_{ii} &\leq \frac{x_i}{2}, \quad 1 \leq i \leq n_x \\
X_{ii} &\leq x_i, \quad n_x + 1 \leq i \leq n \\
Y_{ii} &\leq \frac{y_i}{2}, \quad 1 \leq i \leq n_y \\
Y_{ii} &\leq y_i, \quad n_y + 1 \leq i \leq n.
\end{align*}
\]

We refer to the resulting relaxation as (SDP2).
Claim 17. Let \( n \geq 5 \) and let \( n_y = \lceil \frac{n}{4} \rceil \). Then the optimal value of Problem (SDP2) is given by
\[
\gamma^* = \frac{1}{4} \left( 1 + \frac{1}{n_y - 1} \right).
\]

Proof. We first provide an upper bound on the optimal solution of (SDP2) 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 constraints corresponding to the points in lower left quadrant of the unit square:

\[
\text{(SDPr)} \quad \begin{align*}
\quad \text{maximize} & \quad \gamma \\
\text{subject to} & \quad X_{ii} - 2X_{ij} + X_{jj} + Y_{ii} - 2Y_{ij} + Y_{jj} \geq \gamma, \quad 1 \leq i < j \leq n_y \\
& \quad X_{ii} \leq \frac{x_i}{2}, \quad Y_{ii} \leq \frac{y_i}{2}, \quad 1 \leq i \leq n_y \\
& \quad X \succeq xx^T, \quad Y \succeq yy^T \\
& \quad 0 \leq x_i \leq \frac{1}{2}, \quad 0 \leq y_i \leq \frac{1}{2}, \quad 1 \leq i \leq n_y.
\end{align*}
\]

Note that in the above problem, \( X \) and \( Y \) are \( n_y \times n_y \) matrices. The important property of Problem (SDPr), is its symmetry in \((x, X)\) and \((y, Y)\) variables. Thus, we can employ a similar line of arguments as for (SDP1) to conclude that there exists an optimal solution of (SDPr) with \( x = y, X = Y, X_{ii} = \frac{t}{2}, Y_{ii} = \frac{t}{2}, i = 1, \ldots, n_y, X_{ii} - 2X_{ij} + X_{jj} = \frac{t}{2} \) for all \( 1 \leq i < j \leq n_y \), and \( x_1 = x_2 = \cdots = x_n \). Let \( t = x_i, z = X_{ij}, \) and

\[
\hat{X} = \begin{pmatrix} t/2 - t^2 & z - t^2 & \cdots & z - t^2 \\ z - t^2 & t/2 - t^2 & \cdots & z - t^2 \\ \vdots & \vdots & \ddots & \vdots \\ z - t^2 & z - t^2 & \cdots & t/2 - t^2 \end{pmatrix}.
\]

It follows that (SDPr) simplifies to the following problem:

\[
\begin{align*}
\text{maximize} & \quad 2(t - 2z) \\
\text{subject to} & \quad \hat{X} \succeq 0 \\
& \quad 0 \leq t \leq \frac{1}{2} \quad (29)
\end{align*}
\]

By direct calculation, it can be shown that the \( m \)th order principal minor of \( \hat{X} \) is given by:

\[
M_m = \left( \frac{1}{2} \right)^m (t - 2z)^{m-1} (t + 2(m - 1)z - 2mzt^2).
\]

Since the objective of (29) is to maximize \( t - 2z \), it follows that \( \hat{X} \) is positive semidefinite, if \( t + 2(n_y - 1)z - 2n_yzt^2 \geq 0 \), and at an optimal solution we have \( z = \frac{2mzt^2-t}{2(n_y-1)} \). Therefore, the optimal solution of (29) 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

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

(30)

It is simple to verify that \( \hat{X}_{ii} - 2\hat{X}_{ij} + \hat{X}_{jj} + \hat{Y}_{ii} - 2\hat{Y}_{ij} + \hat{Y}_{jj} \geq \hat{\gamma} = \frac{1}{4}(1 + \frac{1}{n_y-1}) \) for all \( 1 \leq i < j \leq n \). Thus to prove feasibility of (30), it suffices show that \( \hat{X} - \hat{xx}^T \succeq 0 \) and \( \hat{Y} - \hat{yy}^T \succeq 0 \). Let \( \hat{X} = (\frac{1}{4} \hat{X}) \) and
\( \bar{Y} = \begin{pmatrix} 1 & Y^T \end{pmatrix} \). To show \( \bar{X} \geq 0 \) at \( (\bar{x}, \bar{X}) \) (resp. \( \bar{Y} \geq 0 \) at \( (\bar{y}, \bar{Y}) \)), it suffices to factorize \( \bar{X} = \bar{X}_L \bar{L}_x \bar{L}_x^T \) (resp. \( \bar{Y} = \bar{Y}_L D_y \bar{L}_y^T \)), where \( \bar{L}_x \) (resp. \( \bar{L}_y \)) is a lower triangular matrix with ones in the diagonal and \( D_y = \text{diag}(d^y) \), \( d^x \in \mathbb{R}_+^n \) (resp. \( D_y = \text{diag}(d^p), d^p \in \mathbb{R}_+^n \)) is a nonnegative diagonal matrix. Define \( d^x_1 = 1 \) and

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

Let

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

Similarly, let \( L_y = L_x \) and \( d^y_i = d^x_i \) for \( i = 1, \ldots, n_y + 1 \), and \( d^y_i = \frac{1}{4} \), for \( i = n_y + 2, \ldots, n + 1 \). Hence, we have shown that the point defined by (30) is a feasible solution of Problem (SDP2) and this completes the proof. \( \square \)

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 (30), 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 \( x^*_i = y^*_i = X^*_i = Y^*_i = \frac{1}{2} \), for \( 1 \leq i \leq n \), and \( X^*_i = \frac{n-2}{4(n-1)^2}, \) 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 \( i = 1, \ldots, n_y \), \( x^*_i = y^*_i = \frac{1}{4}, \) for \( i = n_y + 1, \ldots, n \), \( X^*_i = \frac{x^*_i}{3}, \) for \( i = 1, \ldots, n_x \), \( X^*_i = \frac{y^*_i}{3}, \) for \( i = 1, \ldots, n_y \), \( Y^*_i = \frac{y^*_i}{3}, \) for \( i = 1, \ldots, n_y \), \( Y^*_i = y_i, \) for \( i = n_y + 1, \ldots, n \), \( X^*_i = Y^*_i = \frac{1}{16} \left( \frac{x^*_i}{n_y-j} \right)^2, \) for \( 1 \leq i < j \leq n, \) \( X^*_i = Y^*_i = \frac{1}{3}, \) for \( 1 \leq i \leq n_y \) and \( n_y + 1 \leq j \leq n, \) \( X^*_i = Y^*_i = \frac{1}{4}, \) 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 (5). Clearly, the optimal solution of Problem (SDP1) given by (28) does not satisfy these constraints. Let us denote by (SDP1ord) the semidefinite optimization problem obtained by adding inequalities (7) to (SDP1). In the following, we first show that Problem (SDP1ord) has a more compact formulation. Subsequently, we analyze the quality of the corresponding bound for the Circle packing problem. Consider the set

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

It can be shown that the projection of the above set onto \( (x, \xi) \) is given by \( \{(x, \xi) : x_j - x_i \geq \xi_{ij}, 1 \leq i < j \leq n \} \), and by Claim 11, this set is the convex hull of \( \{(x, \xi) : (x_j - x_i)^2 \geq \xi_{ij}, 1 \leq i < j \leq n, 0 \leq x_1 \leq \} \).
\[ \ldots x_n \leq 1 \]. This in turn implies that the constraint \( X \succeq xx^T \) in the description of Problem \((\text{SDP1ord})\) is redundant and this problem can be equivalently written as:

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

Clearly, Problem \((\text{SDPord})\) 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 \((\text{SDPord})\) with that of Problem \((\text{MTord}^{\text{tri}})\), as given by Part (iii) of Theorem 2, for \( 3 \leq n \leq 30 \): while the SDP bounds are slightly stronger than the 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 \((\text{MTord}^{\text{tri}})\) is significantly lower than that of \((\text{SDPord})\).

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 \((\text{SDPord})\) is compared with that of Problem \((\text{MTord}^{\text{tri}})\). In Figure 1(b) the optimal value of Problem \((\text{SDPcomb})\) is compared with that of Problem \((\text{MTcomb}^{\text{tri}})\).

**Best SDP relaxations.** We combine the two types of symmetry-breaking constraints discussed above by adding inequalities (9) to Problem \((\text{SDP2})\) and denote the resulting SDP relaxation by \((\text{SDPcomb})\). In Figure 1(b), we compare the the optimal value of Problem \((\text{SDPcomb})\) with that of Problem \((\text{MTcomb}^{\text{tri}})\), 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(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 [10]. 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\(^{tri}\)). 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 (\( N_t \)), 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.

![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\(^{tri}\)) polyhedral relaxations versus the exact optimal solution (exact).](image)

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 \( \text{conv}(\mathcal{P}) \cap \mathcal{K} \) could serve as a good relaxation of \( \text{conv}(\mathcal{P} \cap \mathcal{K}) \). It can be shown that the set \( \text{conv}(\mathcal{P} \cap \mathcal{K}) \) is polyhedral as well. In addition, it can be shown that even for \( n = 3 \), the polyhedron \( \text{conv}(\mathcal{P} \cap \mathcal{K}) \) is strictly contained in \( \text{conv}(\mathcal{P}) \cap \mathcal{K} \). 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 \( \text{conv}(\mathcal{P} \cap \mathcal{K}) \). Therefore, an interesting future research direction is to study the facial structure of \( \text{conv}(\mathcal{P} \cap \mathcal{K}) \) directly, possibly by using ideas from reverse convex programming [5].
Table 1: Effect of the basic single-row (TW) and the best multi-row (MTcombKtri) 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 ($\delta$%)

References


