COMBINATORICA
Akadémiai Kiadó – Springer-Verlag

COMBINATORICA 15 (2) (1995) 151–158

PENNY-PACKINGS WITH MINIMAL SECOND MOMENTS

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Received February 10, 1993
Revised May 5, 1993

We consider the problem of packing n disks of unit diameter in the plane so as to minimize the second moment about their centroid. Our main result is an algorithm which constructs packings that are optimal among hexagonal packings. Using the algorithm, we prove that, except for $n=212$, the n-point packings obtained by Graham and Sloane [1] are optimal among hexagonal packings. We also prove a result that makes precise the intuition that the "greedy algorithm" of Graham and Sloane produces approximately circular packings.

1. Introduction

A set of points $\{P_1,\dots,P_n\}$ in the plane that satisfies

$$(*)\qquad \|P_i - P_j\| \geq 1 \quad \text{for all } i \neq j$$

is called an *n-point packing.* (Here $\|\ \|$ denotes the usual Euclidean distance.) Hereafter we shall refer to the condition $(*)$ as the *disjointness constraint.* The *second moment* U of an n-point packing is defined to be

$$U = \sum_{i=1}^{n} \|P_i - \bar{P}\|^2,$$

where $\bar{P} = n^{-1}\sum_i P_i$ is the centroid of the packing. Let $U(n) = \inf U$, where the infimum is taken over all possible n-point packings. An n-point packing is *optimal* if it attains $U(n)$. We are interested in the problem of determining $U(n)$ and all optimal n-point packings for all positive integers n.

Intuitively, the problem involves packing pennies in the plane as tightly as possible. The disjointness condition means that the pennies cannot overlap.

The main paper on this problem is one by R. L. Graham and N. J. A. Sloane [1]. Graham and Sloane make the following natural conjecture.

Conjecture 1. *For $n \neq 4$ every optimal packing is (up to symmetry) a subset of A_2.*

Here A_2 is the familiar hexagonal lattice that is generated by $(1,0)$ and $(-1/2,\sqrt{3}/2)$. Conjecture 1 seems very difficult. As a first step towards tackling Conjecture 1, we make the following definition.

Mathematics Subject Classification (1991): 52, 05

Definition. An n-point packing is said to be A_2-*optimal* if it is a subset of A_2 and if it has the smallest second moment possible for an n-point subset of A_2.

We can then replace the problem of finding optimal n-point packings with the easier problem of finding A_2-optimal n-point packings. In their paper, Graham and Sloane construct n-point packings with low second moments using two methods: the "greedy algorithm" and the construction of "circular clusters." (We shall define these terms later.) As it turns out, both of these methods generate only subsets of A_2, so it is natural to ask if the packings constructed in [1] are A_2-optimal. Graham and Sloane do not address this question at all, and in fact their methods do not in general yield A_2-optimal packings.

Our main result is an algorithm that is *guaranteed* to produce A_2-optimal n-point packings. Using this algorithm, we prove that all the n-point packings in [1] are in fact A_2-optimal, except for $n=212$. Previously, the A_2-optimality of all of these packings (except for $n \le 5$) was unknown.

We also present a result on the greedy algorithm that makes precise the intuition that the greedy algorithm produces approximately circular n-point packings.

2. Some Preliminaries

We begin with a simple but very useful lemma.

Lemma 1. *Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be packings with n_1 and n_2 points respectively. Let their respective second moments be U_1 and U_2, and let the distance between their centroids be d. Then the second moment U of $\mathcal{P}_1 \cup \mathcal{P}_2$ is given by*

$$U = U_1 + U_2 + \frac{n_1 n_2 d^2}{n_1 + n_2}.$$

Proof. Let $\bar{P}_1$ and $\bar{P}_2$ be the centroids of $\mathcal{P}_1$ and $\mathcal{P}_2$ respectively, and let $\bar{P}$ be the centroid of $\mathcal{P}_1 \cup \mathcal{P}_2$. The distance between $\bar{P}_1$ and $\bar{P}$ is $n_2 d/(n_1 + n_2)$ and the distance between $\bar{P}_2$ and $\bar{P}$ is $n_1 d/(n_1 + n_2)$. By the well-known parallel axis theorem [2], U is given by

$$U = U_1 + U_2 + n_1\left(\frac{n_2 d}{n_1 + n_2}\right)^2 + n_2\left(\frac{n_1 d}{n_1 + n_2}\right)^2 = U_1 + U_2 + \frac{n_1 n_2 d^2}{n_1 + n_2}. \qquad \blacksquare$$

Intuition suggests that optimal packings should be approximately circular. The following proposition confirms this intuition.

Proposition 1. *Given an optimal n-point packing $\mathcal{P}$, let C be the smallest circle that is centered at the centroid $\bar{P}$ of $\mathcal{P}$ and that contains all the points of $\mathcal{P}$. Then given any point Q in C, there exists a point $P \in \mathcal{P}$ such that $\|P - Q\| < 1$.*

Proof. Since the theorem is vacuously true for $n = 1$, we may assume that $n > 1$, so that the radius of C is nonzero. Suppose that $\|P - Q\| \ge 1$ for all $P \in \mathcal{P}$. Let R be a point in $\mathcal{P}$ on the circumference of C, and let O be the centroid of $\mathcal{P} - \{R\}$, so that R, $\bar{P}$ and O are in a straight line, with $\bar{P}$ between R and O. (See Fig. 1.) Consider the set $\mathcal{P}' = \mathcal{P} \cup \{Q\} - \{R\}$. Since $\|P - Q\| \ge 1$ for all $P \in \mathcal{P}$, $\mathcal{P}'$ satisfies

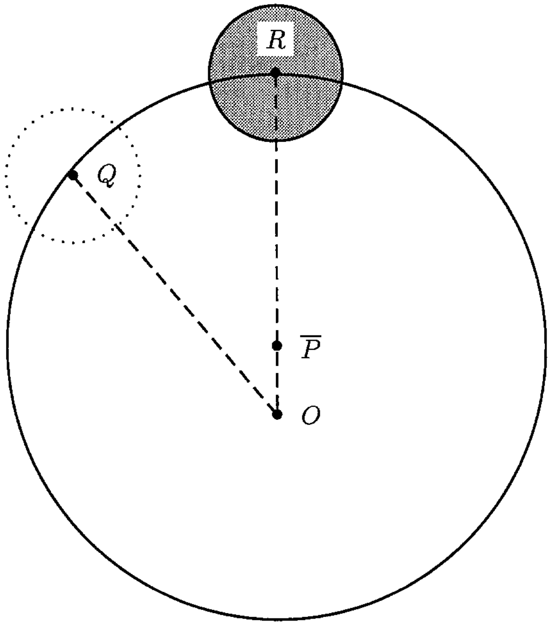

Fig. 1

the disjointness constraint and is therefore an n-point packing. Observe that the distance between Q and O is strictly less than the distance between R and O, so that by Lemma 1 the second moment of $\mathcal{P}'$ is less than that of $\mathcal{P}$, and this implies that $\mathcal{P}$ cannot be optimal. This establishes the desired result. ∎

Definition. A sequence of packings $\mathcal{P}_1$, $\mathcal{P}_2$, $\mathcal{P}_3$, ... is said to be *produced by the greedy algorithm* if $\mathcal{P}_1$ contains a single point and if for $n \geq 2$,

$$\mathcal{P}_n = \mathcal{P}_{n-1} \cup \{P_n\}$$

minimizes U over all choices of P_n that are consistent with the disjointness constraint.

Remark. We shall sometimes talk about a sequence of points that is produced by the greedy algorithm, and we shall also talk about a single n-point packing (as opposed to a sequence of packings) that is produced by the greedy algorithm. These concepts are defined in the obvious way.

Definition. Two points P and Q in an n-point packing are *adjacent* if $\|P-Q\|=1$.

Definition. Let $\mathcal{P}$ be an n-point packing, and let P_1 and P_2 be points of $\mathcal{P}$. We say that P_1 is *connected* to P_2 if there exists a sequence of points $Q_1,\ldots,Q_i \in \mathcal{P}$ such that $Q_1=P_1$, $Q_i=P_2$, and Q_j is adjacent to Q_{j+1} for $j=1,\ldots,i-1$.

The following proposition is tacitly assumed without proof by Graham and Sloane. We state it explicitly for ease of reference but omit the proof since it is straightforward.

Proposition 2. *If $\mathcal{P}_n$ is an n-point packing produced by the greedy algorithm, then $\mathcal{P}_n$ is a connected subset of A_2. For $n>2$, each point in $\mathcal{P}_n$ is adjacent to at least two other points of $\mathcal{P}_n$.* ∎

3. A_2-Optimality

Definition. A *circular cluster* is a set $C \subset A_2$ with the following property: there exists a positive real number r such that C is precisely the set of points in A_2 whose distance from the centroid of C is at most r.

Proposition 3. *All A_2-optimal packings are circular clusters.*

Proof. The proof is almost the same as the proof of Proposition 1. Suppose we have a packing $\mathcal{P}$ that is a subset of A_2. Let $\bar{P}$ be the centroid of $\mathcal{P}$, and let C be the smallest circle centered at $\bar{P}$ that contains all the points of $\mathcal{P}$. Let R be a point of $\mathcal{P}$ that lies on the circumference of C. If $\mathcal{P}$ is not a circular cluster, then there is some point $Q \in A_2$ inside C that is not in $\mathcal{P}$. Arguing as in the proof of Proposition 1, we see that the second moment of $\mathcal{P}' = \mathcal{P} \cup \{Q\} - \{R\}$ is less than that of $\mathcal{P}$. This implies that $\mathcal{P}$ cannot be A_2-optimal, so the proof is complete. ∎

The converse of Proposition 3 is false. In general, for a given n, there is more than one circular cluster, and not all of them are A_2-optimal. (For example, it is easy to check that there are two circular clusters with six points. One is centered at $(1/6, 0)$ and is A_2-optimal, and the other is centered at $(1/2, \sqrt{3}/6)$ and is not A_2-optimal.) However, Proposition 3 does give us a method for finding all A_2-optimal n-point packings for a given n. Observe that every point $P \in A_2$ can be written in the form $a(1,0)+b(-1/2,\sqrt{3}/2)$ where a and b are integers that are uniquely determined by P. Following Graham and Sloane, let us call a and b *oblique coordinates* of P (written $\langle a,b\rangle$). Notice that the oblique coordinates of the centroid of an n-point packing are rational numbers which, if reduced to lowest terms, have denominators that divide n. This means that, up to symmetries of A_2, there is only a finite number of points in the plane that are possible centroids of an A_2-optimal n-point packing. Indeed, it is easy to see that we can restrict our attention to points of the form $\langle a/n, b/n\rangle$ $(a, b \in \mathbb{Z})$ that lie in the triangle with vertices $\langle 0,0\rangle$, $\langle 1/2, 0\rangle$ and $\langle 2/3, 1/3\rangle$. So given n, we can find all A_2-optimal n-point packings as follows:

(a) Consider each possible centroid C in turn.
(b) Let $\mathcal{P}$ be the set of n points in A_2 that are closest to C. It may happen that two or more points of A_2 are equidistant from C, so that $\mathcal{P}$ may not be well-defined. In this case there is no circular cluster with center C so we can ignore C and move on to the next candidate centroid.
(c) Locate the centroid $\bar{P}$ of $\mathcal{P}$. If $C = \bar{P}$ then $\mathcal{P}$ is a circular cluster. Otherwise, we move on to the next candidate centroid.
(d) Having found all the circular clusters using the above procedure, we now calculate the second moment of each circular cluster. The clusters with the lowest second moment are the A_2-optimal n-point packings.

Using a computer we determined the second moment of A_2-optimal n-point packings for all $n \leq 100$ and also for some selected higher values of n. The search confirmed that for $n \leq 350$, all the best known packings published in Graham and Sloane's paper are in fact A_2-optimal, except for $n = 212$. The lowest second moment Graham and Sloane found for $n = 212$ was 6193.0, attained by a circular cluster centered at $\langle 1/2, 0\rangle$. The second moment of an A_2-optimal 212-point packing is actually about 6192.7, attained (for example) by a circular cluster centered at $\langle 9/212, 1/53\rangle$.

4. The Greedy Algorithm

In this section, we shall use the following notation: $P_1, \ldots, P_n$ will denote a sequence of points produced by the greedy algorithm, and $\mathcal{P}_1, \ldots, \mathcal{P}_n$ will denote the corresponding packings. The centroid of $\mathcal{P}_i$ will be denoted by O_i.

The numerical evidence suggests that the greedy algorithm gives approximately circular packings. Although the greedy algorithm does not always give circular clusters (the smallest example is $n = 33$), one has the following result.

Theorem 1. *Suppose that $\mathcal{P}_n$ is an n-point packing produced by the greedy algorithm. Let r_n be the distance from the centroid O_n of $\mathcal{P}$ to the point of $\mathcal{P}$ that is farthest from O_n, and let*

$$c = \left(\frac{\sqrt{3}}{2\pi}\right)^{1/2} + \frac{4}{5} + \delta,$$

where $\delta = 1/\sqrt{1050}$. Then $r_n \leq c\sqrt{n}$.

To prove Theorem 1, we need the following lemma:

Lemma 2. *Let C be a circle with radius r and let n be the number of points of A_2 in the interior C° of C. Then*

$$n \geq \frac{2\pi}{\sqrt{3}}\left(r - \frac{\sqrt{3}}{3}\right)^2.$$

Proof. For each point $P \in A_2$ let H_P be the set of points in the plane that are closer to P than to any other point of A_2. Note that H_P is an open hexagonal region. Let O be the center of C, and let S be the set of points of A_2 that lie in C°. Now let C_1 be the circle with center O and radius $r - \sqrt{3}/3$. Observe that if $P \in A_2$ lies outside C°, then C_1° is disjoint from H_P. So C_1° lies entirely within the area covered by the hexagons associated with the points in S. (Of course we can ignore the area of boundaries of the hexagons since this area is zero.) Now the area of each hexagon is $\sqrt{3}/2$, so

$$\frac{n\sqrt{3}}{2} \geq \pi\left(r - \frac{\sqrt{3}}{3}\right)^2,$$

and the desired result follows. ∎

Proof of Theorem 1. We proceed by induction on n, the number of points in the packing. Using the results from [1], one may easily check that the theorem is true for $n \le 350$, so now let n be some integer greater than 350. Let $P_1, \dots, P_n$ be a sequence of n points produced by the greedy algorithm. For all $k \le n$, let r_k be the distance from O_k to the point in $\mathcal{P}_k$ that is farthest from O_k, and let t_k be r_k minus the distance between O_k and the point of A_2 nearest to O_k that does not coincide with any of the points in $\mathcal{P}_k$.

As our induction hypothesis, we assume that $r_k \le c\sqrt{k}$ and $t_k \le 4c\sqrt{k}/5$ for all $k < n$. To simplify the notation, let $y = \|O_{n-1} - O_n\|$, and let $D = \|O_n - P_n\|$. By Proposition 2 and Lemma 1, P_n must coincide with a point of A_2 that is as close as possible to O_{n-1}, i.e., at a distance $r_{n-1} - t_{n-1}$ from O_{n-1}. Since O_n lies on the line between O_{n-1} and P_n, we see that

$$D = \|O_n - P_n\| = r_{n-1} - t_{n-1} - \|O_{n-1} - O_n\| = r_{n-1} - t_{n-1} - y.$$

Observe that the circle S with radius $D' \stackrel{\text{def}}{=} r_{n-1} + y$ and center O_n entirely encloses the circle with radius r_{n-1} and center O_{n-1}. Hence S contains all the points of $\mathcal{P}_{n-1}$. Let

$$m = \max\{D', \|O_n - P_n\|\} = \max\{D', D\}.$$

Then a circle with radius m and center O_n will contain P_n in addition to all the points of $\mathcal{P}_{n-1}$. It follows that $r_n \le m$. Note also that $r_n \ge D$.

Let us now prove that $t_n \le 4c\sqrt{n}/5$. Suppose that $D \ge D'$. Then $t_{n-1} \le -2y \le 0$, and $D \le r_n \le m = D$, i.e., $r_n = D$. Let C_1 be the circle with center O_{n-1} and radius r_{n-1}, let C_2 be the circle with center O_n and radius $r_n = D$, and let C_3 be the circle with center O_{n-1} and radius $r_{n-1} - t_{n-1}$. (See Fig. 2.) Note that, by definition of t_{n-1}, every point of A_2 that lies strictly inside C_3 (and consequently C_2) must coincide with some point of $\mathcal{P}_{n-1}$. This implies that $t_n \le 0 < 4c\sqrt{n}/5$, as required. So we may assume that $D < D'$. Then $r_n \le m = D'$. Every point of A_2 whose distance from O_{n-1} is less than $r_{n-1} - t_{n-1}$ coincides with some point of $\mathcal{P}_{n-1}$, so every point of A_2 whose distance from O_n is less than $r_{n-1} - t_{n-1} - y = D$ coincides with some point of $\mathcal{P}_{n-1} \subset \mathcal{P}_n$. In other words,

$$t_n \le r_n - D \le D' - D = r_{n-1} + y - (r_{n-1} - t_{n-1} - y) = t_{n-1} + 2y.$$

Now by definition of O_n, $D/y = n - 1$, i.e.,

$$y = \frac{r_{n-1} - t_{n-1}}{n}.$$

Combining this with $t_n \le t_{n-1} + 2y$ and the induction hypothesis yields

$$t_n \le \frac{2r_{n-1} + (n-2)t_{n-1}}{n} \le \left(2 + \frac{4}{5}(n-2)\right)\frac{c\sqrt{n-1}}{n}.$$

Now since $n > 350$,

$$\begin{aligned} n + \frac{1}{2} &\le n + \frac{1}{2} + \frac{3}{8(n-1)} - \frac{1}{8(n-1)^2} \\ &= (n-1+1)\left(1 + \frac{1}{2(n-1)} - \frac{1}{8(n-1)^2}\right) \le n\sqrt{1 + \frac{1}{n-1}}. \end{aligned}$$

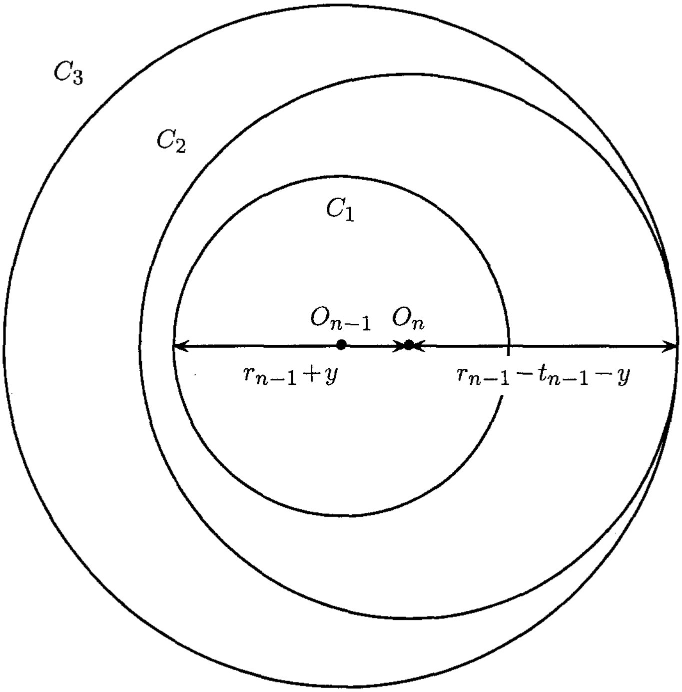

Fig. 2

So

$$t_n \leq \frac{4}{5}\left(\frac{5}{2}+n-2\right)\frac{c\sqrt{n-1}}{n} \leq \frac{4}{5}\left(n\sqrt{1+\frac{1}{n-1}}\right)\frac{c\sqrt{n-1}}{n} = \frac{4}{5}c\sqrt{n}.$$

Now let us show that $r_n \leq c\sqrt{n}$. Define

$$r_n' \stackrel{\text{def}}{=} r_n - t_n.$$

Every point of A_2 that lies in the interior of the circle C with radius r_n' and center O_n coincides with some point of $\mathcal{P}_n$. By Lemma 2, this means that the number of points of $\mathcal{P}_n$ in the interior of C is at least

$$\frac{2\pi}{\sqrt{3}}\left(r_n' - \frac{\sqrt{3}}{3}\right)^2.$$

We can obtain an upper bound for r_n by noting that, in view of Proposition 2, the worst possible case occurs when
(a) r_n' is as small as possible, and
(b) the points of $\mathcal{P}_n$ that do not lie in C are lined up in a single file F along a radius extending outwards from the perimeter of C.

The length of F is at most the total number of points in $\mathscr{P}_n$ minus the number of points of $\mathscr{P}_n$ in the interior of C. It follows that

$$r_n \le n - \frac{2\pi}{\sqrt{3}}\left(r_n' - \frac{\sqrt{3}}{3}\right)^2 + r_n' = n - \frac{2\pi}{\sqrt{3}}\left(r_n - t_n - \frac{\sqrt{3}}{3}\right)^2 + r_n - t_n.$$

Rearranging, we see that

$$\begin{aligned} r_n &\le \left(\frac{\sqrt{3}}{2\pi}(n - t_n)\right)^{1/2} + t_n + \frac{\sqrt{3}}{3} \le \left[\left(\frac{\sqrt{3}}{2\pi}\right)^{1/2} + \frac{4}{5}\right]\sqrt{n} + \frac{\sqrt{3}}{3} \\ &\le \left[\left(\frac{\sqrt{3}}{2\pi}\right)^{1/2} + \frac{4}{5} + \frac{1}{\sqrt{1050}}\right]\sqrt{n} = c\sqrt{n}, \end{aligned}$$

since $n > 350$. ∎

Acknowledgments This work was done under the supervision of Dr. Joseph A. Gallian at the University of Minnesota, Duluth with the financial support of the National Science Foundation (grant number DMS 9000742) and the National Security Agency (grant number MDA 904-88-H-2027).

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