A numerical search for the worst-packing shapes

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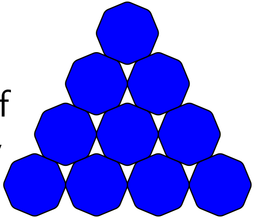
Confrence on the occasion of Jorge Urrutia's 60th birthday
November 15, 2013

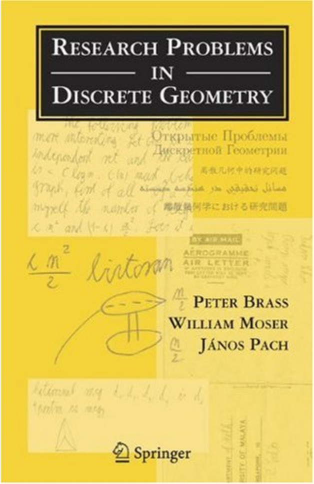


From Hilbert's 18$^{\text{th}}$ Problem

"How can one arrange most densely in space an infinite number of equal solids of a given form, e.g., spheres with given radii or regular tetrahedra with given edges, that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as large as possible?"

$$\delta(C) = \text{optimal packing fraction}$$

Least Efficient Shapes for Packing



1.2 The Least Economical Convex Sets for Packing

The closer the packing density of a convex body C is to 1, the larger the number of congruent copies of C that can be packed into a given big container. Therefore, the least economical convex bodies for packing are those whose packing density is minimum.

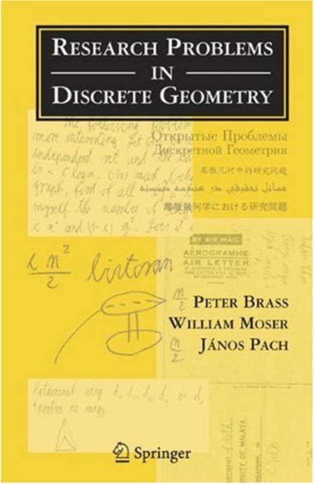
Problem 1 *Is the least economical convex body for packing in the plane centrally symmetric? More precisely, is it true that for any plane convex body C there exists a centrally symmetric convex body C' such that $\delta(C') \leq \delta(C)$?*

A result of G. Kuperberg and W. Kuperberg [KuK90] suggests that the answer to this question is probably in the negative. It is possible that the worst convex body from the point of view of economical packing in the plane is the regular heptagon (whose densest known packing is of density 0.8926...; see also [Bl83]).

Problem 2 *What is the minimum of $\delta(C)$ over all convex bodies C in the plane?*

Chakerian and Lange [ChL71] proved that every plane convex body C is contained in a quadrilateral Q with area$(Q) \leq \sqrt{2}\,$area(C). Since every quadrilateral tiles the plane, this implies that

Least Efficient Shapes for Packing

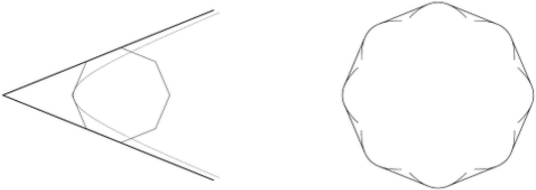


Conjecture 3 *(Reinhardt [Re34]) For every centrally symmetric convex body C in the plane,*

$$\delta(C) = \delta_L(C) \geq \frac{8 - 4\sqrt{2} - \ln 2}{2\sqrt{2} - 1} = 0.90241418\ldots,$$

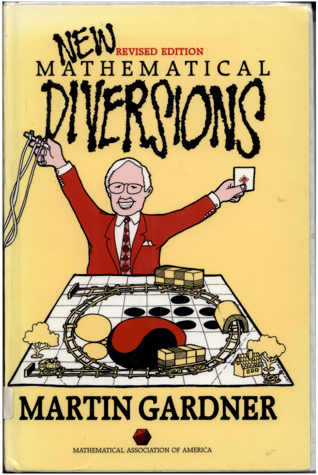
with equality only for the so-called smoothed octagon.

The "smoothed octagon" results from a regular octagon by cutting off each vertex v_i with a hyperbolic arc from the hyperbola that is tangential to $v_i v_{i-1}$ and $v_i v_{i+1}$ and has the lines $v_{i-1}v_{i-2}$ and $v_{i+1}v_{i+2}$ as asymptotes. Nazarov [Na86] proved that Reinhardt's smoothed octagon is, in a certain sense, locally optimal.



THE SMOOTHED OCTAGON

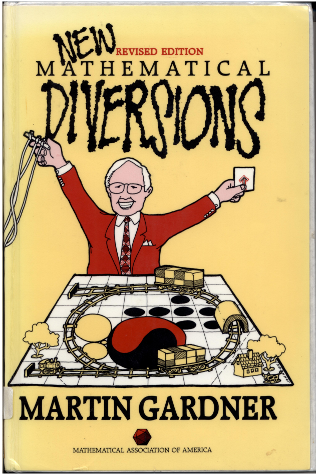
Ulam's Conjecture



"Stanislaw Ulam told me in 1972 that he suspected the sphere was the worst case of dense packing of identical convex solids, but that this would be difficult to prove."

1995 postscript to the column "Packing Spheres"

Ulam's Last Conjecture



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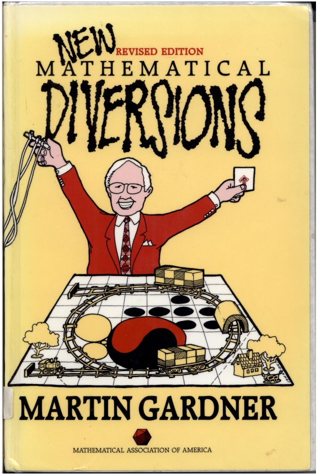

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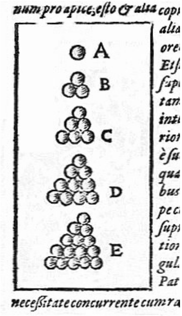
Related conjecture: any *centrally-symmetric* convex shape can be packed using *only translations* at a higher density than spheres.

1995 postscript to the column "Packing Spheres"

Sphere packing in $\mathbb{R}^3$



Conjecture (Kepler)

Every nonoverlapping arrangement of spheres in $\mathbb{R}^3$ fills at most $\pi/\sqrt{18} = 0.7405$ of space.

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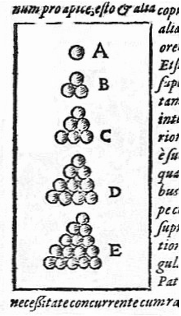
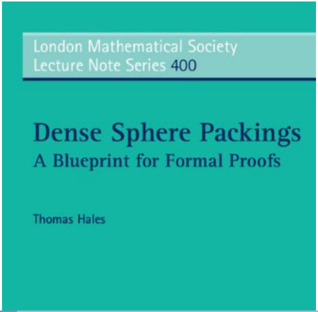


Conjecture (Kepler)

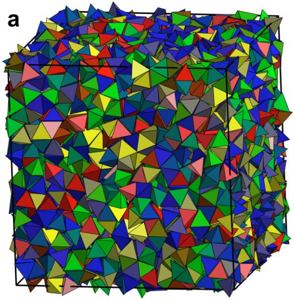
Every nonoverlapping arrangement of spheres in $\mathbb{R}^3$ fills at most $\pi/\sqrt{18} = 0.7405$ of space.

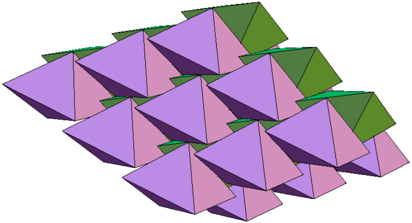
- Computational proof of Kepler's conjecture by Thomas Hales.
- Involved solving around 100,000 LP problems.



Computational search in packing

Tetrahedra:

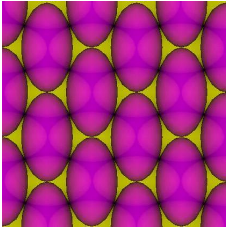




- Conway & Torquato conjectured in 2006 that $\delta(T) < \delta(B) = 0.7405$.
- A sequence of numerically discovered structures (2008–2009) showed that $\delta(T) \geq 0.8563$.

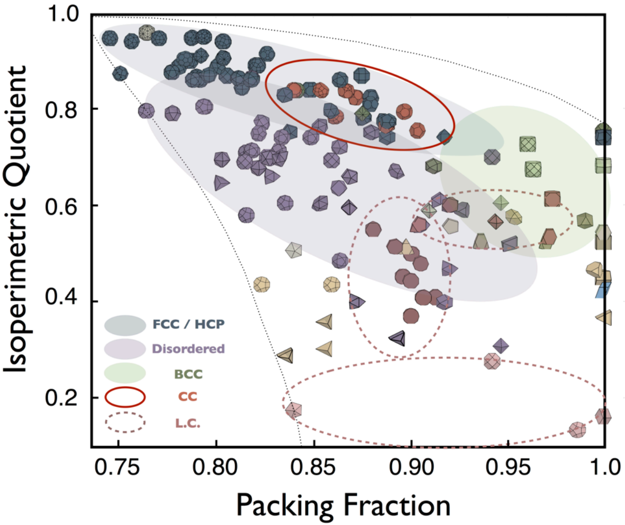
Computational search in packing

Ellipsoids:



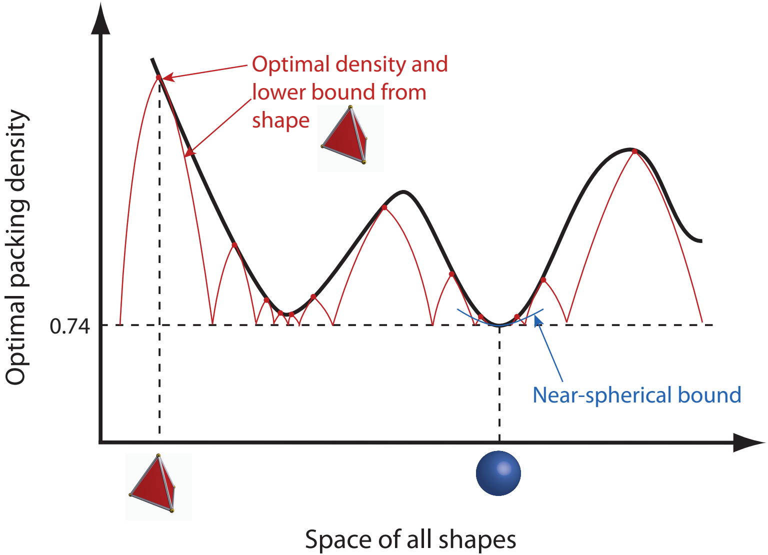
- $\delta(E) \geq \delta(B)$ for ellipsoids of high enough aspect ratio (Bezdek & Kuperberg 1991).
- Numerically discovered structure achieves $\delta(E) \geq \delta(B)$ for all ellipsoids E, and $\delta(E) \geq 0.7707$ for all ellipsoids of high enough aspect ratio (Donev et al. 2004).

Packing non-spherical shapes



Damasceno, Engel, and Glotzer, 2012.

Verification strategy



Local minimality

Theorem (YK)

The 3D sphere is a local minimum of the optimal translative packing fraction among convex, centrally symmetric bodies.

YK, arXiv:1212.2551

Local minimality

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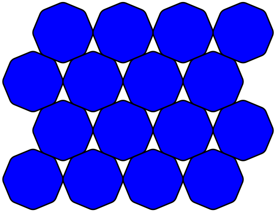
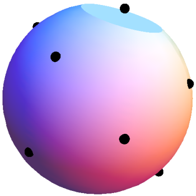
The 3D sphere is a local minimum of the optimal translative packing fraction among convex, centrally symmetric bodies.

In dimensions $d = 2, 4, 5, 6, 7, 8$, and 24, the sphere is not a local minimum.





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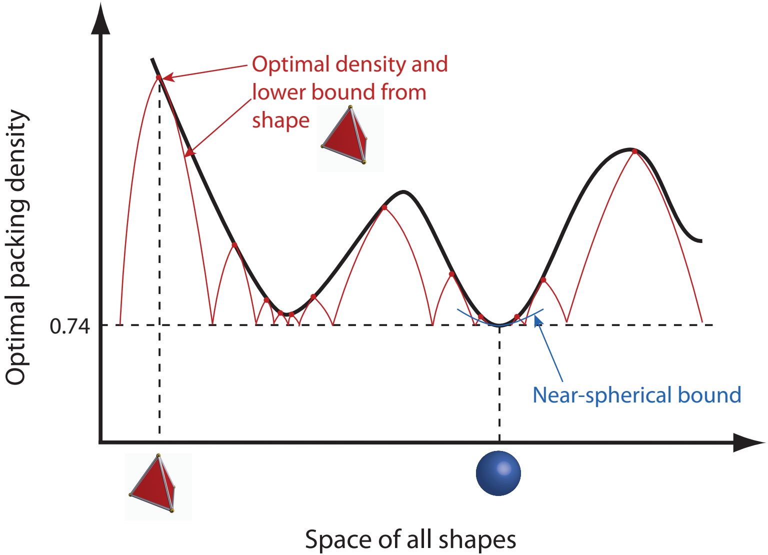

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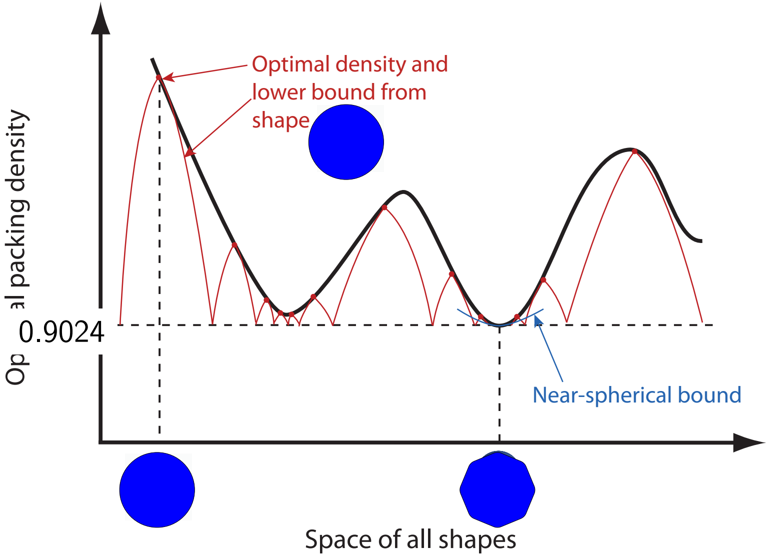
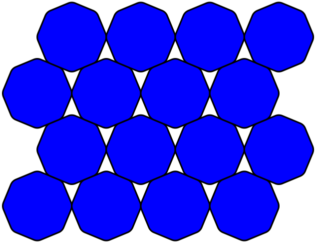


Reinhardt's conjecture – previous results



$\delta(M) = 0.9024$

Theorem (V. Ennola, 1961)

For any c.s. planar convex body C, $\delta(C) \geq 0.8813$.

Theorem (P. P. Tammela, 1970)

$\delta(C) \geq 0.8926$.

Theorem (F. Nazarov, 1986)

The smoothed octagon is a local minimum.

V. Ennola, J. London Math. Soc s1-36 (1961), 135
P. P. Tammela, Izv. Vysš. Učebn. Zaved. Mat. 1970 (1970), 103
F. Nazarov, J. Soviet Math. 43 (1988), 2687

Branch and Bound algorithm

want:
$\delta(C) \geq 0.9204$

$\mathcal{K}_0 = \{\text{all shapes}\}$

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$\delta(C) \geq 0.71$ for all $C \in \mathcal{K}_0$

Branch and Bound algorithm

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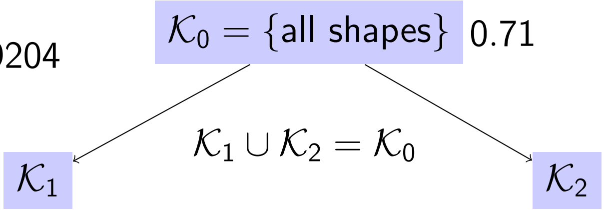


Branch and Bound algorithm

want:

$\delta(C) \geq 0.9204$

$\mathcal{K}_0 = \{\text{all shapes}\}$ 0.71

$\mathcal{K}_1 \cup \mathcal{K}_2 = \mathcal{K}_0$

$\mathcal{K}_1$ $\mathcal{K}_2$

$\delta(C) \geq 0.94$ for all $C \in \mathcal{K}_1$

Branch and Bound algorithm

want:

$\delta(C) \geq 0.9204$

$\mathcal{K}_0 = \{\text{all shapes}\}$ 0.71

$\mathcal{K}_1 \cup \mathcal{K}_2 = \mathcal{K}_0$

~~$\mathcal{K}_1$~~ $\mathcal{K}_2$

$\delta(C) \geq 0.94$ for all $C \in \mathcal{K}_1$

Branch and Bound algorithm

want:
$\delta(C) \geq 0.9204$

$\mathcal{K}_0 = \{\text{all shapes}\}$ 0.71

$\mathcal{K}_1 \cup \mathcal{K}_2 = \mathcal{K}_0$

0.94 ~~$\mathcal{K}_1$~~

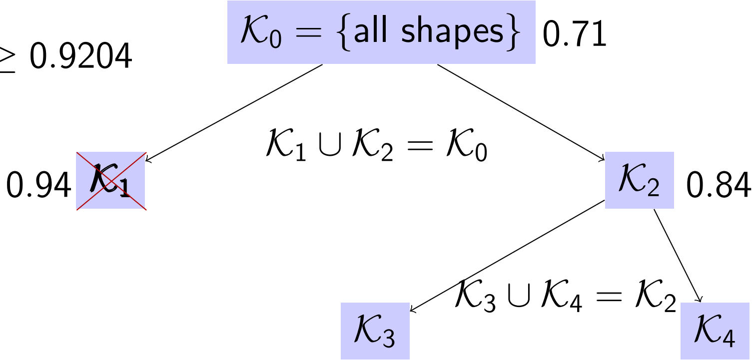
$\mathcal{K}_2$

$\delta(C) \geq 0.84$ for all $C \in \mathcal{K}_2$

Branch and Bound algorithm

want:

$\delta(C) \geq 0.9204$



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want:

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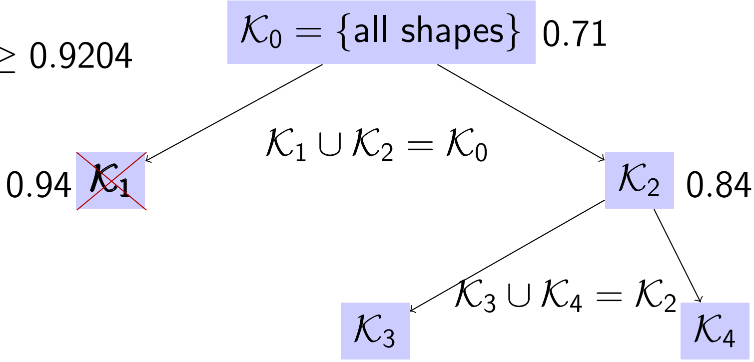

$\delta(C) \geq 0.86$ for all $C \in \mathcal{K}_3$

Branch and Bound algorithm

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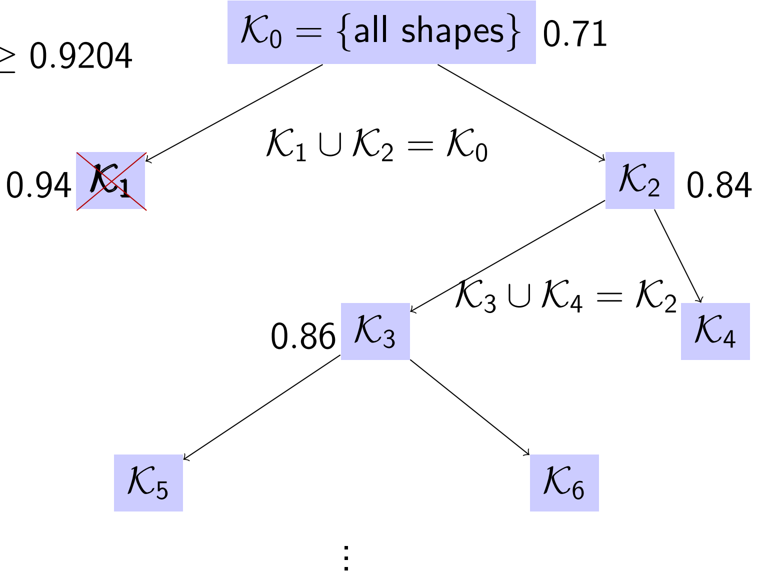

Branch and Bound algorithm

To demonstrate that $\delta(C) \geq \delta_0$ for all $C \in \mathcal{K}_0$.

(1) Seed a stack with an object representing $\mathcal{K}_0$.

(2) If the stack is empty, then done.

(3) Else, pop the top object, representing a collection $\mathcal{K}_i$ from the stack.

(4) If it can be shown directly that $\delta(C) \geq \delta_0$ for all $C \in \mathcal{K}_i$, then go to (2).

(5) Else, split $\mathcal{K}_i = \mathcal{K}' \cup \mathcal{K}''$, and push $\mathcal{K}'$ and $\mathcal{K}''$ onto the stack.

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Branch and Bound algorithm

To demonstrate that $\delta(C) \geq \delta_0$ for all $C \in \mathcal{K}_0$.

(1) Seed a stack with an object **representing** $\mathcal{K}_0$.

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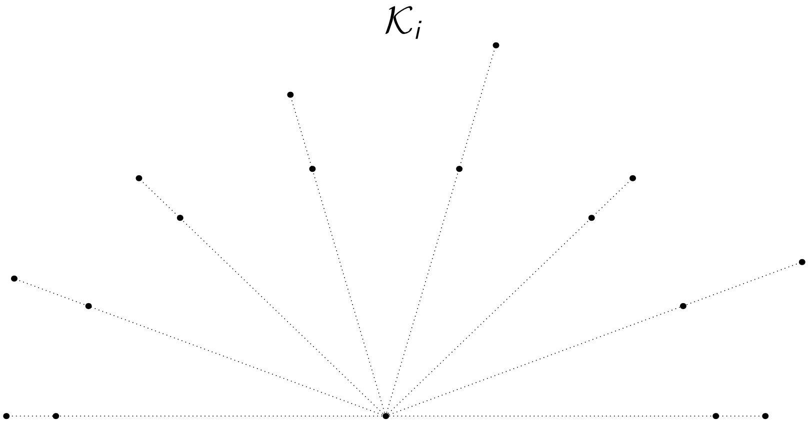
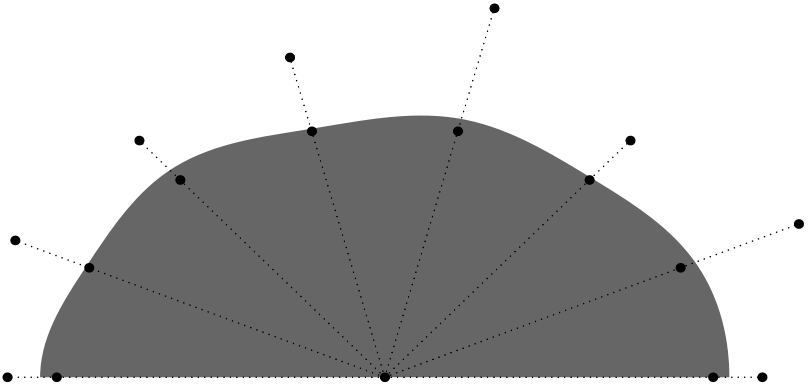
Node representation



Node representation

$C \in \mathcal{K}_i$



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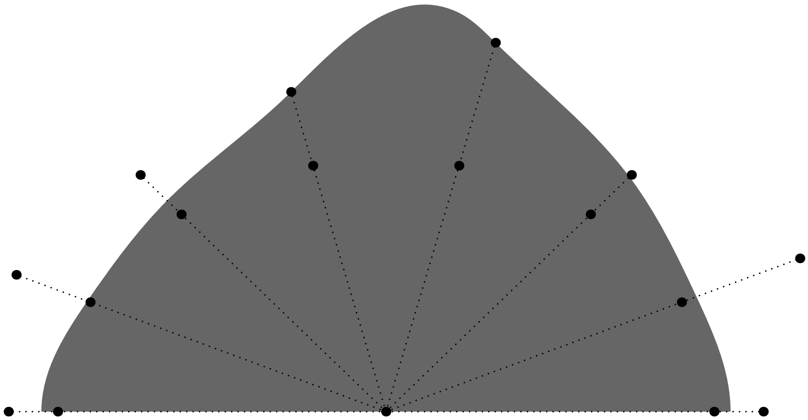

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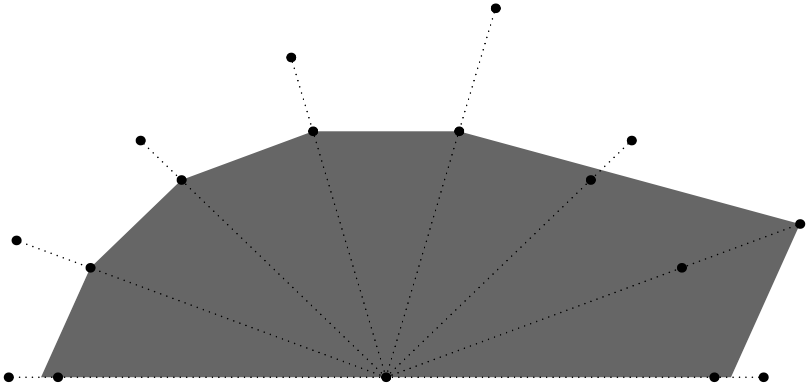

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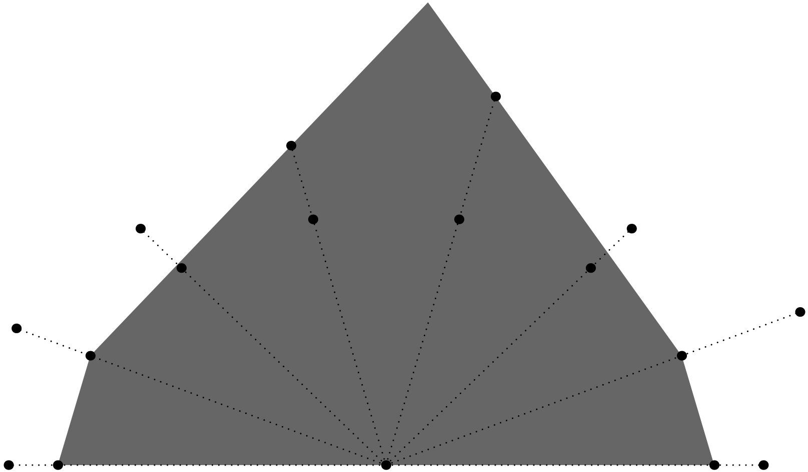

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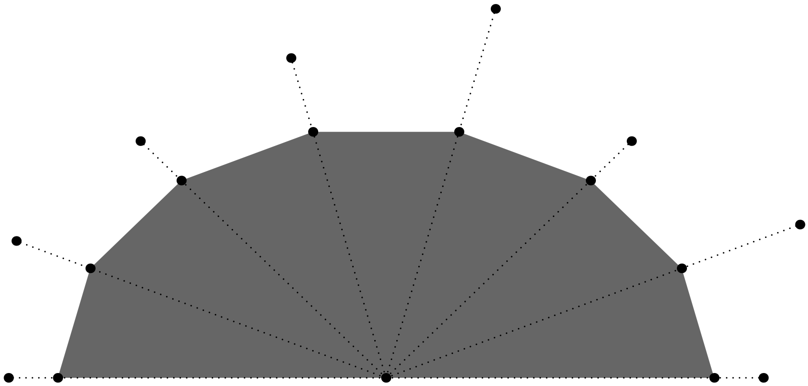
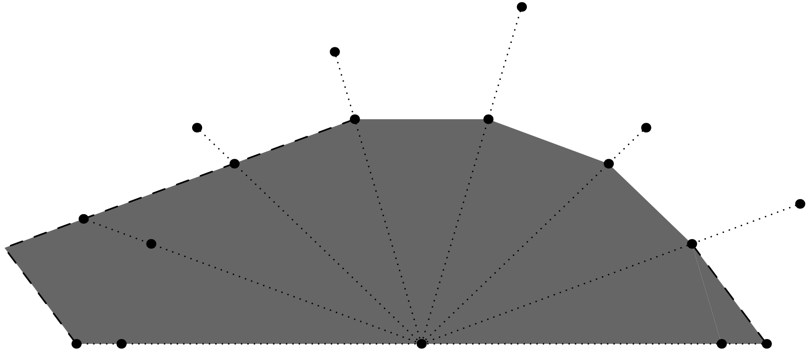
Bound setting – minimal body

$$C_{\min} = \bigcap_{C \in \mathcal{K}_i} C$$



Bound setting – maximal body

$$\bigcup_{C \in \mathcal{K}_i} C$$



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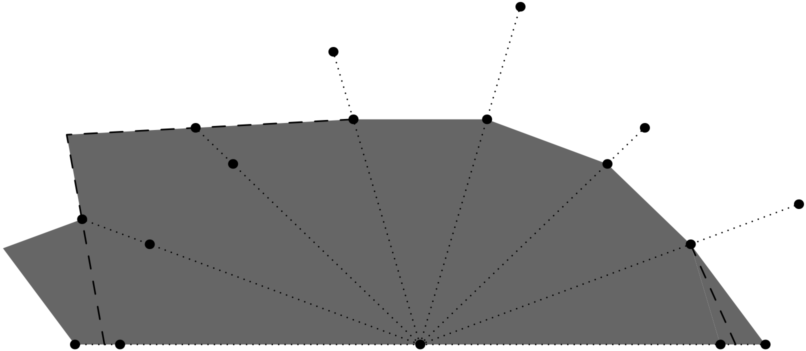

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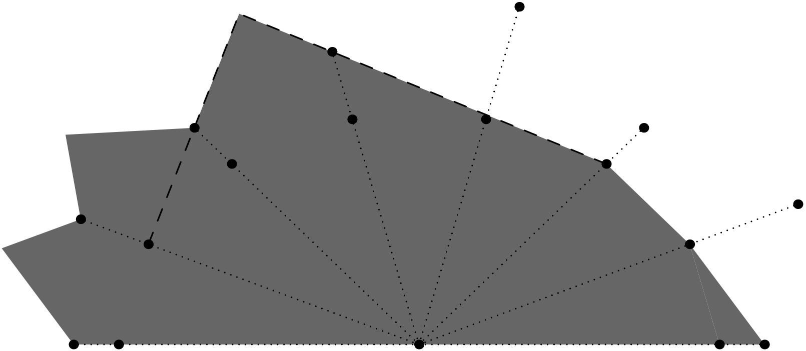

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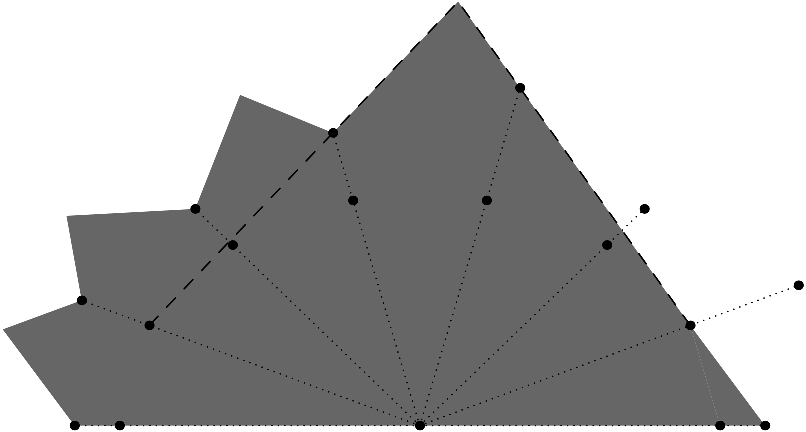

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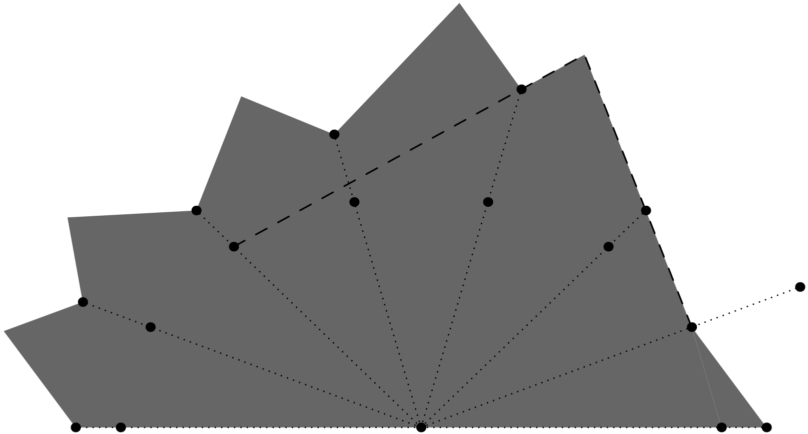

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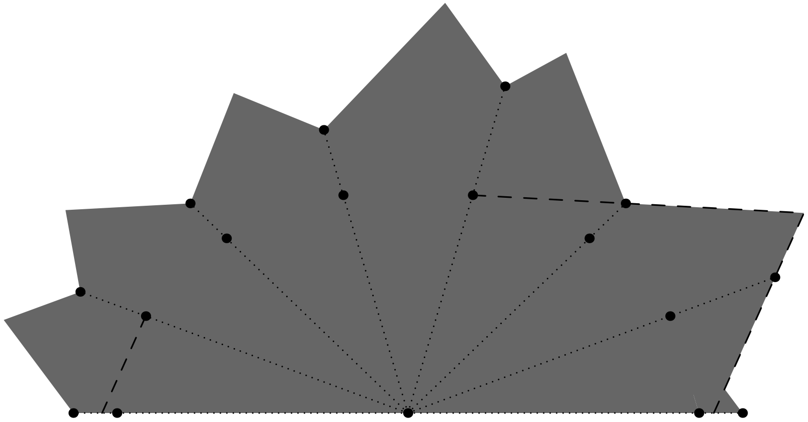

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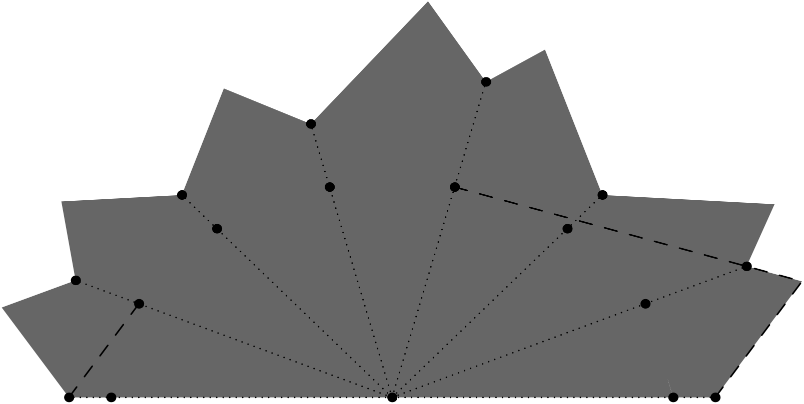
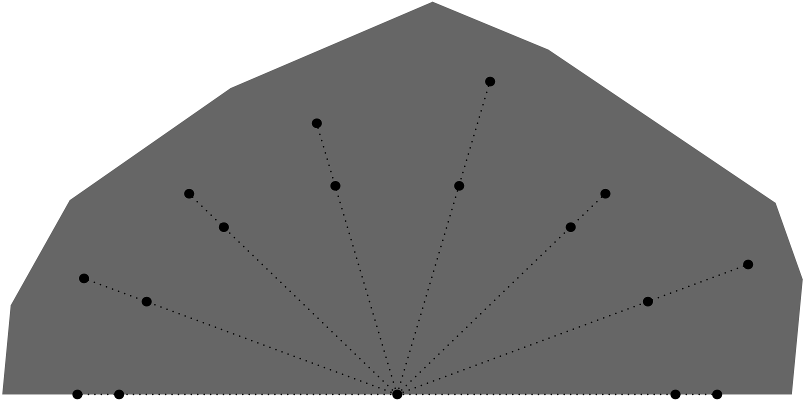


Bound setting – maximal body

$$C_{\max} = \mathrm{conv} \bigcup_{C \in \mathcal{K}_i} C$$



Bound setting

Because $C \subseteq C_{\max}$, and $\text{area}(C) \geq \text{area}\, C_{\min}$,

$$\delta(C) \geq \frac{\delta(C_{\max})\, \text{area}(C_{\min})}{\text{area}(C_{\max})}$$

for all $C \in \mathcal{K}_i$.

D. M. Mount & R. Silverman, J. Algorithms 11 (1990), 564.

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for all $C \in \mathcal{K}_i$.

$O(n)$ algorithm to compute $\delta(C_{\max})$.

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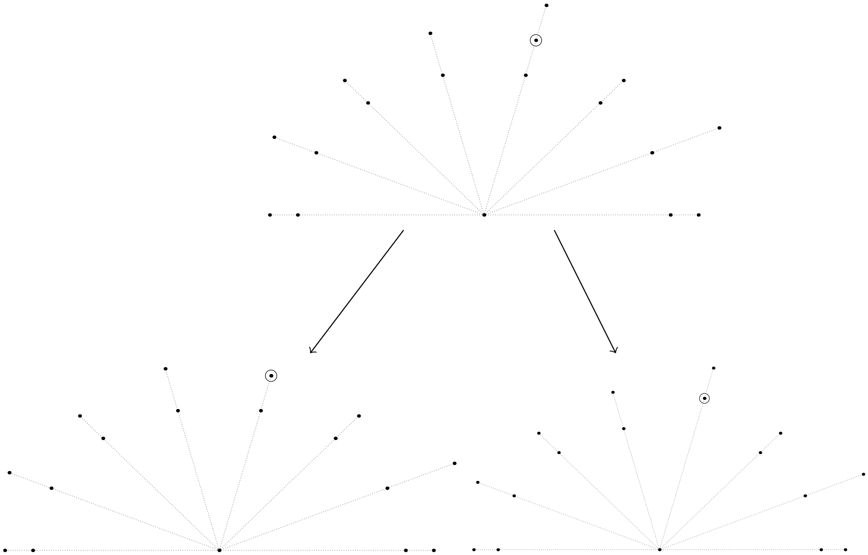
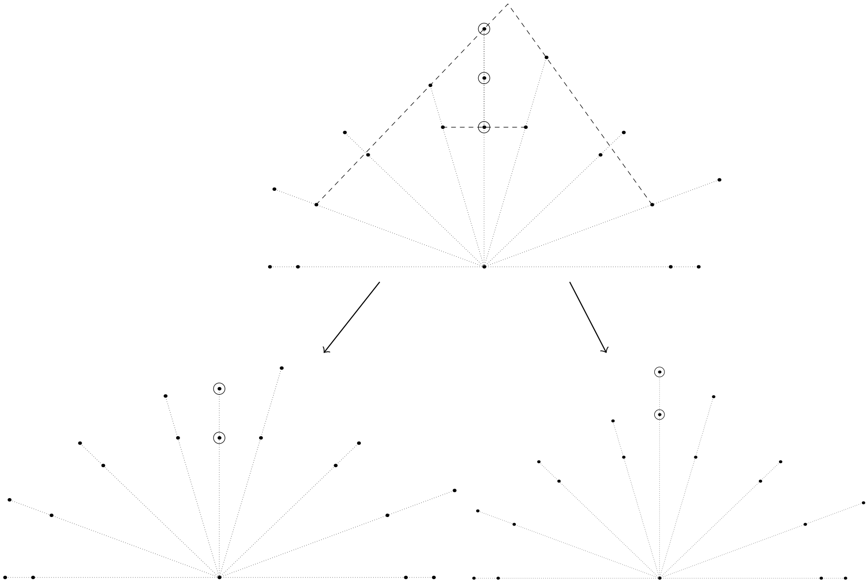
Splitting: no new radii



Splitting: adding a radius



Results

Recall:

Disks: $\delta(B) = 0.9069$.
Conjecture: $\delta(C) \geq 0.9024$ for all C.
Ennola: $\delta(C) \geq 0.8813$ for all C.
Tammela: $\delta(C) \geq 0.8926$ for all C.

δ_0	0.8820	0.8850	0.8870	0.8890
iterations	3.2×10^4	3.3×10^5	1.8×10^6	1.1×10^7
δ_0	0.8910	0.8930	0.8950	0.8960
iterations	7.1×10^7	8.0×10^8	3.8×10^{10}	4.3×10^{11}