Bounds on packing density via slicing

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Motivation

I point out the following question, . . . important to number theory and perhaps sometimes useful to physics and chemistry: How can one arrange most densely in space an infinite number of equal solids of given form, e.g., spheres with given radii or regular tetrahedra with given edges (or in prescribed position), that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?

-David Hilbert

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- A *local* upper bound for the density of regular pentagons in $\mathbb{R}^2$.

- An upper bound for the density of infinite polycylinders in $\mathbb{R}^n$.

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Idea

A packing defines a family of foliations that can be used to estimate the volume of slices.

Density

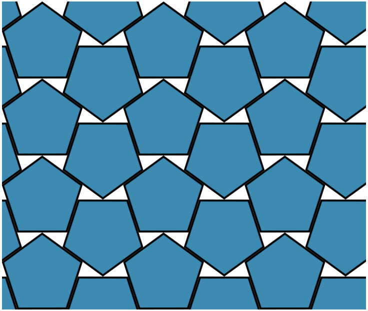
A *packing* of a region $X \subseteq \mathbb{R}^n$ by objects $C_i \subseteq X$ is a countable family $\mathscr{C} = \{C_i\}_{i \in I}$ with disjoint interiors.

The *upper density* ρ^+ of a packing $\mathscr{C}$ in $\mathbb{R}^n$ will be defined as

$$\rho^+(\mathscr{C}) = \limsup_{r \to \infty} \frac{\mathrm{Vol}(r\mathbb{B}^n \cap \mathscr{C})}{\mathrm{Vol}(r\mathbb{B}^n)},$$

where $\mathbb{B}^n$ is the unit n-ball centered at 0.

Pentagons



The best lower bound for the density of pentagon packings and the conjectured maximal density configuration is shown. This packing has a density of $(5-\sqrt{5})/3 = 0.921311\ldots$. Only in the past few years has a reasonable upper bound of $0.98103\ldots$ been produced as a corollary to a more general method.

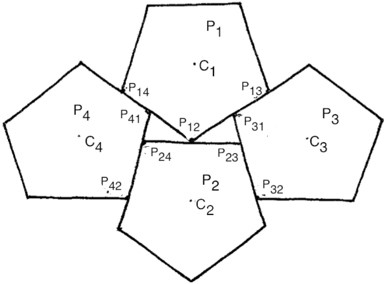
Nonlinear Program

The problem of finding the densest packing of pentagons can be phrased as a nonlinear program:

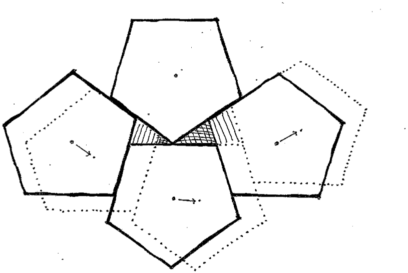
Maximize the density of a configuration of pentagons subject to the condition that the pentagons do not intersect.

Nonlinear Program

Let $\mathscr{M}(\mathscr{P})$ be the configuration space of four pentagons. The coordinate system introduced on $\mathscr{M}(\mathscr{P})$ is not the naive parameterization where all pentagons are independent, but rather a coupled system.



Pentagon labels



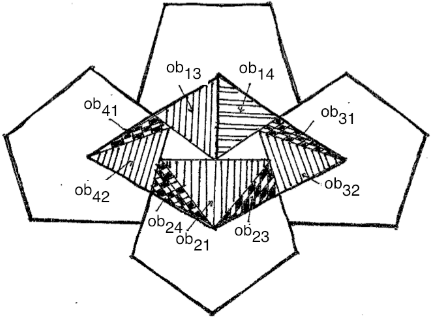
One-parameter family

Nonlinear Program

The objective function for the nonlinear program is defined in in terms of the areas and corresponds to the density function on a neighborhood of the conjectured optimal configuration of four pentagons. The constituent functions (ob_{ij}) are the areas of various triangular regions of the pentagons and FT, the area of the convex hull of $\{c_1, c_2, c_3, c_4\}$. The objective function may be written as

$$\sum_{i=1}^{4} \frac{\mathrm{Area}(FT(\mathcal{P}) \cap P_i)}{\mathrm{Area}(FT(\mathcal{P}))} - \frac{5-\sqrt{5}}{3}.$$

Nonlinear Program



Constituent functions of the objective function.

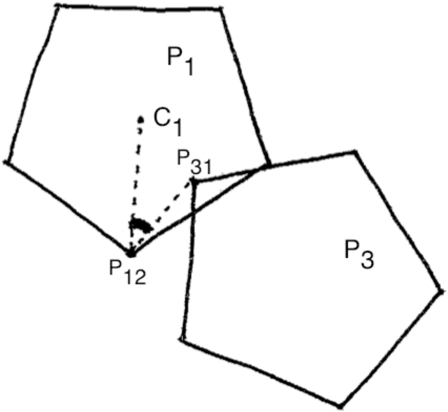
Nonlinear Program

The constraint functions for the nonlinear program are non-intersection conditions on the pentagons. Locally, it is sufficient to require that no vertex of a pentagon be in the interior of another. Let the vertex of P_i that is in contact with P_j be the p_{ij}. The constraint that a vertex of P_k does not lie in P_j may be considered as an angle constraint, written as

$$\mathrm{Angle}\{c_i - p_{ij}, p_{ki} - p_{ij}\} - \frac{3\pi}{10} \geq 0$$

for appropriate choices of i, j, k in $\{1, 2, 3, 4\}$.

Nonlinear Program



Violation of an angle constraint.

Nonlinear Program

This program is HARD. Trying to solve the nonlinear program numerically crashes the Mathematica kernel. But, there is a linear program that can be solved numerically and indicates a local maximum at 0.

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Numerically, the second order terms have the correct sign. A restricted bordered Hessian test indicates 0 is a local max. There are some directions where the objective function is geometrically known to be constant or linear.

Conical Program

The pentagon nonlinear program is special, in that it satisfies certain assumptions that allow it to be sliced and analyzed. In general,

Theorem

a nonlinear program

$$\max_{x \in \mathbb{R}^n} f(x) \ \textit{subject to } g_r(x) \geq 0, r \in I$$

satisfying the following assumptions, has an isolated local maximum at 0 with f(0) = 0. □

Conical Program

Assumptions

- *The index set I is a finite set.*
- *The vector e_1 is the standard unit vector $\{1, 0, \ldots, 0\}$ in $\mathbb{R}^n$.*
- *For r in I, the objective and constraint functions f and g_r are analytic functions on a neighborhood of 0.*
- *Assume $f(0) = g_r(0) = 0$ for all r in I.*
- *Let $F(t) = \nabla f(te_1)$.*
- *Let $G_r(t) = \nabla g_r(te_1)$.*

Conical Program

Assumptions

- *The linear program*

$$\max_{x \in \mathbb{R}^n} F(0) \cdot x \ \mathit{subject\ to}\ G_r(0) \cdot x \geq 0, r \in I$$

  has a bounded solution and that the maximum is attained at 0.

- *The set of solutions in* $\mathbb{R}^n$ *to*

$$F(0) \cdot x = 0 \ \mathit{subject\ to}\ G_r(0) \cdot x \geq 0, r \in I$$

  is

$$E := \{te_1 : t \in \mathbb{R}\}.$$

- *Let* H *be the orthogonal complement of* E *so that* $\mathbb{R}^n = E \oplus H$.

Conical Program

Assumptions

- *Assume there is an* $\epsilon > 0$ *so the functions* $g_r(te_1) = 0$ *for all* $t \in (-\epsilon, \epsilon)$*, for all* r *in* I*.*
- *Assume* $\frac{\partial}{\partial t} f(0) = 0$*,* $\frac{\partial^2}{\partial t^2} f(0) < 0$*.*

Sketch of Proof

Lemma

Given the assumptions, the linear program

$$\max_{x \in H} F(0) \cdot x \;\; subject \;\; to \;\; G_r(0) \cdot x \geq 0, r \in I$$

has a unique maximum at $x = 0$

Sketch of Proof

Proof.

From the assumptions, the linear program

$$\max_{x\in\mathbb{R}^n} F(0)\cdot x \text{ subject to } G_r(0)\cdot x \geq 0, r \in I$$

is maximized exactly on E. The feasible set

$$\{x : G_r(0)\cdot x \geq 0, r \in I \text{ and } x \in H\}$$

is a subset of the feasible set $\{x : G_r(0)\cdot x \geq 0, r \in I\}$. Thus, the program

$$\max_{x\in H} F(0)\cdot x \text{ subject to } G_r(0)\cdot x \geq 0, r \in I$$

is maximized exactly on the (non-empty) intersection

$$E \cap \{x : G_r(0)\cdot x \geq 0, r \in I\} \cap H = 0.$$

Sketch of Proof

Definition

A ***finitely generated cone*** is a subset of $\mathbb{R}^n$ which is the non-negative span of a finite set of non-zero vectors $\{v_1, \dots v_m\}$ in $\mathbb{R}^n$, which are called the ***generators*** of the cone.

Definition

A ***conical linear program*** is a linear program with a constraint set that is a finitely generated cone.

The linear programs described throughout this section are always constrained to be on the intersection of half-spaces with 0 on the boundary. These are conical programs.

Definition

For a cone C, the set $C^p := \{x \in \mathbb{R}^n : v \cdot x \leq 0 \text{ for all } v \in C\}$ is the ***polar cone*** of C.

Sketch of Proof

Lemma

A conical linear program with $F \neq 0$ given by

$$\max_{x \in \mathbb{R}^n} F \cdot x \;\; subject\ to\ G_r \cdot x \geq 0, r \in I$$

(a) has a unique maximum at $x = 0$ iff F is in the interior of the polar cone C^p of $C = \{x : G_r \cdot x \geq 0, r \in I\}$ (b) has a bounded solution iff F is in the polar cone C^p of $C = \{x : G_r \cdot x \geq 0, r \in I\}$ and attains its maximum exactly on the span of the generators v_i such that $F \cdot v_i = 0$.

Sketch of Proof

Proof.

If F is in the interior of the polar cone C^p, then $F \cdot v_i < 0$ for all generators v_i. Therefore $F \cdot x$ is uniquely maximized in C at the vertex. If F is on the boundary of the polar cone, then $F \cdot x$ is maximized in C exactly on the span of the generators v_i for which $F \cdot v_i = 0$ as $F \cdot v_j < 0$ otherwise. If F is outside the polar cone, then $F \cdot v_i > 0$ for some generator v_i. Then $F \cdot x$ is unbounded in C. □

Sketch of Proof

Lemma

Given the assumptions, there exists $\epsilon > 0$ such that for all t in $(-\epsilon, \epsilon)$, the linear program

$$\max_{y_t \in H} F(t) \cdot y_t$$

subject to

$$G_r(t) \cdot y_t \geq 0, r \in I$$

has a unique maximum at $y_t = 0$.

Sketch of Proof

Proof.

The program for $t \in (-\epsilon, \epsilon)$, for y_t in H, for each fixed t in $(-\epsilon, \epsilon)$, for some $\epsilon > 0$, can be written as a conical program on all of $\mathbb{R}^n$ with a cone C_t in $\mathbb{R}^n$ of co-dimension ≥ 1 by introducing further constraints $e_1 \cdot y_t \geq 0$ and $-e_1 \cdot y_t \geq 0$. By previous lemmas, $F(0)$ is in the polar cone of $C_0 = \{y_0 : G_r(0) \cdot y_0 \geq 0, e_1 \cdot y_0 \geq 0, -e_1 \cdot y_0 \geq 0\}$. As $f, g_r \in C^\omega$, the condition of $F(t)$ being in the interior of the polar cone C_t^p is open and the condition of the feasible set $C_t = \{y_t : G_r(t) \cdot y_t \geq 0, e_1 \cdot y_t \geq 0, -e_1 \cdot y_t \geq 0\}$ being conical is open. Therefore, by a previous lemma, the program has a unique maximum at $y_t = 0$ for each fixed t in $(-\epsilon, \epsilon)$ for some $\epsilon > 0$. $\square$

Sketch of Proof

Lemma

Given the assumptions and ϵ *as in the previous lemmas, for all* $t \in (-\epsilon, \epsilon)$ *there exists* $\delta(t) > 0$ *and a cube* $Q(t) \subset \mathbb{R}^n$ *of side length* $2\delta(t)$ *such that*

$$\{(F(t) + Q(t)) \cap (\partial(C_t^p) + Q(t))\} = \emptyset.$$

Proof.

This follows from a previous lemma, which shows $F(t)$ is in the interior of the polar cone C_t^p. Then $F(t)$ and the boundary of C_t^p can be separated and the existence of Q is trivial. $\square$

Sketch of Proof

Corollary

Given the assumptions and ϵ *as in previous lemmas, for all* $t \in (-\epsilon, \epsilon)$,

$$(F(t) + \Delta) \cdot y_t \leq 0$$

whenever y_t *satisfies*

$$(G_r(t) + \Delta_r) \cdot y_t \geq 0, r \in I \text{ and } e_1 \cdot y_t \geq 0, -e_1 \cdot y_t \geq 0$$

where Δ *and* Δ_r *are any points in the* $2\delta(t)$*-cube* $Q(t)$ *and* y_t *is in* H.

Proof.

By a previous lemma, $F(t) + \Delta$ is in the interior of the polar cone $C^p_{t,\Delta}$, where
$C_{t,\Delta} = \{y_t : (G_r(t) + \Delta_r) \cdot y_t \geq 0, e_1 \cdot y_t \geq 0, -e_1 \cdot y_t \geq 0, r \in I\}$. □

Sketch of Proof

Lemma

Given the assumptions and ϵ as in the previous lemmas, for all $t \in (-\epsilon, \epsilon)$, let $y_t = x - te_1 \in H$. Choose $\Delta = \Delta(y_t)$ and $\Delta_r = \Delta_r(y_t)$ in the $2\delta(t)$-cube $Q(t)$ to be the corner given by the sign of $x - te_1 = y_t$. Then there is an ϵ_t for which

$$(F(t) + \Delta(y_t)) \cdot y_t \leq 0 \implies f(x) - f(te_1) \leq 0$$

and

$$(G_r(t) + \Delta_r(y_t)) \cdot y_t \leq 0 \implies g_r(x) - g_r(te_1) = g_r(x) \leq 0$$

for all $\|y_t\| \leq \epsilon_t$.

Sketch of Proof

Proof.

This follows from the local expansions of the nonlinear program. By this choice of $\Delta(y_t)$ and $\Delta_r(y_t)$,

$$f(x) - f(te_1) = F(t)\cdot(x - te_1) + O(t^2) = F(t)\cdot y_t + O(t^2)$$
$$\le F(t)\cdot y_t + \delta(t)\|y_t\|_1 = (F(t) + \Delta(y_t))\cdot y_t$$

and

$$g_r(x) = g_r(x) - g_r(te_1) = G_r(t)\cdot(x - te_1) + O(t^2) = G_r(t)\cdot y_t + O(t^2)$$
$$\le G_r(t)\cdot y_t + \delta(t)\|y_t\|_1 = (G_r(t) + \Delta_r(y_t))\cdot y_t.$$

□

Sketch of Proof

By the previous lemmas, for t in $(-\epsilon, \epsilon)$, the program

$$\max_{y_t \in H} (F(t) + \Delta) \cdot y_t \text{ subject to } (G_r + \Delta_r) \cdot y_t$$

is uniquely maximized at $y_t = 0$ for any choice of Δ, Δ_r in the $2\delta(t)$ cube $Q(t)$. Combined with previous lemmas, there is an ϵ_t neighborhood of 0 where $f(y_t + te_1)$ is less than $f(te_1)$ on

$$\cup_{\Delta_r \in Q(t)} \{y_t : (G_r + \Delta_r) \cdot y_t \geq 0, r \in I, y_t \in H\},$$

which contains the feasible set $\{y_t : g_r(y_t + te_1) \geq 0, r \in I, y_t \in H\}$. Therefore the nonlinear programs $f(y_t + te_1)$ subject to $g_r(y_t + te_1) \geq 0$, $y_t \in H$, which are parameterized by t in $(-\epsilon, \epsilon)$, have local maxima at $y_t = 0$. This gives the following:

Sketch of Proof

Theorem

Given the assumptions, a fixed t *in* $(-\epsilon, \epsilon)$ *and choosing* Δ *and* Δ_r *as in the previous lemmas, for* x *satisfying* $g_r(x) \geq 0$ *for all* r *in* I *and* $y_t = x - te_1$ *in* H*, there exist linear programs*

$$\max_{y_t \in H} (F(t) + \Delta(y_t)) \cdot y_t \ \ subject\ to\ (G_r(t) + \Delta_r(y_t)) \cdot y_t \geq 0$$

that give solutions to the nonlinear programs

$$\max_{x \in H + te_1} f(x) \ \ subject\ to\ g_r(x) \geq 0$$

in an ϵ_t *neighborhood of* te_1 *in* $H + te_1$. □

Sketch of Proof

By choice of a sufficiently small ϵ and a minimal non-zero ϵ_t, the previous theorem gives an open neighborhood of 0 in which the maximum value of the original nonlinear program occurs on E. The assumptions for the first and second t-derivatives at 0 shows 0 to be a local maximum for the nonlinear program

$$\max_{x \in \mathbb{R}^n} f(x) \text{ subject to } g_r(x) \geq 0.$$

Theorem

A nonlinear program satisfying the assumptions has an isolated local maximum at 0 with f(0) = 0. □

Change of Pace

Analysis $\rightarrow$ Geometry!

Change of Pace

Analysis $\rightarrow$ Geometry!

Recall the cylinder packing problem from 7 months 2 weeks ago.

Packing Polycylinders

Definition

A ***polycylinder*** is a set isometric to $\mathbb{D}^2 \times \mathbb{R}^n$ in $\mathbb{R}^{n+2}$.

Definition

A ***polycylinder packing*** is a countable family

$$\mathscr{C} = \{C_i\}_{i \in I}$$

of polycylinders $C_i \subset \mathbb{R}^{n+2}$ with mutually disjoint interiors.

Packing Polycylinders

Definition

The ***upper density*** $\delta^+(\mathscr{C})$ of a packing $\mathscr{C}$ of $\mathbb{R}^n$ is defined to be

$$\delta^+(\mathscr{C}) = \limsup_{r\to\infty} \frac{\mathrm{Vol}(\mathscr{C} \cap r\mathbb{B}^n)}{\mathrm{Vol}(r\mathbb{B}^n)}.$$

Note that this notion can be generalized further by replacing $\mathbb{B}^n$ with an arbitrary convex body K.

Definition

The ***upper packing density*** $\delta^+(C)$ of an object C is the supremum of $\delta^+(\mathscr{C})$ over all packings $\mathscr{C}$ of $\mathbb{R}^n$ by C.

Packing Polycylinders

Definition

A ***d-flat*** is a d-dimensional affine subspace of $\mathbb{R}^n$.

Definition

The ***parallel dimension*** $dim_{\|}\{F, \ldots, G\}$ of a collection of flats $\{F, \ldots, G\}$ is the dimension of their maximal parallel sub-flats.

Definition

Two disjoint d-flats are ***parallel*** if their parallel dimension is d, that is, if every line in one is parallel to a line in the other.

Packing Polycylinders

For a collection of flats $\{F, \ldots, G\}$, consider each flat as a system of linear equations. The corresponding homogeneous equations determine a collection of linear subspaces $\{F_\infty, \ldots, G_\infty\}$. The parallel dimension is the dimension of their intersection $F_\infty \cap \cdots \cap G_\infty$.

Packing Polycylinders

Lemma

A pair of disjoint n-flats in $\mathbb{R}^{n+k}$ with $n \geq k$ has parallel dimension strictly greater than $n - k$.

Proof.

By homogeneity of $\mathbb{R}^{n+k}$, let $F = F_\infty$. As F_∞ and G are disjoint, G contains a non-trivial vector $\mathbf{v}$ such that $G = G_\infty + \mathbf{v}$ and $\mathbf{v}$ is not in $F_\infty + G_\infty$. It follows that

$$dim(\mathbb{R}^{n+k}) \geq dim(F_\infty + G_\infty + \mathrm{span}(\mathbf{v})) > dim(F_\infty + G_\infty)$$

$$= dim(F_\infty) + dim(G_\infty) - dim(F_\infty \cap G_\infty).$$

Count dimensions to find $n + k > n + n - dim_{\|}(F_\infty, G_\infty)$. □

Packing Polycylinders

Corollary

A pair of disjoint n-flats in $\mathbb{R}^{n+2}$ has parallel dimension at least $n-1$.

Packing Polycylinders

Definition

The ***core*** a_i of a polycylinder C_i isometric to $\mathbb{D}^2 \times \mathbb{R}^n$ in $\mathbb{R}^{n+2}$ is the distinguished n-flat defining C_i as the set of points at most distance 1 from a_i.

In a packing $\mathscr{C}$ of $\mathbb{R}^{n+2}$ by polycylinders, the previous lemma shows that, for every pair of polycylinders C_i and C_j, one can choose parallel $(n-1)$-dimensional subflats $b_i \subset a_i$ and $b_j \subset a_j$ and define a product foliation

$$\mathscr{F}^{b_i,b_j} : \mathbb{R}^{n+2} \to \mathbb{R}^{n-1} \times \mathbb{R}^3$$

with $\mathbb{R}^3$ leaves that are orthogonal to b_i and to b_j. Given a point x in a_i, there is a distinguished $\mathbb{R}^3$ leaf $F_x^{b_i,b_j}$ that contains the point x. The foliation $\mathscr{F}^{b_i,b_j}$ restricts to foliations of C_i and C_j with right-circular-cylinder leaves.

Packing Polycylinders

Definition

In a packing $\mathscr{C}$ of $\mathbb{R}^{n+2}$ by polycylinders, the ***Dirichlet cell*** D_i associated to a polycylinder C_i is the set of points in $\mathbb{R}^{n+2}$ no further from C_i than from any other polycylinder in $\mathscr{C}$.

The Dirichlet cells of a packing partition $\mathbb{R}^{n+2}$, because $C_i \subset D_i$ for all polycylinders C_i. To bound the density $\delta^+(\mathscr{C})$, it is enough to fix an i in I and consider the density of C_i in D_i. For the Dirichlet cell D_i, there is a slicing as follows.

Definition

Given a fixed a polycylinder C_i in a packing $\mathscr{C}$of $\mathbb{R}^{n+2}$ by polycylinders and a point x on the core a_i, the plane p_x is the 2-flat orthogonal to a_i and containing the point x. The ***Dirichlet slice*** d_x is the intersection of D_i and p_x.

Note that p_x is a sub-flat of $F_x^{b_i,b_j}$ for all j in I.

Packing Polycylinders

For any point x on the core a_i of a polycylinder C_i, a result of Bezdek and Kuperberg applies to the Dirichlet slice d_x.

Lemma

A Dirichlet slice is convex and, if bounded, a parabola-sided polygon.

Packing Polycylinders

Proof.

Construct the Dirichlet slice d_x as an intersection. Define d^j to be the set of points in p_x no further from C_i than from C_j. Then the Dirichlet slice d_x is realized as

$$d_x = \{\cap_{j\in I} d^j\}.$$

Each arc of the boundary of d_x in p_x is given by an arc of the boundary of some d^j in p_x. The boundary of d^j in p_x is the set of points in p_x equidistant from C_i and C_j. Since the foliation $\mathscr{F}^{b_i,b_j}$ is a product foliation, the arc of the boundary of d^j in p_x is also the set of points in p_x equidistant from the leaf $C_i \cap F_x^{b_i,b_j}$ of $\mathscr{F}^{b_i,b_j}|_{C_i}$ and the leaf $C_j \cap F_x^{b_i,b_j}$ of $\mathscr{F}^{b_i,b_j}|_{C_j}$. This reduces the analysis to the case of a pair cylinders in $\mathbb{R}^3$. It follows that d^j is convex and the boundary of d_j in p_x is a parabola; the intersection of such sets d^j in p_x is convex, and a parabola-sided polygon if bounded. $\square$

Packing Polycylinders

Let $S_x(r)$ be the circle of radius r in p_x centered at x.

Lemma

The vertices of d_x are not closer to $S_x(1)$ than the vertices of a regular hexagon circumscribed about $S_x(1)$.

Proof.

A vertex of d_x occurs where three or more polycylinders are equidistant, so the vertex is the center of a $(n+1)$-ball B tangent to three polycylinders. Thus B is tangent to three disjoint unit $(n+2)$-balls B_1, B_2, B_3. By projecting into the affine hull of the centers of B_1, B_2, B_3, it is immediate that the radius of B is no less than $2/\sqrt{3}-1$. $\square$

Packing Polycylinders

Lemma

Let y and z be points on the circle $S_x(2/\sqrt{3})$. If each of y and z is equidistant from C_i and C_j, then the angle yxz is smaller than or equal to $2\arccos(\sqrt{3}-1) = 85.8828\ldots^\circ$.

Proof.

The existence of a supporting hyperplane of C_i that separates $\mathrm{int}(C_i)$ from $\mathrm{int}(C_j)$ suffices. $\square$

Packing Polycylinders

Planar objects satisfying the previous lemmas have area no less than $\sqrt{12}$. As the bound holds for all Dirichlet slices, it follows that $\delta^+(\mathbb{D}^2 \times \mathbb{R}^n) \leq \pi/\sqrt{12}$ in $\mathbb{R}^{n+2}$. The product of the dense disk packing in the plane with $\mathbb{R}^n$ gives a polycylinder packing in $\mathbb{R}^{n+2}$ that achieves this density. Combining this with the results of Thue for $n = 0$, Bezdek and Kuperberg for $n = 1$, it follows that

Theorem

$\delta^+(\mathbb{D}^2 \times \mathbb{R}^n) \leq \pi/\sqrt{12}$ *for all natural numbers* n.