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Convex Maximization Formulation of General Sphere Packing Problem

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Abstract. We consider a general sphere packing problem which is to pack nonoverlapping spheres (balls) with the maximum volume into a convex set. This problem has important applications in science and technology. We prove that this problem is equivalent to the convex maximization problem which belongs to a class of global optimization. We derive necessary and sufficient conditions for inscribing a finite number of balls into a convex compact set. In two dimensional case, the sphere packing problem is a classical circle packing problem. We show that 200 years old Malfatti's problem [11] is a particular case of the circle packing problem. We also survey existing algorithms for solving the circle packing problems as well as their industrial applications.

Keywords: sphere packing problem, convex maximization, optimality conditions, Malfatti's problem.

1. Introduction

The sphere packing problem is one of the most applicable areas in mathematics which finds numerous applications in science and technology.

Sphere packing problem with one sphere is called the design centering problem. A practical application of the design centering problem in the diamond industry has been discussed in [13]. The industry needs to cut the largest diamond of a prescribed form inside a rough stone. This form can often be described by a ball. The quality control problem which arise in a fabrication process where the quality of manufactured item is measured can be reduced to the design centering problem [17].

Two dimensional sphere packing problem is circle packing problem. Circle packing problems finds applications in circular cutting problems, communication networks, facility location and dashboard layout. The circular cutting problem is to cut out from a rectangular plate as many circular pieces as possible of N different radii.

In [10] it has been shown that the circular cutting problem is NP-hard and the authors propose heuristic methods and algorithms for solving it. In [9] Fraser and George consider a container loading problem for pulp industries which reduces to the circle packing problem. For solving this problem, the authors implemented a heuristic approach.

In [1] Dowsland considers the problem of packing cylindrical units into a rectangular container. Under some assumptions, the author shows that the problem is equivalent to the circle packing problem and proposes a simulated annealing method to solve it.

In [7] Erkut introduced the p-dispersion problem which consider the optimized location of a set of points that represent facilities to be found. In [2] it is shown that the continuous p-dispersion problem and the circle packing problems are equivalent. A local search methods were used to solve this problem.

Martin in [12] showed that the robot communication problem is equivalent to the circle packing problem.

Drezner in [2] considers the facility layout problem reduced to a circle packing problem where facilities are modeled as circles. Different optimization methods and algorithms [3] are used for solving the problem.

In general, the circle packing problems are reduced to difficult nonconvex optimization problems which cannot be handled effectively by analytical approaches. Moreover, the complexity of the circle packing problems increases rapidly as a number of circles increases. Thus, only heuristic type methods are available for high dimensional cases (N > 50).

The circle packing problem has also important applications in automated radiosurgical treatment planning [18; 19]. Gamma-rays are focused on a common center creating high radiation dose spherical volume. The key problem in the gamma knife treatment is how to place spheres in the tumor of arbitrary shape.

2. Formulation of Sphere Packing Problem

Let $B(x^0, r)$ be a ball with a center $x^0 \in \mathbb{R}^n$ and radius $r \in \mathbb{R}$.

$$B(x^{0}, r) = \{ x \in \mathbb{R}^{n} | ||x - x^{0}|| \le r \},$$
(2.1)

here $\|\cdot\|$ is Euclidean norm.

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The *n*-dimensional volume of the Euclidean ball $B(x^0, r)$ is [8, 14]

$$V(B) = \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2}+1)} r^{n},$$
(2.2)

where Γ is Leonhard Euler's gamma function.

Define the set D as follows:

$$D = \{ x \in \mathbb{R}^n | g_i(x) \le 0, i = \overline{1, m} \},$$

$$(2.3)$$

where $g_i : \mathbb{R}^n \to \mathbb{R}, i = \overline{1, m}$, are convex functions. Assume that D is a compact set which is not congruent to a sphere and $intD \neq \emptyset$. Clearly, D is a convex set in \mathbb{R}^n .

For further purpose, let us introduce the functions $\varphi_i : \mathbb{R}^{n+1} \to \mathbb{R}, i = \overline{1, m}$, for $x \in \mathbb{R}^n$ and r with help of vectors $h \in \mathbb{R}^n$.

$$\varphi_i(x,r) = \max_{\|h\| \le 1} g_i(x+rh), r > 0, i = \overline{1,m}.$$
(2.4)

Lemma 1. $B(x^0, r) \subset D$ if and only if

$$\max_{1 \le i \le m} \varphi_i(x^0, r) \le 0.$$
(2.5)

Proof. Necessity. Let $y \in B(x^0, r)$ and $y \in D$. The point $y \in B(x^0, r)$ can be presented as $y = x^0 + rh, h \in \mathbb{R}^n, ||h|| \le 1$. Then condition $y \in D$ implies that

$$g_i(x^0 + rh) \le 0, \forall h \in \mathbb{R}^n : ||h|| \le 1, i = \overline{1, m}$$

Consequently, $\max_{1 \le i \le m} \varphi_i(x^0, r) \le 0.$

Sufficiency. Let condition (2.4) be satisfied, and on the contrary, assume that there exists $\tilde{y} \in B(x^0, r)$ such that $\tilde{y} \notin D$. Then we have $\tilde{h} \in \mathbb{R}^n$ so that $\tilde{y} = x^0 + r\tilde{h}, \|\tilde{h}\| \leq 1$. Since $\tilde{y} \notin D$, there exists $j \in \{1, 2, ..., m\}$ such that $g_j(x^0 + r\tilde{h}) > 0$ which contradicts (5).

Denote by $u^1, u^2, \ldots u^k$ centers of the spheres inscribed in D defined by (2.3). Let r_1, r_2, \ldots, r_k be their corresponding radii. Now we consider a problem of maximizing a total volume of k non-overlapping spheres (balls) inscribed in $D \subset \mathbb{R}^n$. This problem in the literature [9] is often called sphere packing problem for different spheres.

Now we formulate the following optimization problem :

$$\max_{(u,r)} V = \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2}+1)} \sum_{i=1}^{k} r_i^n,$$
(2.6)

subject to:

$$\varphi_i(u^j, r_j) \le 0, i = \overline{1, m}, j = \overline{1, k}, \tag{2.7}$$

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$$||u^{i} - u^{j}||^{2} \ge (r_{i} + r_{j})^{2}, i, j = \overline{1, k}, \ i < j,$$
(2.8)

$$r_1 \ge 0, r_2 \ge 0, \dots, r_k \ge 0. \tag{2.9}$$

The function V, which is convex as a sum of convex functions r_i^n defined on the positive orthant of \mathbb{R} , denotes the total volume of all spheres inscribed in D. Conditions (2.7) describe that all spheres are in D while conditions (2.8) secure non-overlapping case of balls. Denote by $S \subset \mathbb{R}^{(n+1)k}$ the feasible set of problem (2.6)-(2.9). $(u,r) \in S \subset \mathbb{R}^{(n+1)k}$, where (u,r) = $(u^1, u^2, ..., u^k, r_1, r_2, ..., r_k), u^i = (u_1^i, u_2^i, ..., u_n^i), i = \overline{1, k}$. Denote problem (2.6)-(2.9) by SP(n, m, k), where n, m and k are its parameters.

Theorem 1. Let $(\overline{u}, \overline{r}) \in S$ be a solution of SP(n, m, k). Then $(\overline{u}, \overline{r})$ is a solution to sphere packing problem.

Proof. By the condition of theorem, we have the following inequalities $V(\overline{u},\overline{r}) \geq V(u,r)$ for all $(u,r) \in S$.

According to (2.6), V is the total volume of balls. Taking into account conditions (2.7)-(2.9) which describe non-overlapping spheres inscribed in the convex set D, we conclude that $(\overline{u}, \overline{r})$ is a solution to the sphere packing problem proving the assertion.

Then problem SP(n, m, k) can be written as:

$$\max_{(u,r)\in S} V \tag{2.10}$$

The problem is convex maximization problem and the global optimality conditions of A.Strekalovsky [15] applied to this problem are following.

Theorem 2. Let $(\overline{u}, \overline{r}) \in S$ satisfy $V'(\overline{r}) \neq 0$. Then $(\overline{u}, \overline{r})$ is a solution to problem (2.10) if and only if

$$\langle V'(y), r-y \rangle \le 0 \text{ for all } y \in E_{V(\overline{r})}(V)$$
 (2.11)

and $(u, r) \in S$,

where $E_c(V) = \{y \in \mathbb{R}^{(n+1)k} \mid V(y) = c\}$ is the level set of V at c and V'(y) is the gradient of V at y. Here \langle, \rangle denotes the scalar product of two vectors in $\mathbb{R}^{(n+1)k}$.

Condition (2.11) can be written as

$$\sum_{i=1}^{k} y_i(r_i - y_i) \le 0, \ \forall y \in E_{V(\overline{r})}(V) =$$
$$= \{ y \in \mathbb{R}^{(n+1)k} \mid \sum_{i=1}^{k} y_i^2 = \sum_{i=1}^{k} \overline{r}_i^2 \}, (u, r) \in S$$

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Let D be a polyhedral set given by the following linear inequalities.

$$D = \{x \in \mathbb{R}^n | \langle a^i, x \rangle \le b_i, i = \overline{1, m}\}, a^i \in \mathbb{R}^n, b_i \in \mathbb{R}.$$

Assume that D is compact. Then the functions $\varphi_i(x,r)$ in (2.4) are computed in the following way.

$$\varphi_i(x,r) = \max_{\|h\| \le 1} g_i(x+rh) = \max_{\|h\| \le 1} [\langle a^i, x+rh \rangle - b_i] = \max_{\|h\| \le 1} [\langle a^i, x \rangle + r \langle a^i, h \rangle - b_i] = \langle a^i, x \rangle + r \|a^i\| - b_i, i = \overline{1, m}.$$

Then the problem (2.6)-(2.9) has the form

$$\max_{(u,r)} V = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)} \sum_{i=1}^{k} r_i^n$$
(2.12)

subject to:

$$\langle a^i, u^j \rangle + r_j \|a^i\| \le b_i, i = \overline{1, m}, j = \overline{1, k},$$
(2.13)

$$||u^{i} - u^{j}||^{2} \ge (r_{i} + r_{j})^{2}, i, j = \overline{1, k}, \ i < j,$$
(2.14)

$$r_1 \ge 0, r_2 \ge 0, \dots, r_k \ge 0. \tag{2.15}$$

If we set $r_j = r, j = 1, 2, ..., k$, then problem (2.12)-(2.15) is reduced to the classical packing problem of inscribing k equal spheres into D with maximum volume:

$$\max_{(u,r)} V = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)} kr^n$$
(2.16)

subject to:

$$\langle a^i, u^j \rangle + r \|a^i\| \le b_i, i = \overline{1, m}, j = \overline{1, k},$$
(2.17)

$$\|u^{i} - u^{j}\|^{2} \ge 4r^{2}, i, j = \overline{1, k}, \ i < j,$$
(2.18)

$$r \ge 0. \tag{2.19}$$

The design centering problem [13; 17] can be formulated as circle packing problems (2.12)-(2.15) and (2.16)-(2.19) for different and equal radii.

The most practical sphere packing problems [9; 10] are formulated for box constraints. For instance, if D is a box set, $D = \{x \in \mathbb{R}^n | \alpha_i \leq x_i \leq \beta_i, i = \overline{1, n}\}$ then problem (2.16)-(2.19) is equivalent to the problem of inscribing k equal spheres into a box set which is formulated as:

$$\max_{(u,r)} V = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)} kr^n$$
(2.20)

subject to:

$$u_i^j + r \le \beta_i, i = \overline{1, n}, j = \overline{1, k},$$
(2.21)

$$-u_i^j + r \le -\alpha_i, i = \overline{1, n}, j = \overline{1, k},$$
(2.22)

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$$\|u^{i} - u^{j}\|^{2} \ge 4r^{2}, i, j = \overline{1, k}, \ i < j,$$
(2.23)

$$r \ge 0. \tag{2.24}$$

If we set n = 2, m = 3 and k = 3 in problem (2.12)-(2.15), then problem SP(2,3,3) becomes Malfatti's problem which was first formulated in 1803 [11]. Indeed, the problem has the form:

$$\max_{(u,r)} V = \pi \sum_{i=1}^{3} r_i^2$$
(2.25)

subject to:

$$\langle a^i, u^j \rangle + r_j \|a^i\| \le b_i, i, j = 1, 2, 3,$$
 (2.26)

$$||u^{i} - u^{j}||^{2} \ge (r_{i} + r_{j})^{2}, i, j = 1, 2, 3, i \ne j,$$
(2.27)

$$r_1 \ge 0, r_2 \ge 0, r_3 \ge 0. \tag{2.28}$$

The original Malfatti's and its extended four circle problem SP(2,3,4) as well its three dimensional problem SP(3,4,3) were solved numerically in [4–6].

Note that problem SP(n, m, k) for a polyhedral set can be reduced to D.C. programming (minimization of difference of two convex functions) with d.c.constraints so that one can apply D.C programming approach [16] for finding a local maximum point. Indeed, let us put convex constraints (2.13) in the set Q:

$$Q = \{(u,r) \in \mathbb{R}^{(n+1)k} \mid \langle a^i, u^j \rangle + r_j ||a^i|| \le b_i, \ i = \overline{1, m}, j = \overline{1, k}\}.$$

Then problem SP(n, m, k) can be reformulated as:

$$\min_{(u,r)} f_0 = -\frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)} \sum_{i=1}^k r_i^n, \quad (u,r) \in Q,$$
(2.29)

subject to:

$$f_{ij} = \|u^i - u^j\|^2 - (r_i + r_j)^2 \ge 0, i, j = \overline{1, k}, \ i < j,$$
(2.30)

$$r_1 \ge 0, r_2 \ge 0, \dots, r_k \ge 0, \tag{2.31}$$

where f_0 and f_{ij} are D.C. functions which are differences of two convex functions.

Computational algorithms for solving the problem SP(n, m, k) based on D.C programming will be discussed in a next paper.

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Conclusion

We have examined the general sphere packing problem which is to pack non-overlapping spheres into a convex set with the maximum volume from a view point of theory of convex maximization. We prove that a solution of a new formulated convex maximization problem is a solution to the sphere packing problem for a polyhedral set.

We show that the classical circle packing problems, the design centering and Malfatti's problems [11] are particular cases of the general packing problem. We also survey recent advances of the packing problems and their industrial applications.

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Постановка задачи выпуклой оптимизации как общей задачи упаковки сфер

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Аннотация. Рассмотрена общая задача упаковки сфер, которая заключается в упаковке непересекающихся сфер (шаров) с максимальным объемом в выпуклое множество. Эта проблема имеет важные приложения в науке и технике. Доказано, что эта задача эквивалентна выпуклой задаче максимизации, которая принадлежит классу глобальной оптимизации. Получены необходимые и достаточные условия для вписывания конечного числа шаров в выпуклый компакт. В двумерном случае задача упаковки сфер является классической задачей упаковки кругов. Показано, что 200-летняя задача Мальфатти [11] является частным случаем задачи упаковки кругов. Также рассмотрены существующие алгоритмы для решения задач упаковки кругов и их промышленное применение.

Ключевые слова: задача упаковки сферы, выпуклая оптимизация, условия оптимальности, проблема Мальфатти.

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