

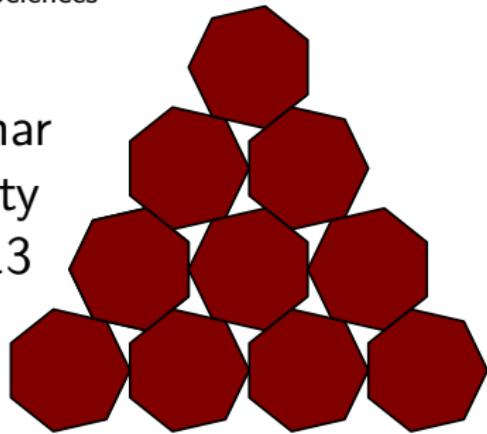


Pessimal Shapes for Packing

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Soft Matter Seminar
New York University
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The Miser's Problem

A miser is required by a contract to deliver a chest filled with gold bars, arranged as densely as possible. The bars must be identical, convex, and much smaller than the chest. What shape of gold bars should the miser cast so as to part with as little gold as possible?



Optima and *pessima*

Optimal packing
shapes are trivial



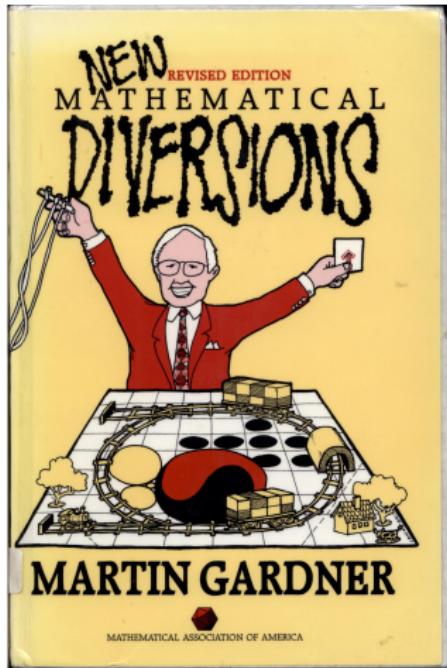
Optima and *pessima*

Optimal packing
shapes are trivial



Is the sphere the
pessimal convex
shape?

Ulam's Conjecture

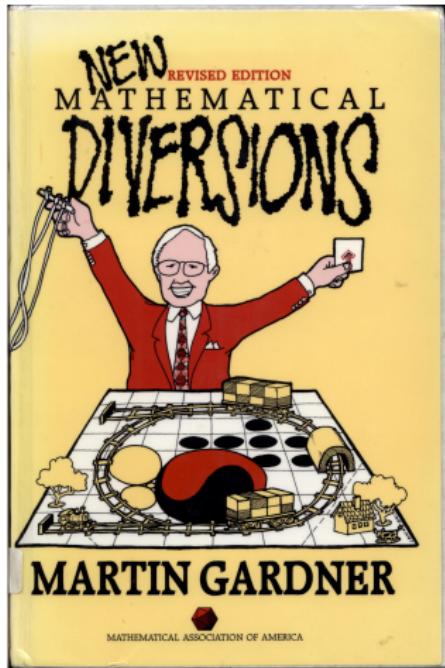


“Stanislaw Ulam told me in 1972 that he suspected the sphere was the worst case of dense packing of identical convex solids, but that this would be difficult to prove.”

$$\phi(B) = \pi/\sqrt{18} = 0.7405$$

1995 postscript to the column “Packing Spheres”

Ulam's Last Conjecture

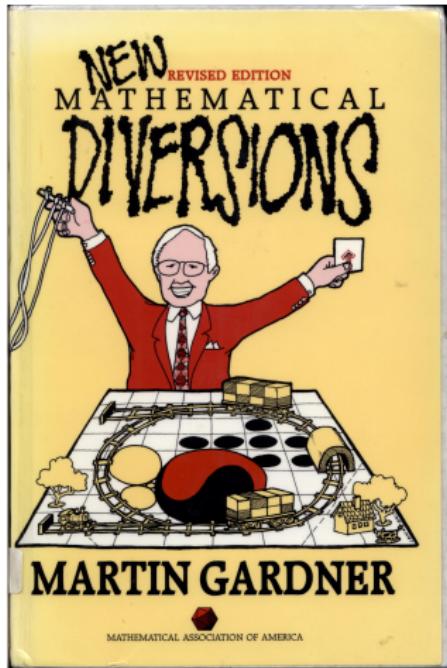


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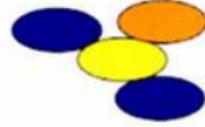
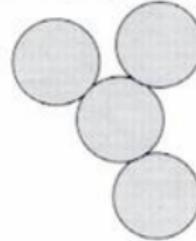
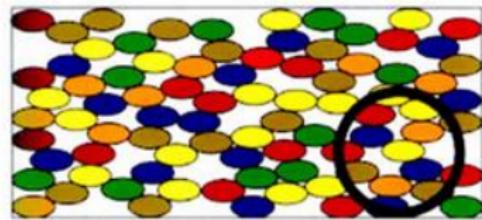
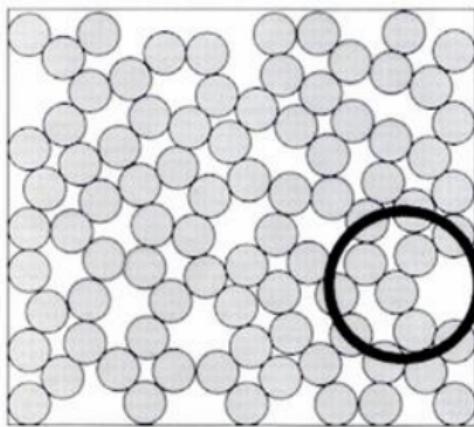
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$$\phi(B) = \pi/\sqrt{18} = 0.7405$$

Naive motivation: sphere is the least free solid (three degrees of freedom vs. six for most solids).

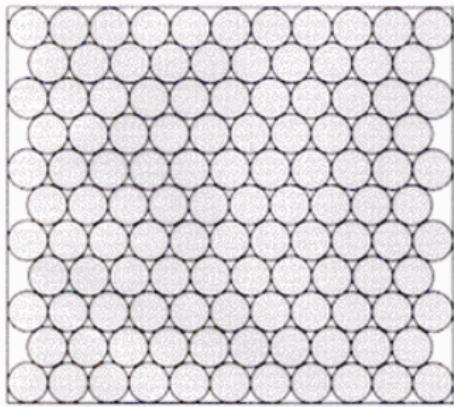
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Using rotation to unjam a packing

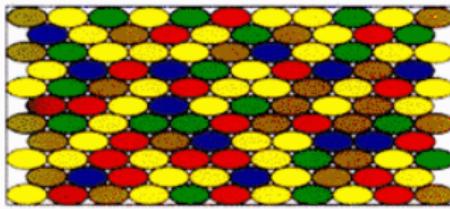


P. Chaikin

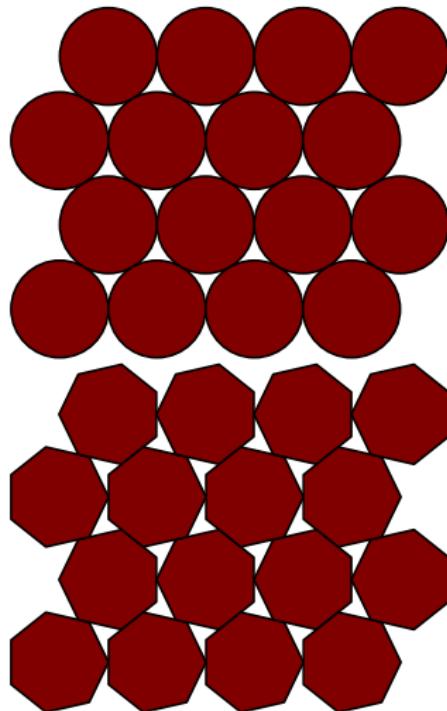
Using rotation to unjam a packing



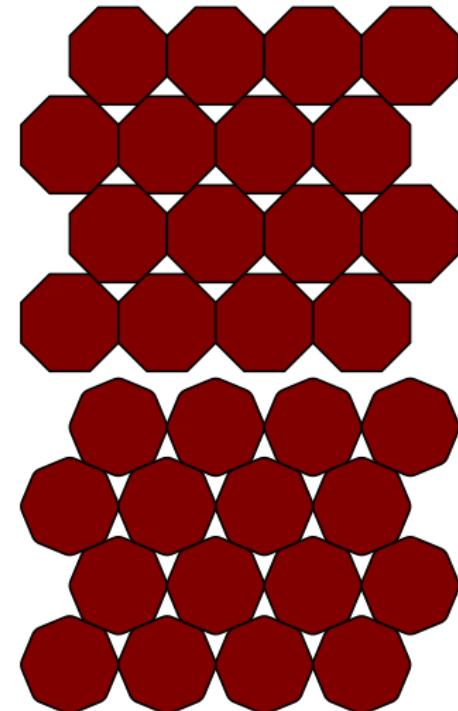
M&M® aspect ratio 1.91



In 2D disks are not worst



0.9069

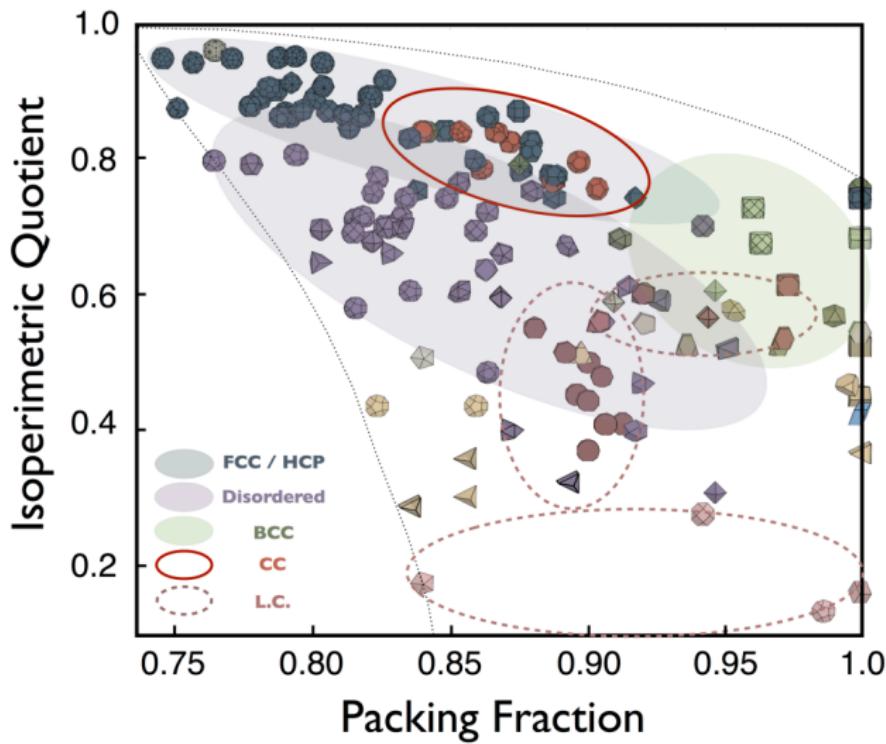


0.9062

0.9024

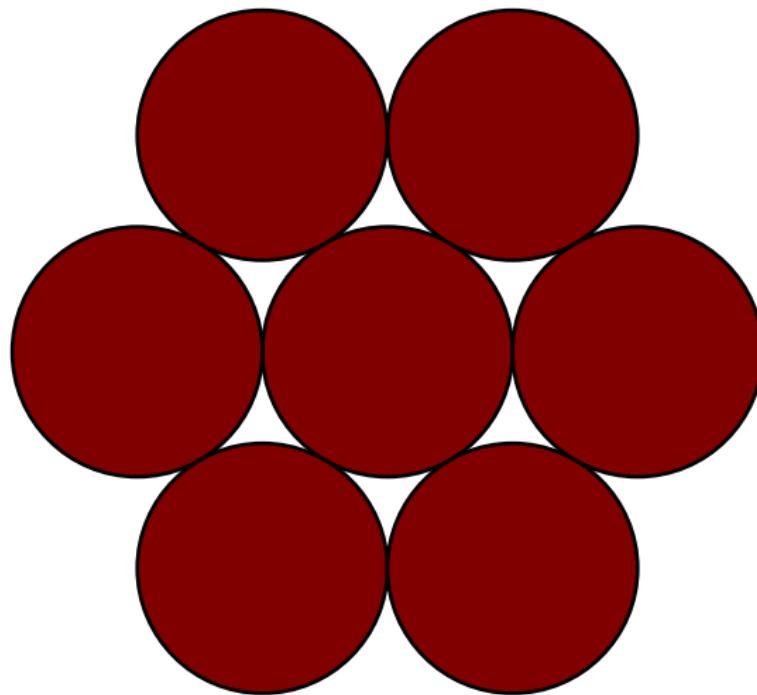
0.8926(?)

Packing non-spherical shapes

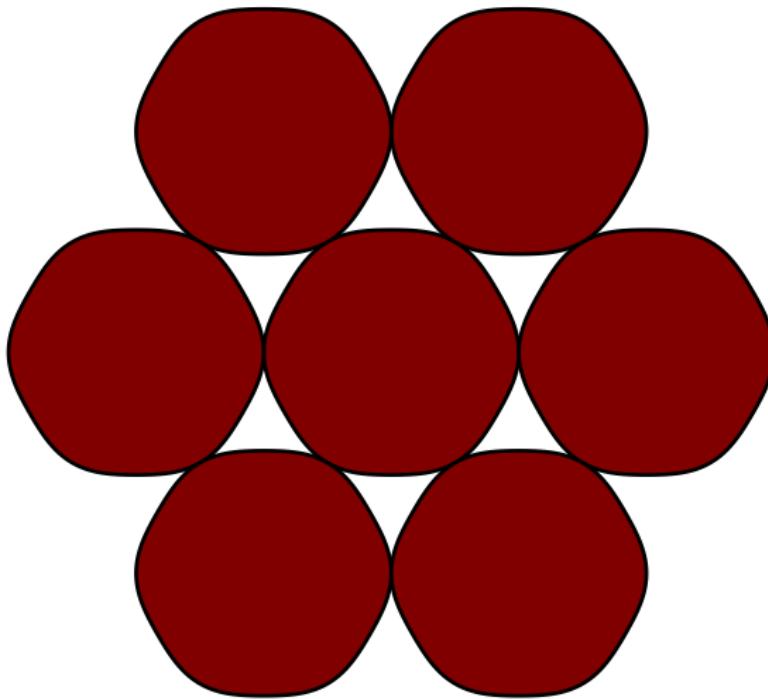


Damasceno, Engel, and Glotzer, 2012.

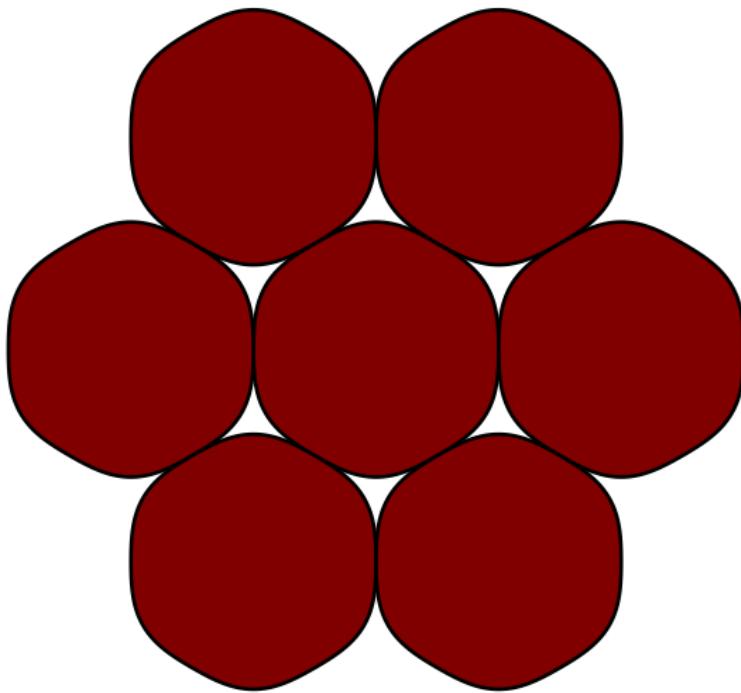
Why can we improve over circles?



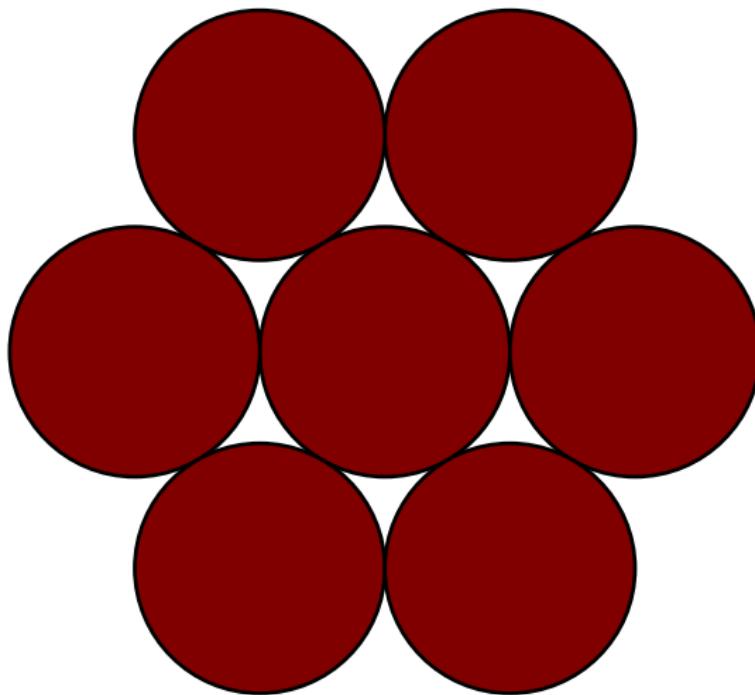
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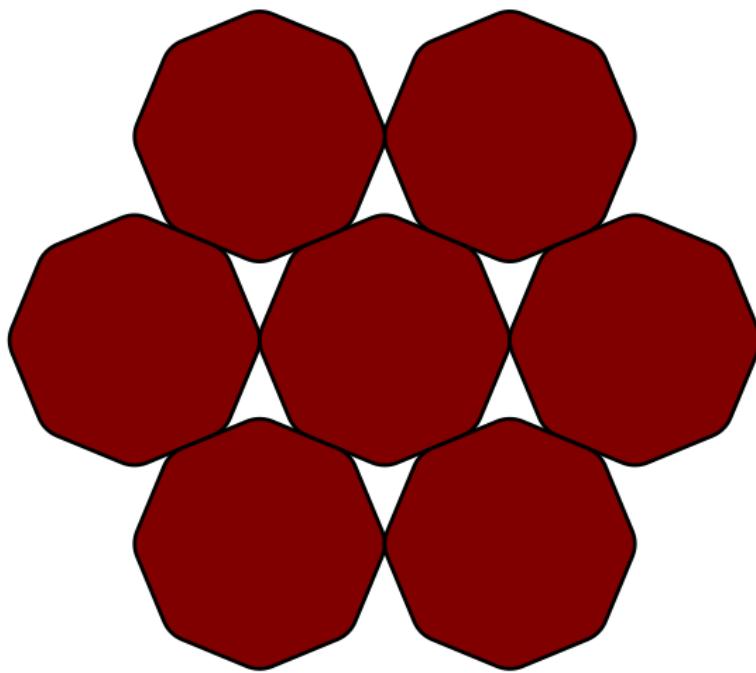
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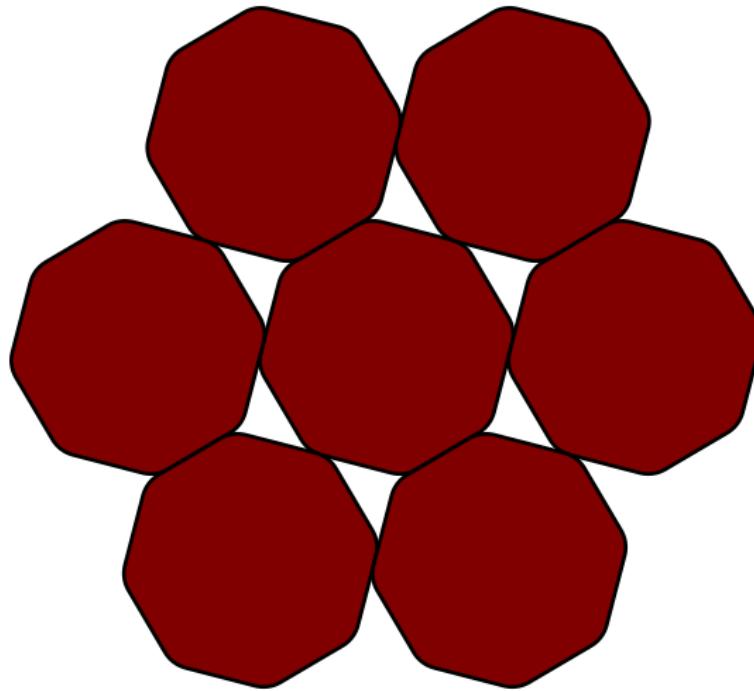
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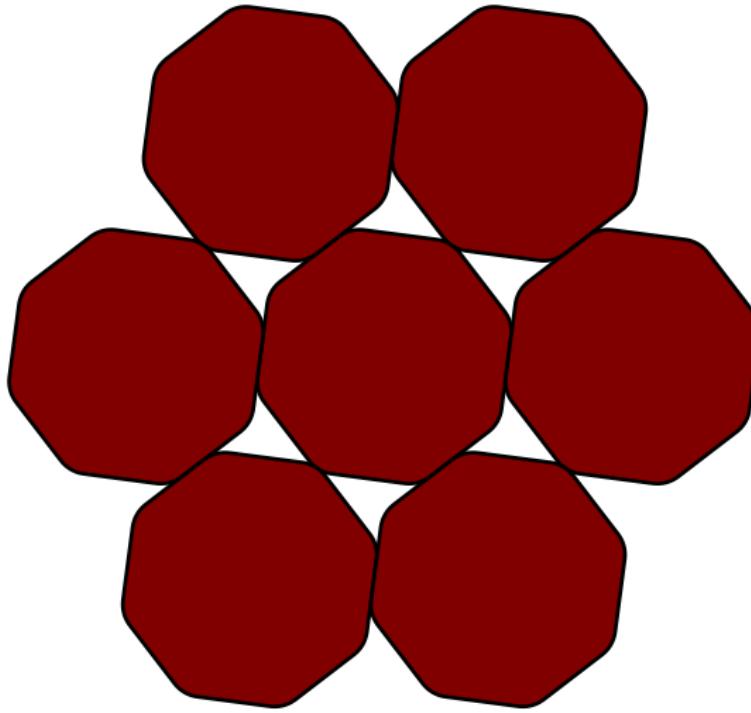
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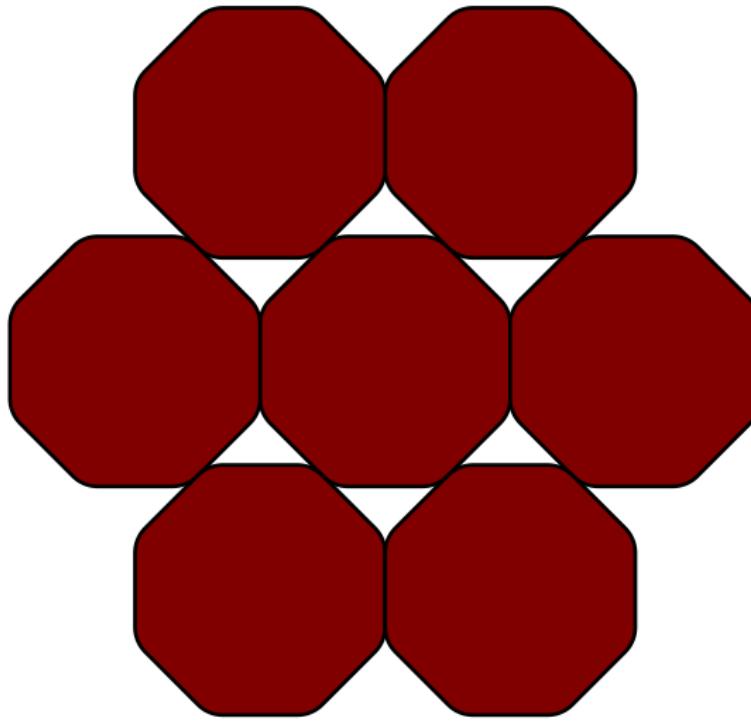
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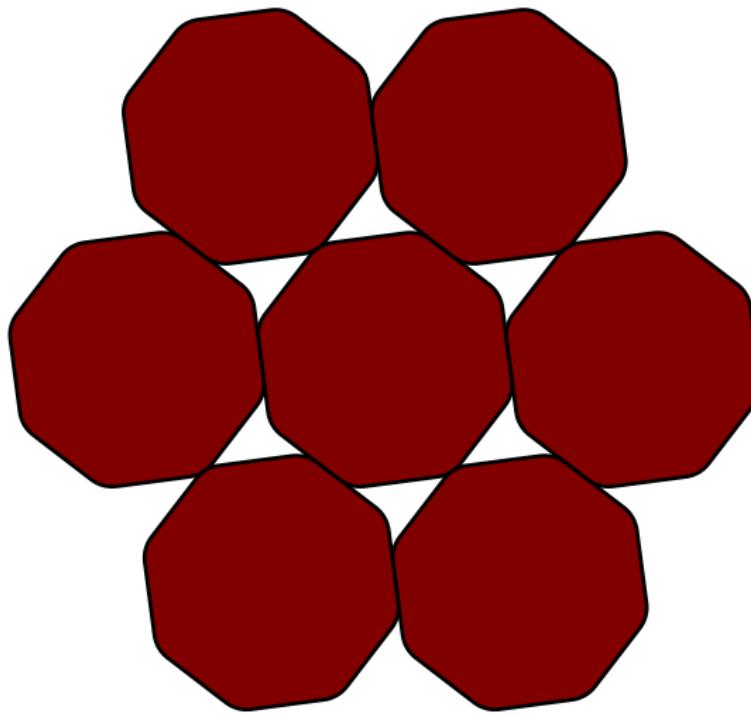
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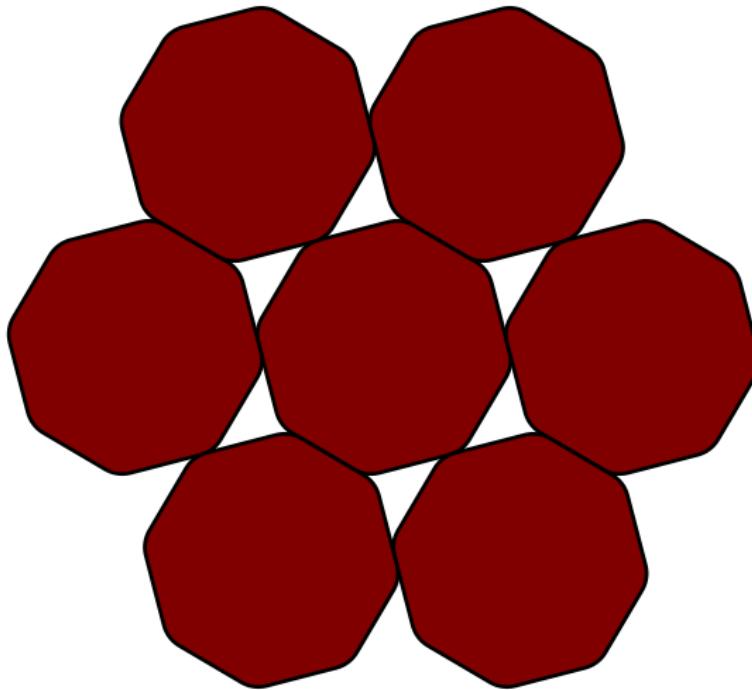
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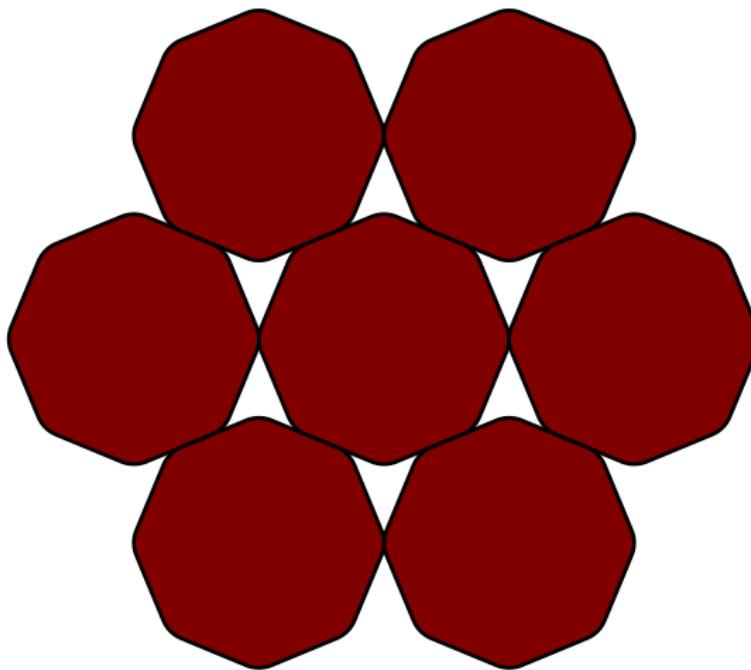
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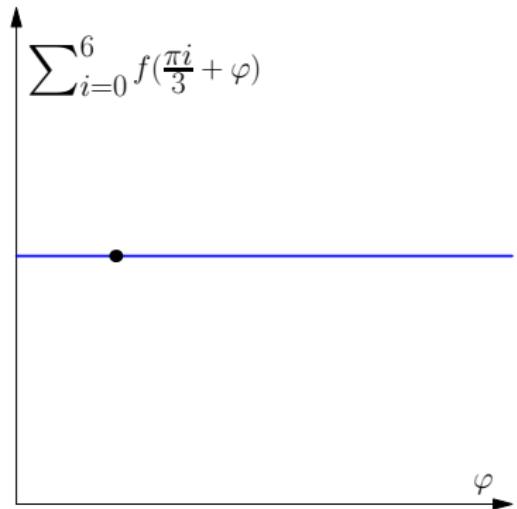
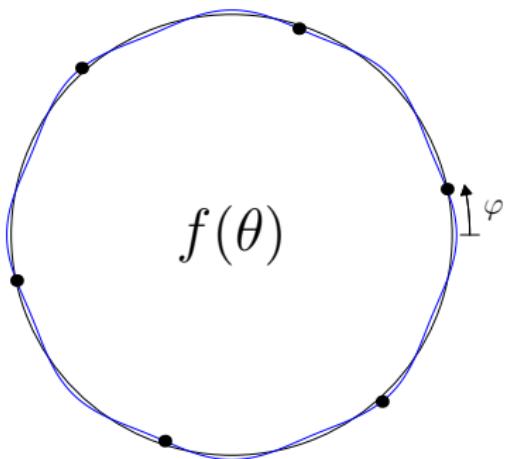
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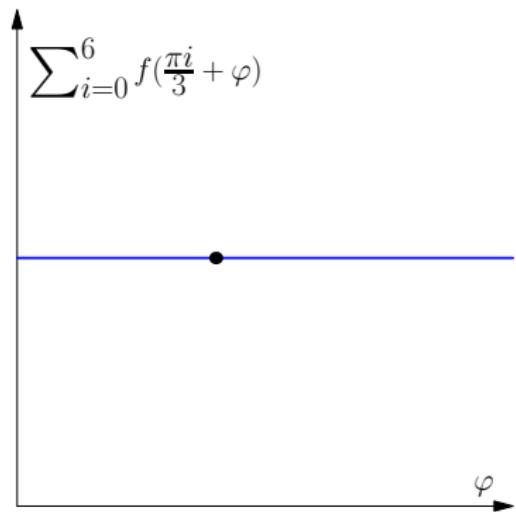
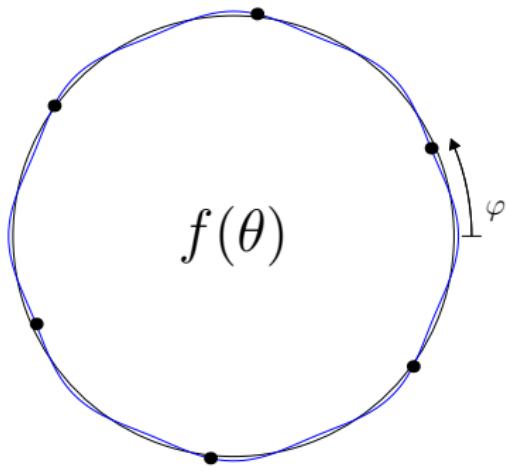
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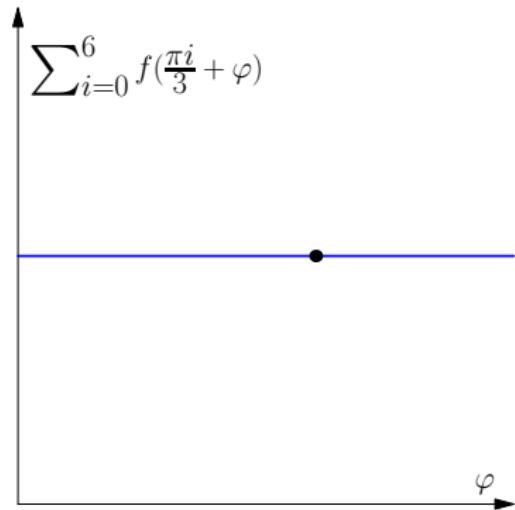
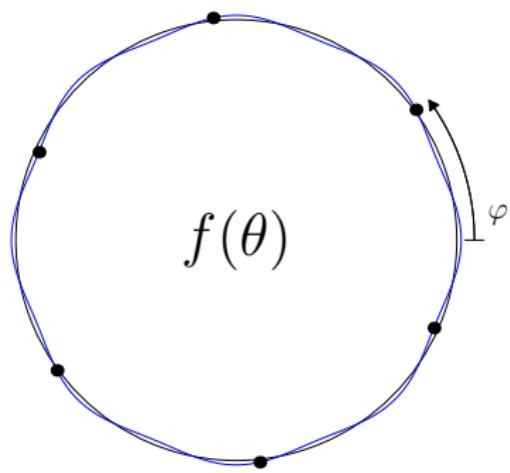
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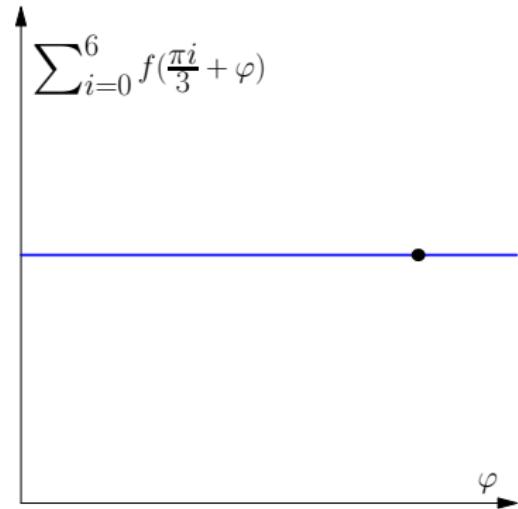
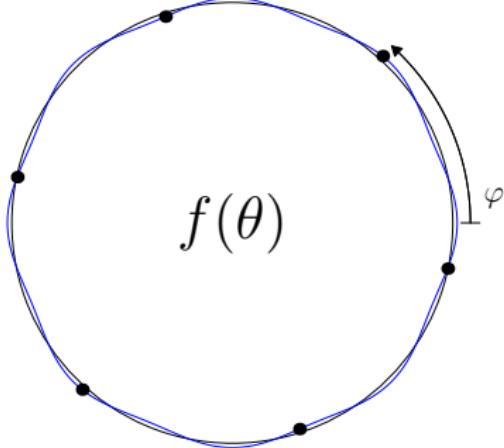
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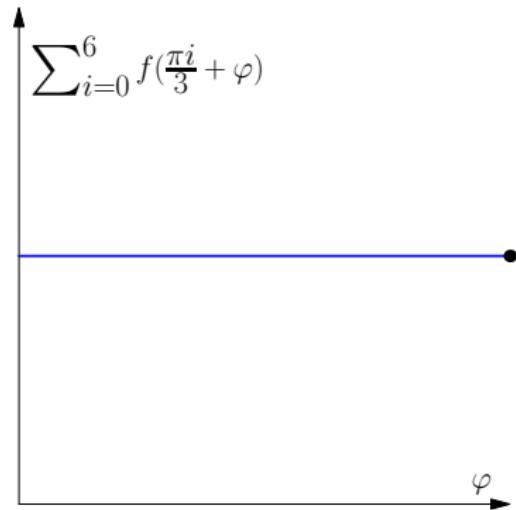
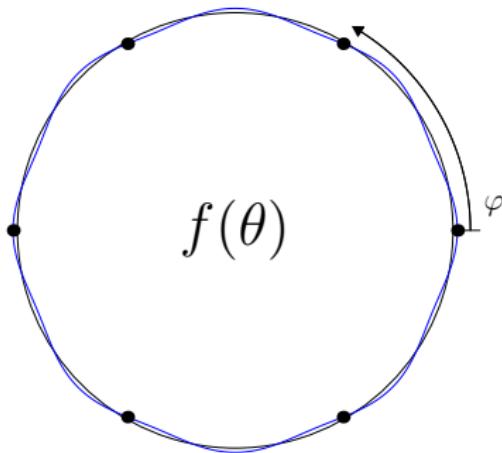
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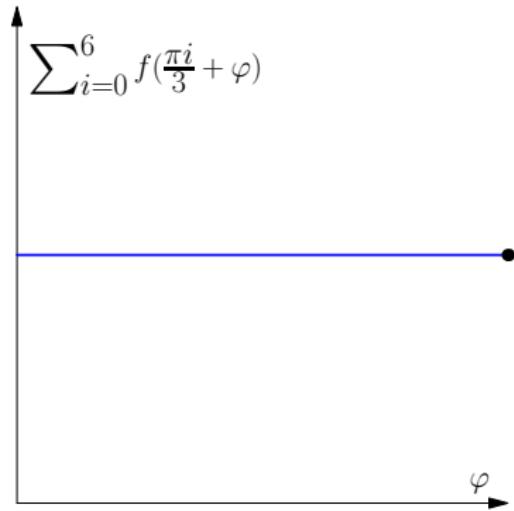
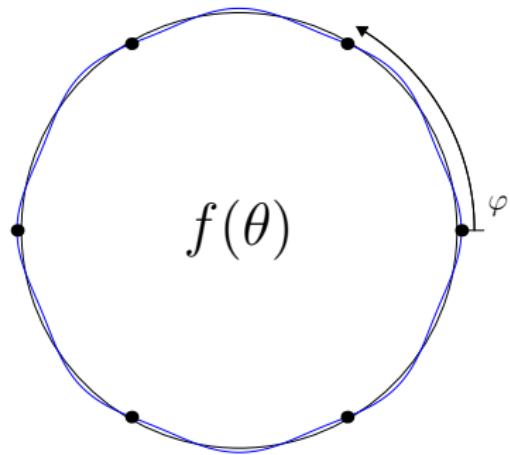
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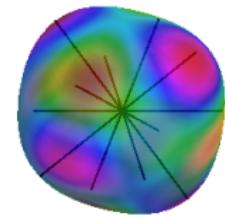
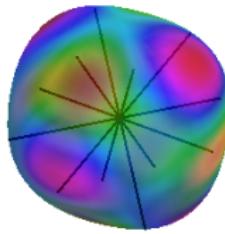
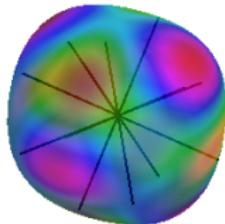


Why can we improve over circles?



$$f(\theta) = 1 + \epsilon \cos(8\theta)$$

Why can we not improve over spheres?



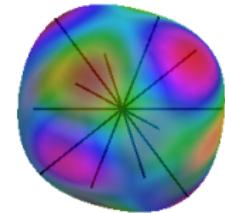
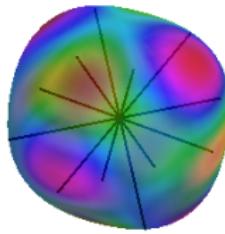
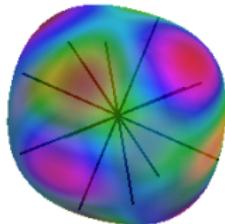
Lemma

Let f be an even function $S^2 \rightarrow \mathbb{R}$.

$\sum_{i=1}^{12} f(R\mathbf{x}_i)$ is independent of R if and only if the expansion of $f(\mathbf{x})$ in spherical harmonics terminates at $l = 2$.

YK, arXiv:1212.2551

Why can we not improve over spheres?



Lemma

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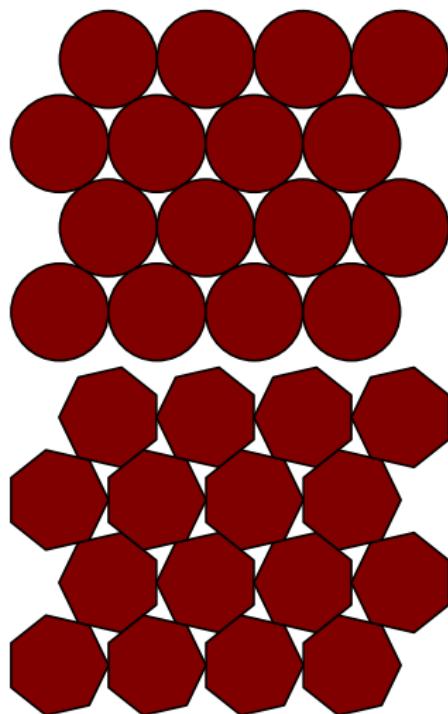
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Theorem (YK)

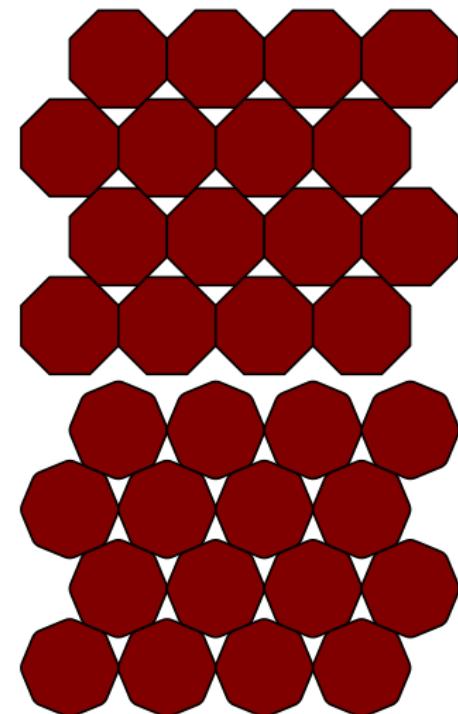
The sphere is a local minimum of the optimal packing fraction among convex, centrally symmetric bodies.

YK, arXiv:1212.2551

In 2D disks are not worst



0.9069

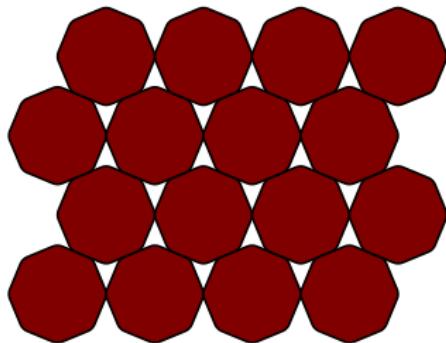


0.9062

0.9024

0.8926(?)

Reinhardt's conjecture



0.9024

Conjecture (K. Reinhardt, 1934)

The smoothed octagon is an absolute minimum of the optimal packing fraction among convex, centrally symmetric bodies.

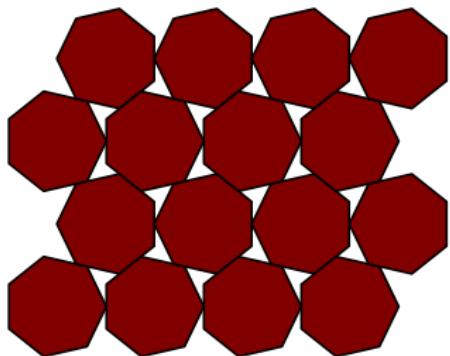
Theorem (F. Nazarov, 1986)

The smoothed octagon is a local minimum.

K. Reinhardt, *Abh. Math. Sem., Hamburg, Hansischer Universität, Hamburg 10* (1934), 216

F. Nazarov, *J. Soviet Math.* 43 (1988), 2687

Regular heptagon is locally worst packing



0.8926(?)

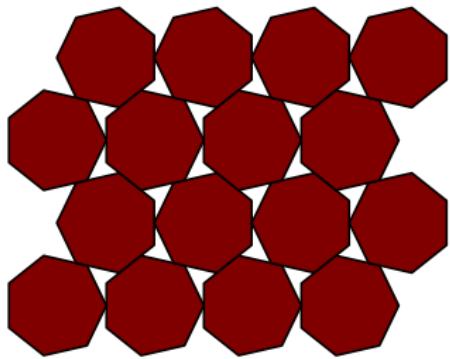
Theorem (YK)

Any convex body sufficiently close to the regular heptagon can be packed at a filling fraction at least that of the “double lattice” packing of regular heptagons.

Note: it is not proven, but highly likely, that the “double lattice” packing is the densest packing of regular heptagons.

YK, arXiv:1305.0289

Regular heptagon is locally worst packing



0.8926(?)

Theorem (YK)

Any convex body sufficiently close to the regular heptagon can be packed at a filling fraction at least that of the “double lattice” packing of regular heptagons.

Conjecture

The regular heptagon is an absolute minimum of the optimal packing fraction among convex bodies.

YK, arXiv:1305.0289

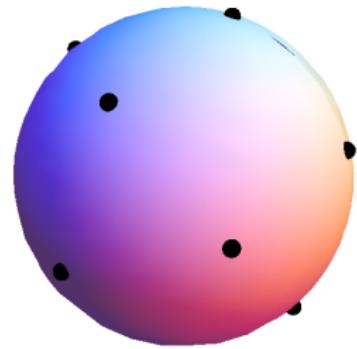
Higher dimensions

- In 2D, the circle is not a local minimum of packing fraction among c. s. convex bodies.
- In 3D, the sphere is a local minimum of packing fraction among c. s. convex bodies.
- What can we say about spheres in higher dimensions?

Higher dimensions

- In 2D, the circle is not a local minimum of packing fraction among c. s. convex bodies.
- In 3D, the sphere is a local minimum of packing fraction among c. s. convex bodies.
- What can we say about spheres in higher dimensions?
- Note that in $d > 3$ we do not know the densest packing of spheres.
- But we do know the densest (Bravais) *lattice* packing in $d = 4, 5, 6, 7, 8$, and 24.

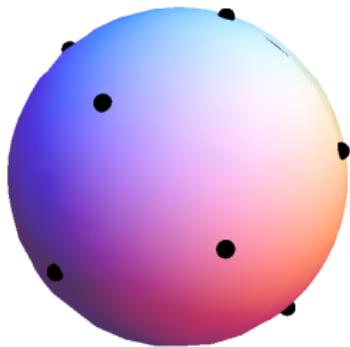
Extreme Lattices



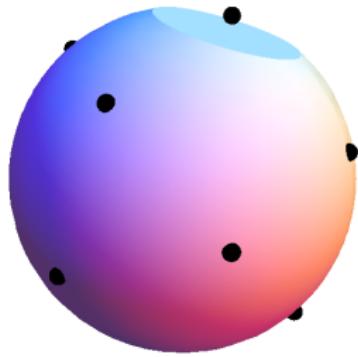
Contact points
 $S(\Lambda)$ of the
optimal lattice.

A lattice Λ is *extreme* if and only if
 $\|T\mathbf{x}\| \geq \|\mathbf{x}\|$ for all $\mathbf{x} \in S(\Lambda) \implies$
 $\det T \geq 1$ for $T \approx 1$.

Extreme Lattices



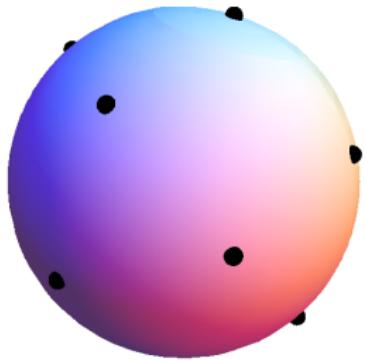
A lattice Λ is *extreme* if and only if $\|T\mathbf{x}\| \geq \|\mathbf{x}\|$ for all $\mathbf{x} \in S(\Lambda) \Rightarrow \det T \geq 1$ for $T \approx 1$.



In $d = 6, 7, 8, 24$, the optimal lattice is *redundantly extreme*, and so the ball is not locally pessimal.

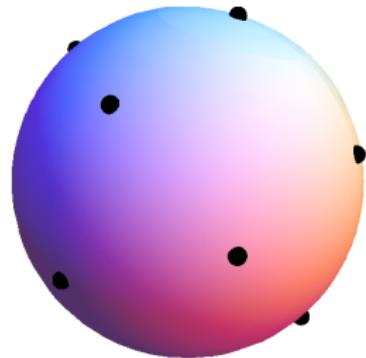
YK, arXiv:1212.2551

$d = 4$ and $d = 5$

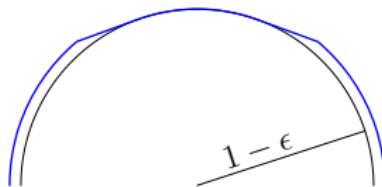


In $d = 4, 5$, if $\|T\mathbf{x}\| \geq \|\mathbf{x}\|$ for all $\mathbf{x} \in S(\Lambda) \setminus \{\mathbf{x}_0\}$, and $\|T\mathbf{x}_0\| > (1 - \epsilon)\|\mathbf{x}_0\|$, then $1 - \det T < C\epsilon^2$ (compared with $C\epsilon$ for $d = 2, 3$).

$d = 4$ and $d = 5$



In $d = 4, 5$, if $\|T\mathbf{x}\| \geq \|\mathbf{x}\|$ for all $\mathbf{x} \in S(\Lambda) \setminus \{\mathbf{x}_0\}$, and $\|T\mathbf{x}_0\| > (1 - \epsilon)\|\mathbf{x}_0\|$, then $1 - \det T < C\epsilon^2$ (compared with $C\epsilon$ for $d = 2, 3$).



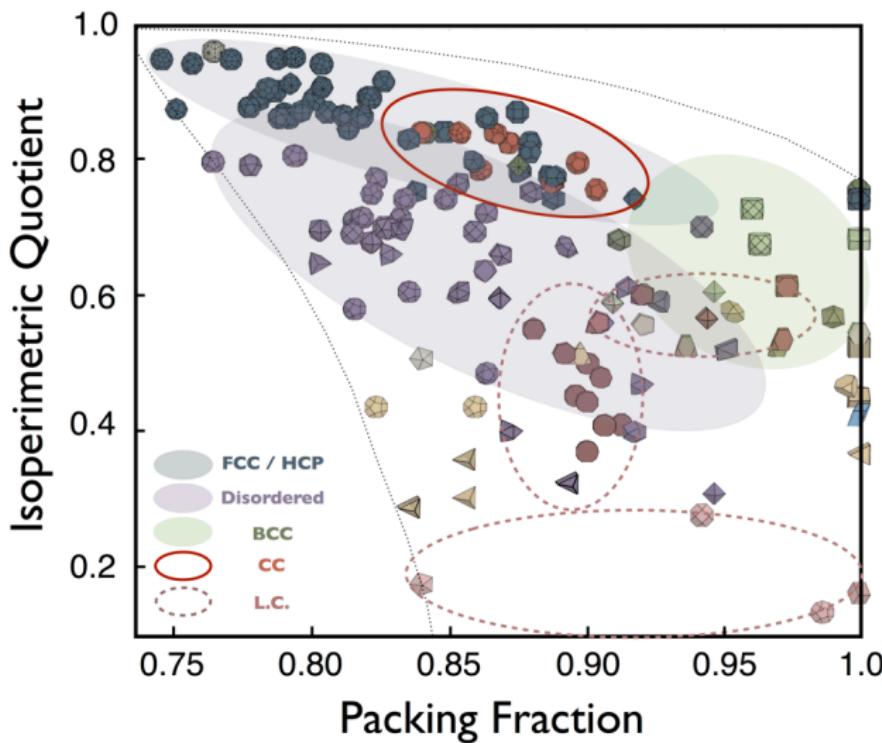
$$(\rho(K) - \rho(B))/\rho(B) \sim \epsilon^2$$
$$(V(B) - V(K))/V(B) \sim \epsilon$$

The ball is not locally pessimal.

Summary of local pessimality results

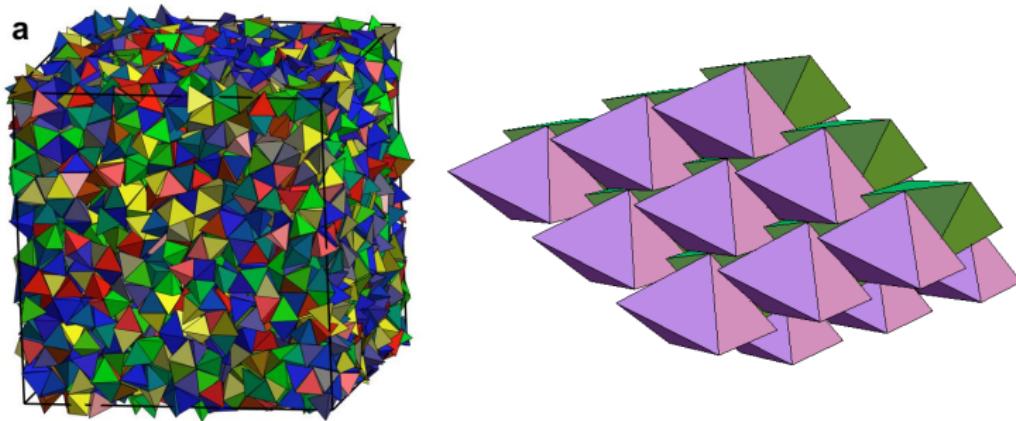
- In $d = 2$, the heptagon is a local pessimum, assuming the “double lattice” packing of heptagons is their densest packing. The disk is not a local pessimum.
- In $d = 3$, the ball is a local pessimum among centrally symmetric bodies.
- In higher dimensions, at least with respect to Bravais lattice packing of centrally symmetric bodies, the ball is not a local pessimum.

Global pessimality?



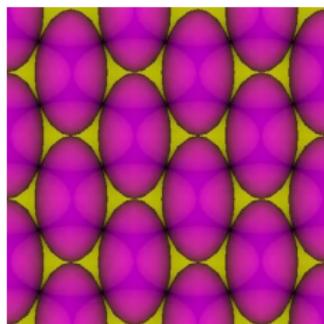
Damasceno, Engel, and Glotzer, 2012.

Tetrahedra



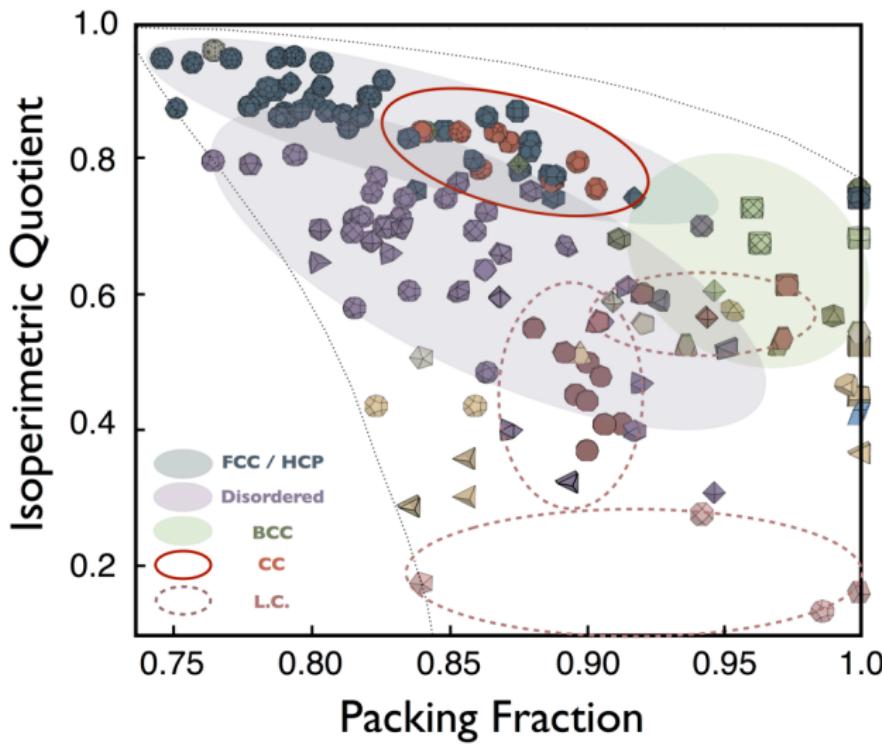
- Conway & Torquato suggested in 2006 that $\phi(T) < \phi(B) = 0.7405$.
- A sequence of experimentally and numerically discovered structures showed that $\phi(T) \geq 0.8563$.

Ellipsoids



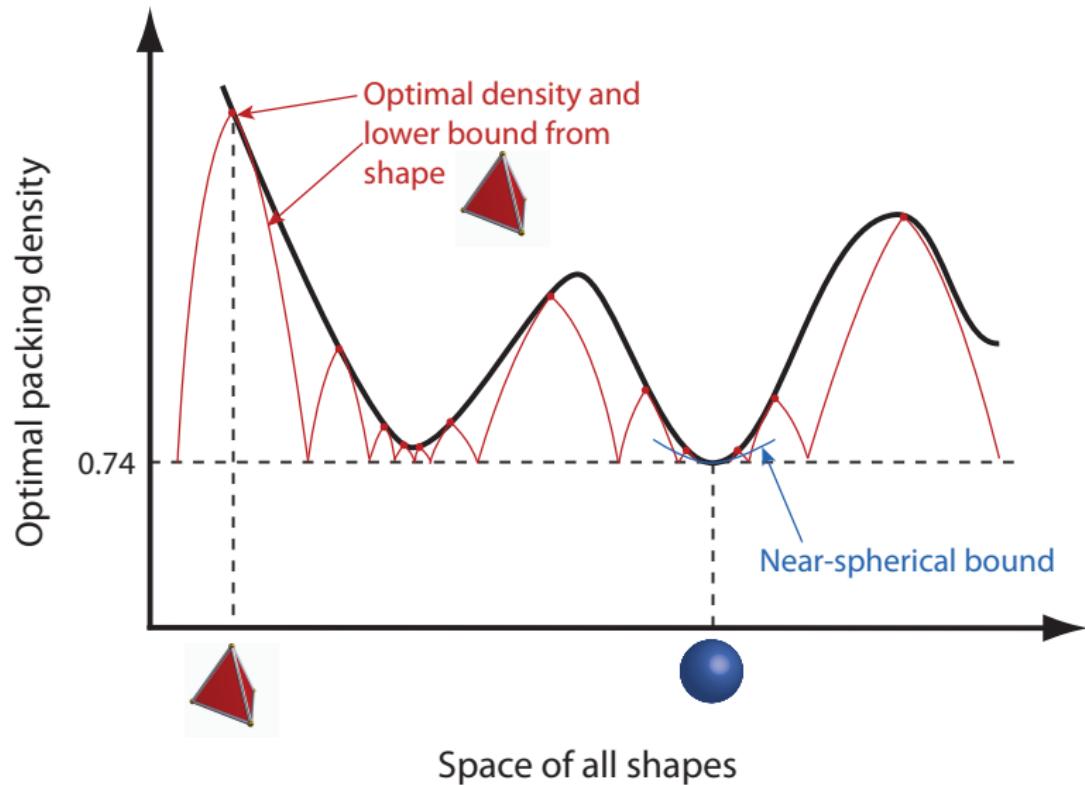
- $\phi(E) \geq \phi(B)$ for ellipsoids of high enough aspect ratio (Bezdek & Kuperberg 1991).
- True also for arbitrarily spherical ellipsoids?
- Numerically discovered structure achieves $\phi(E) \geq \phi(B)$ for all ellipsoids E (Donev et al. 2004).

Global pessimality?



Damasceno, Engel, and Glotzer, 2012.

Verification strategy



Branch and Bound algorithm

want:

$$\phi(C) \geq 0.7405$$

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

Branch and Bound algorithm

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$$\phi(C) \geq 0.7405$$

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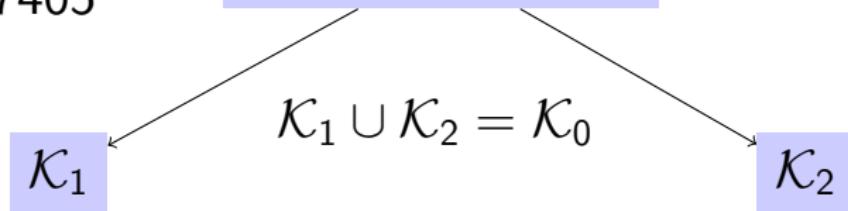
$$\phi(C) \geq 0.60 \text{ for all } C \in \mathcal{K}_0$$

Branch and Bound algorithm

want:

$$\phi(C) \geq 0.7405$$

$$\mathcal{K}_0 = \{\text{all shapes}\} \quad 0.60$$

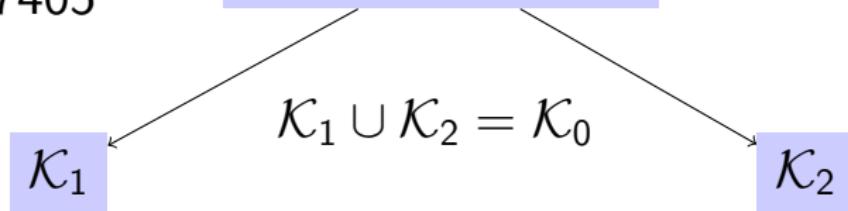


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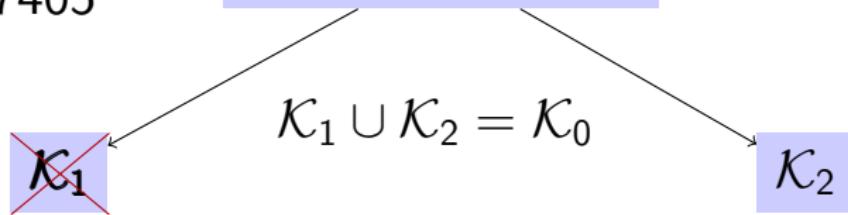
$$\phi(C) \geq 0.80 \text{ for all } C \in \mathcal{K}_1$$

Branch and Bound algorithm

want:

$$\phi(C) \geq 0.7405$$

$$\mathcal{K}_0 = \{\text{all shapes}\} \quad 0.60$$

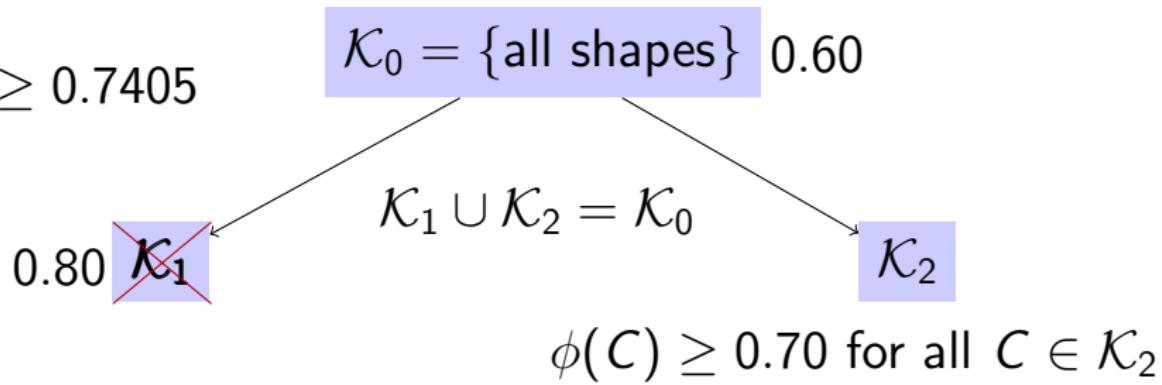


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Branch and Bound algorithm

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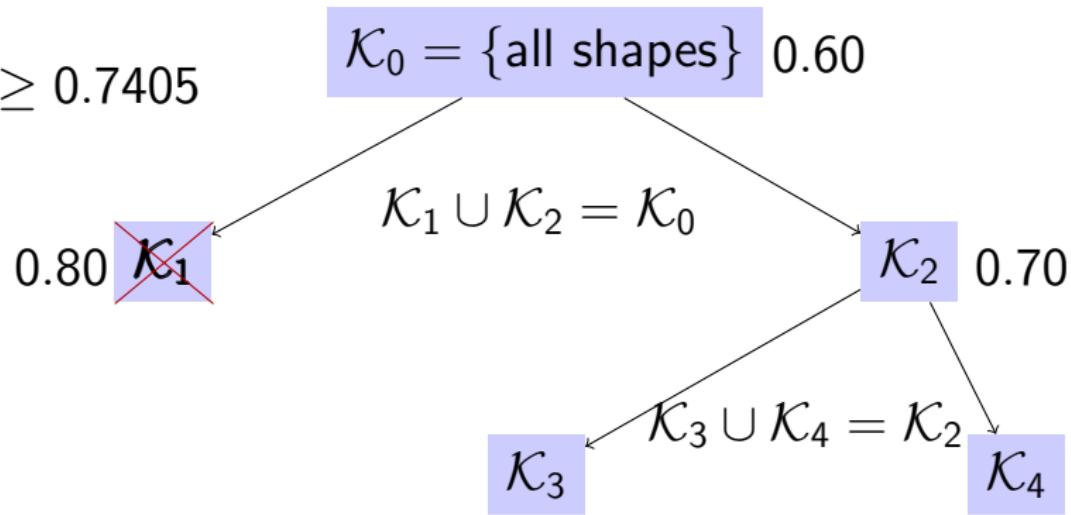
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Branch and Bound algorithm

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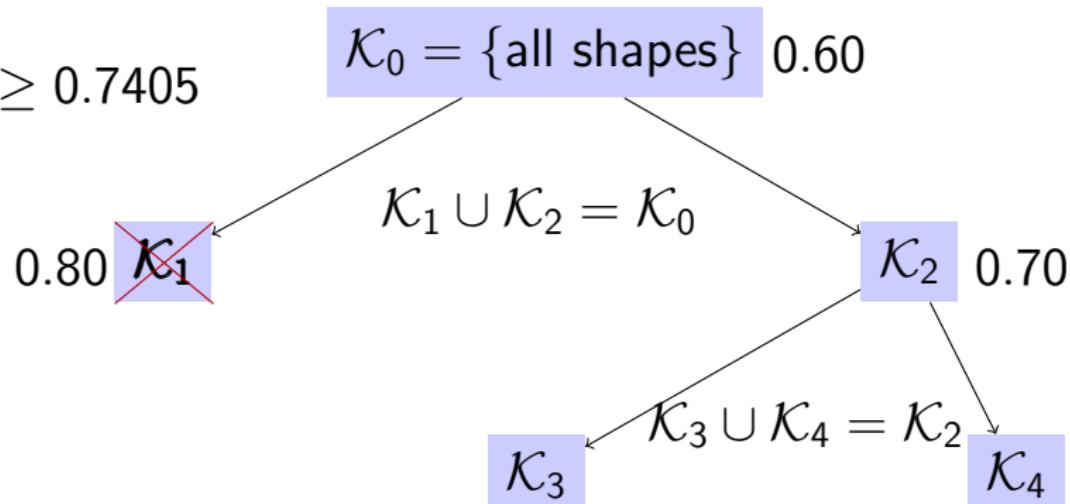
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Branch and Bound algorithm

want:

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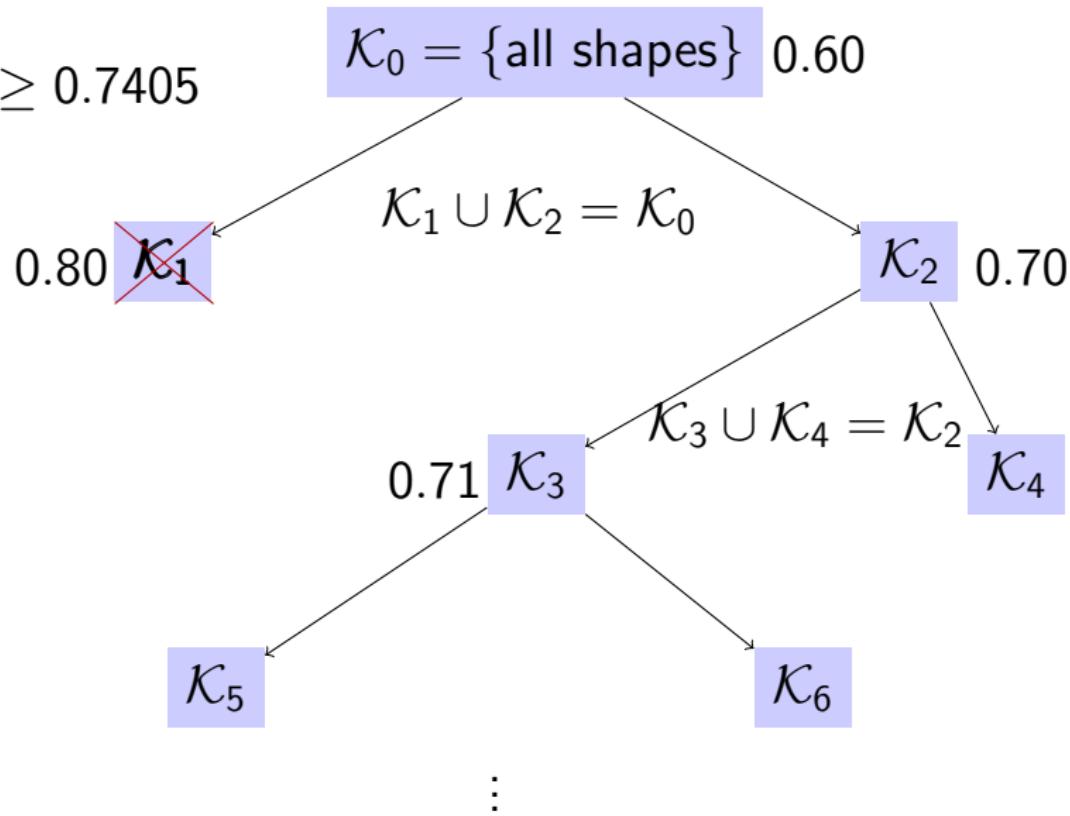


$$\phi(C) \geq 0.71 \text{ for all } C \in \mathcal{K}_3$$

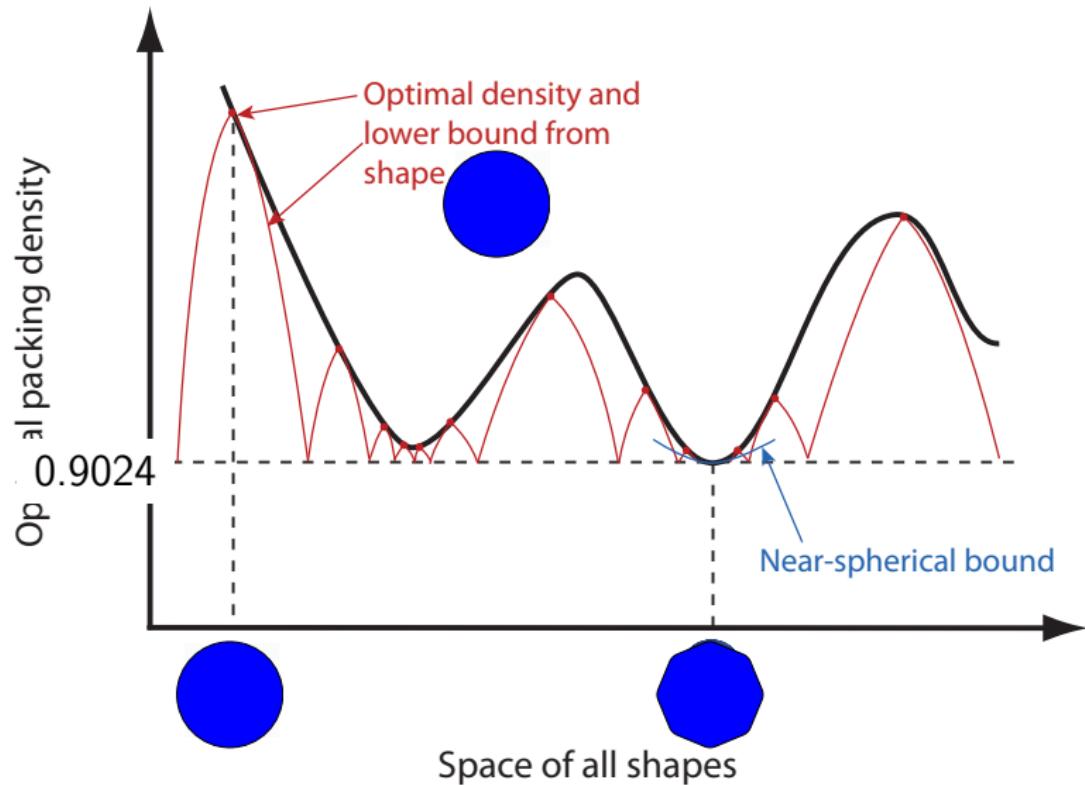
Branch and Bound algorithm

want:

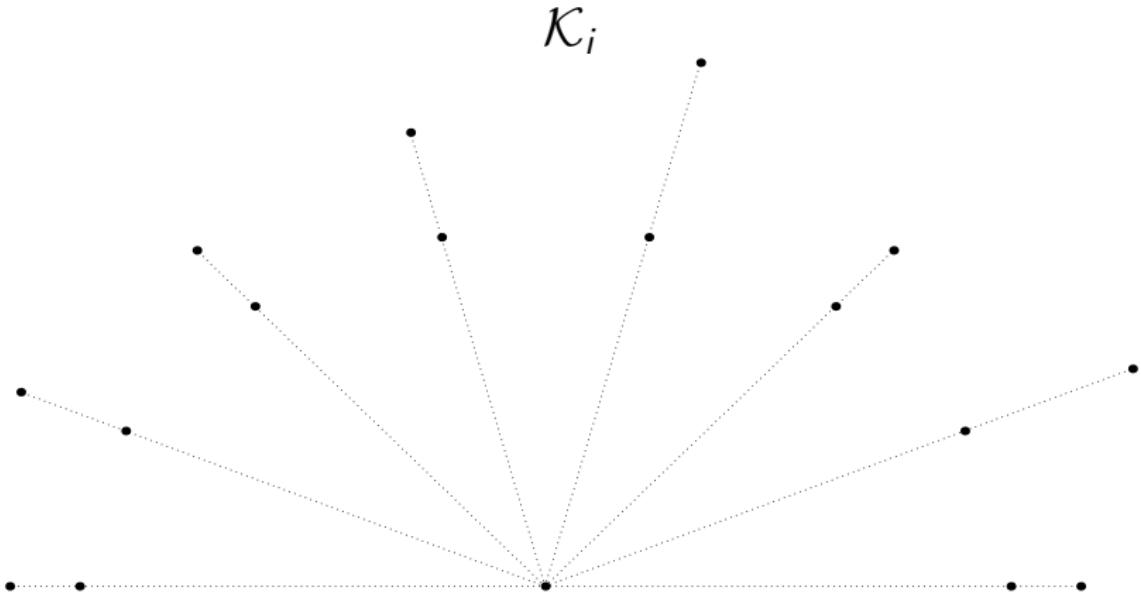
$$\phi(C) \geq 0.7405$$



Verification strategy

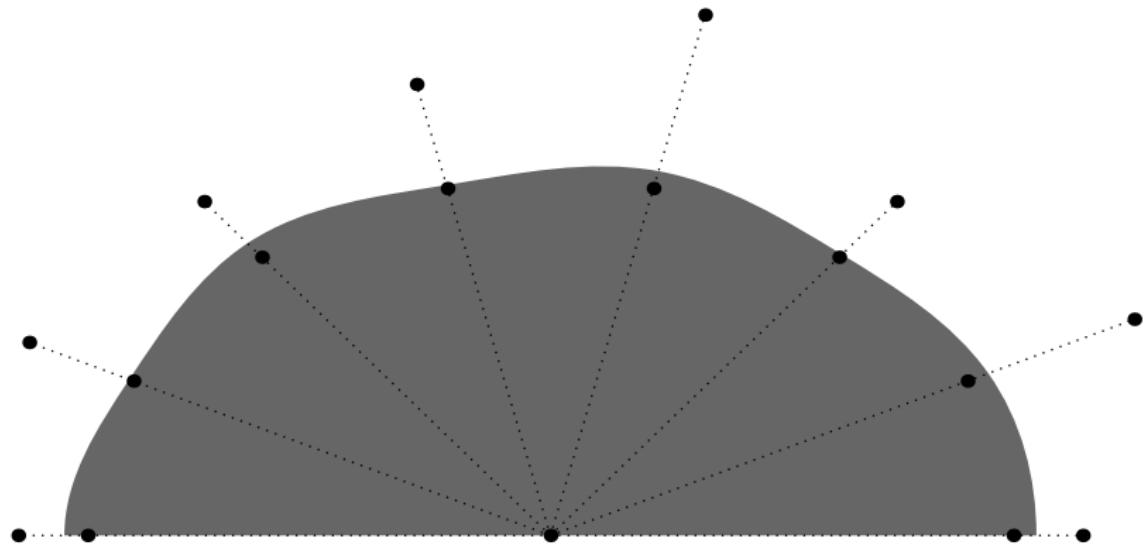


Node representation



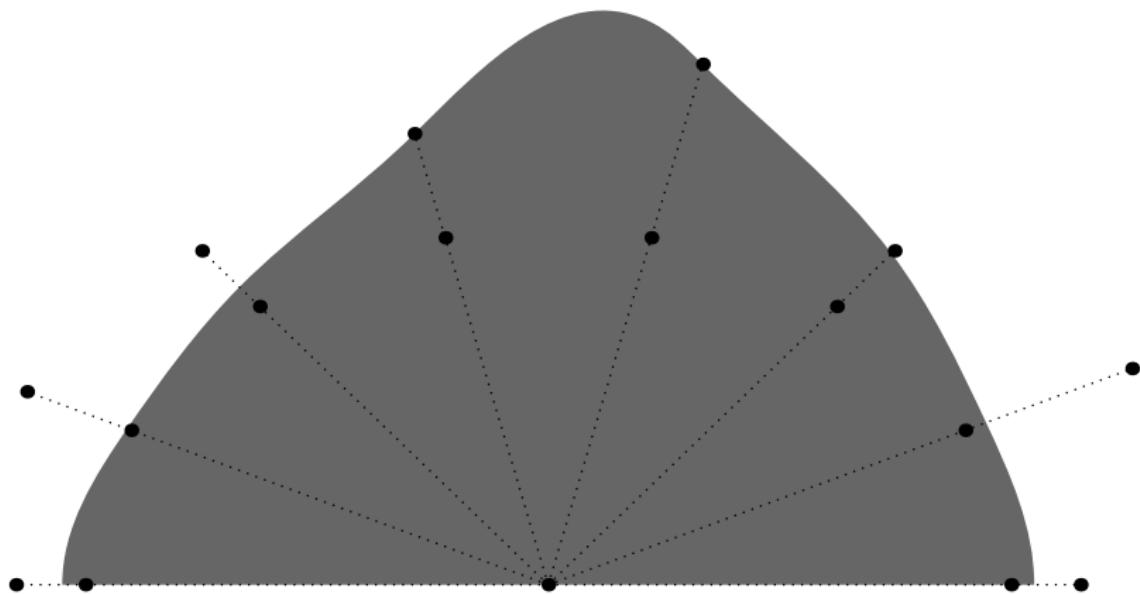
Node representation

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



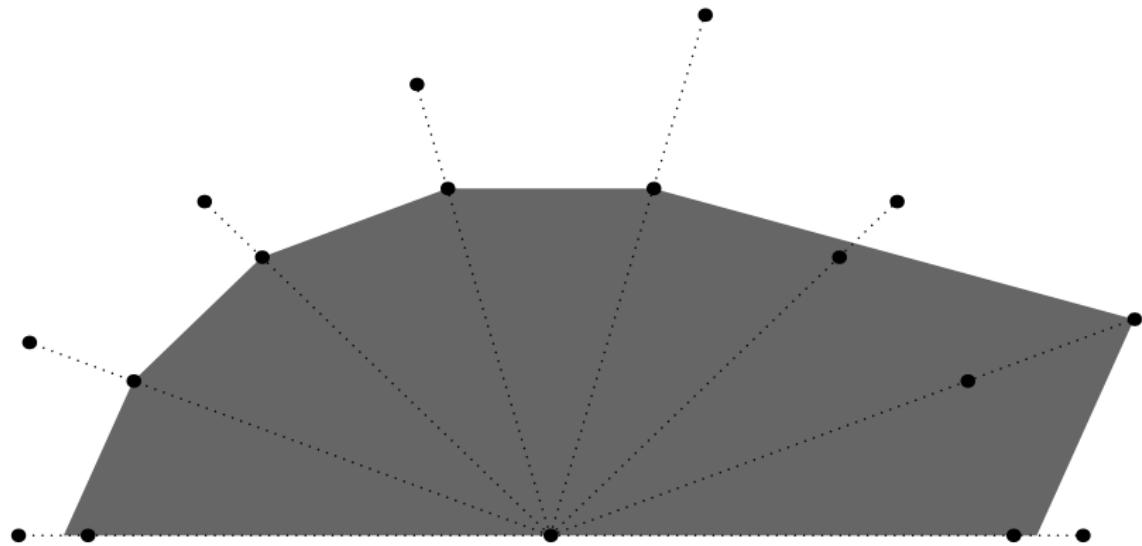
Node representation

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



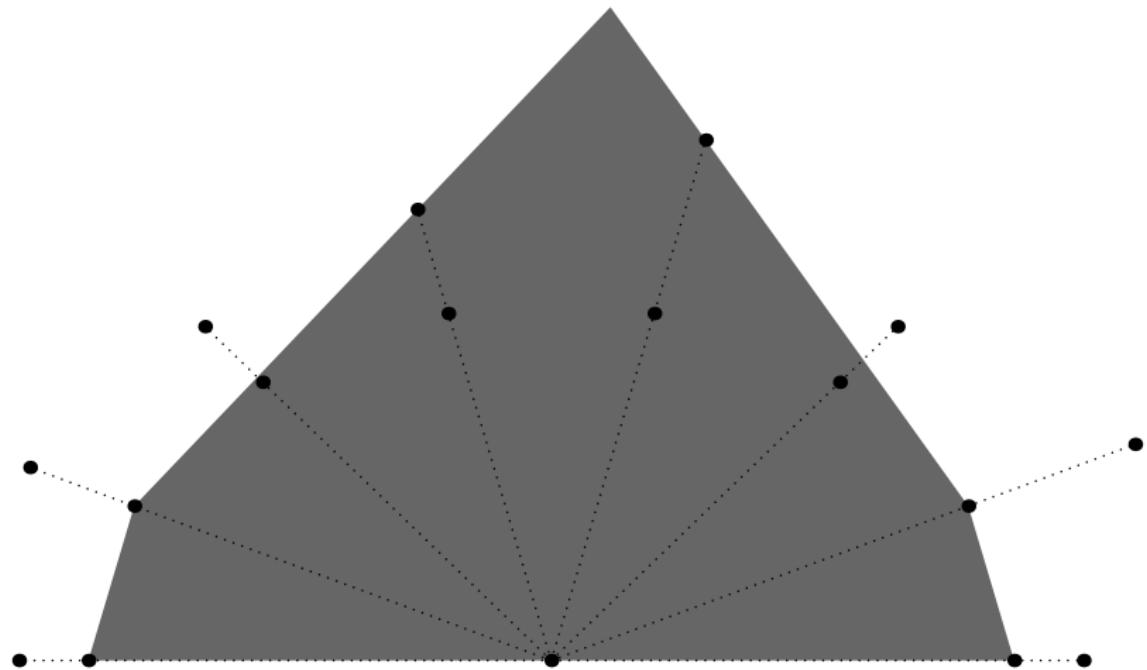
Node representation

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



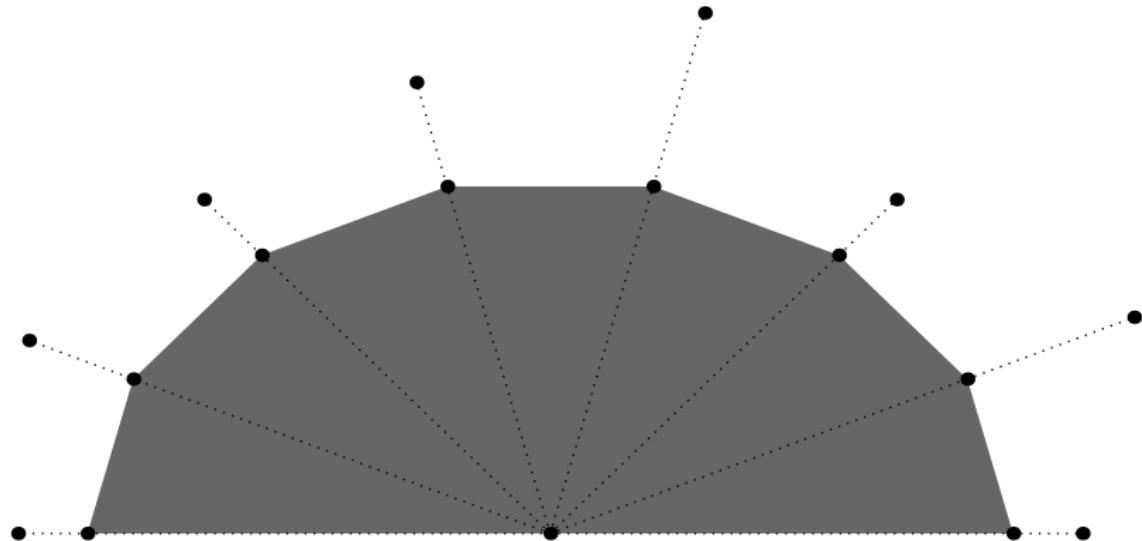
Node representation

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



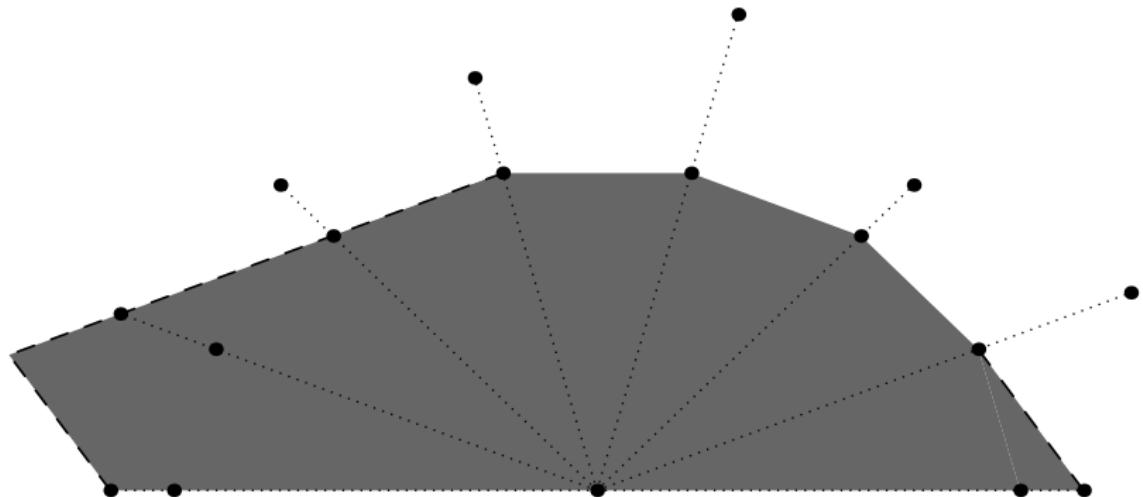
Bound setting – minimal body

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



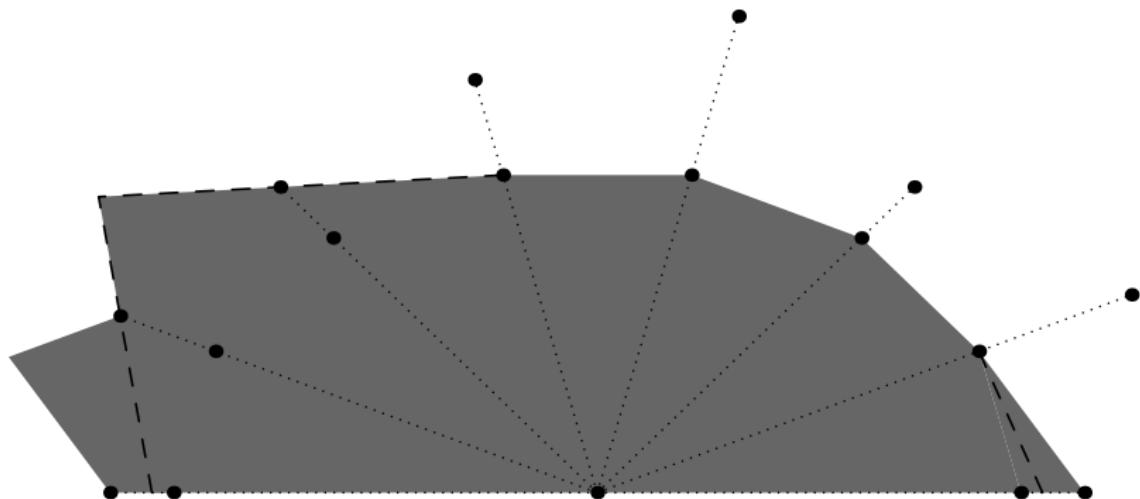
Bound setting – maximal body

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



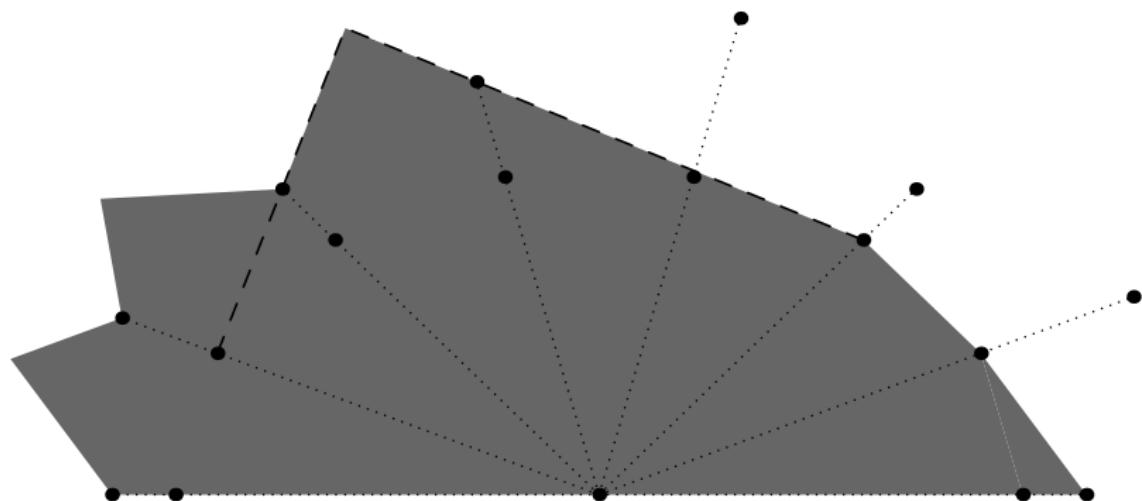
Bound setting – maximal body

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

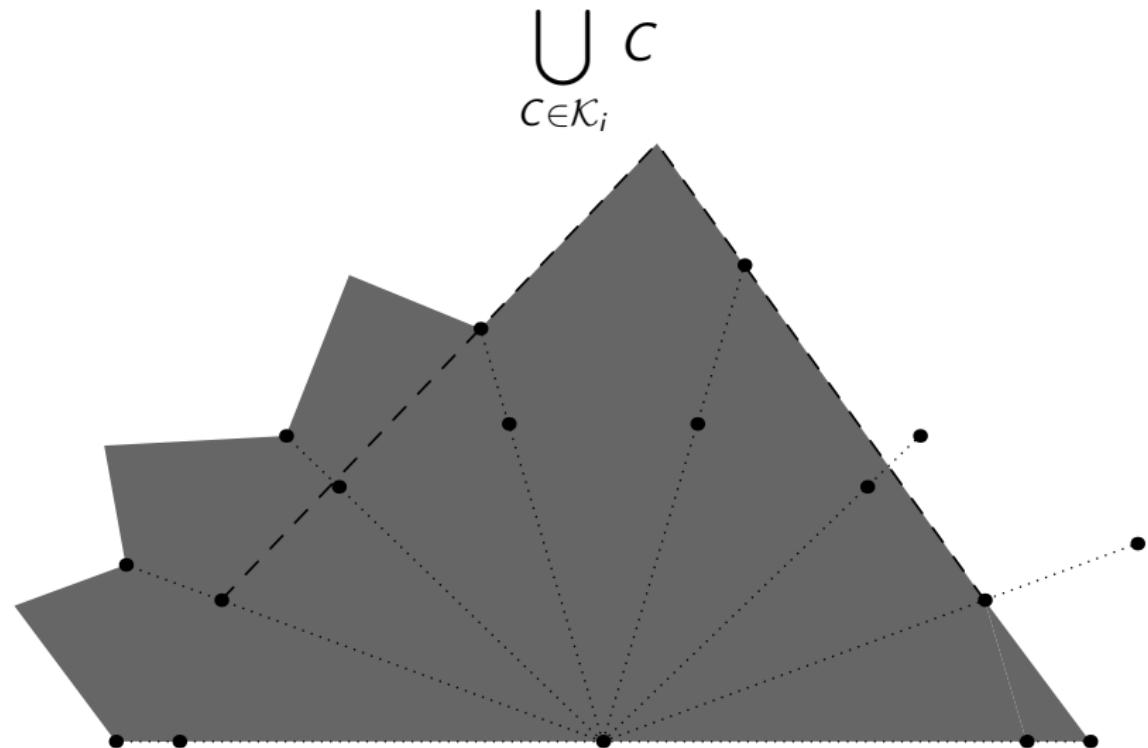


Bound setting – maximal body

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

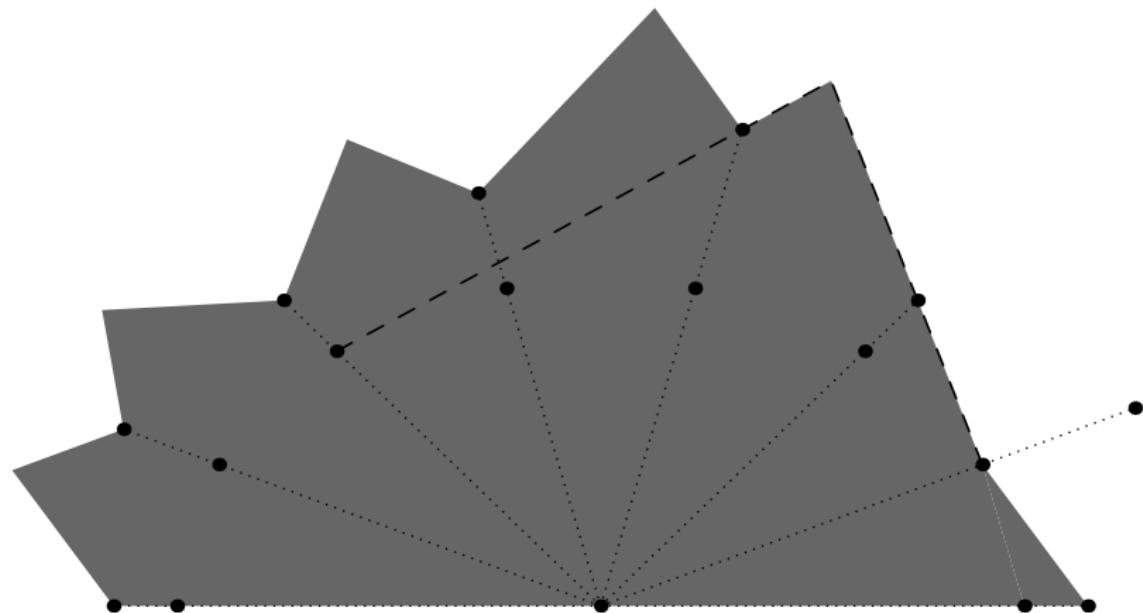


Bound setting – maximal body

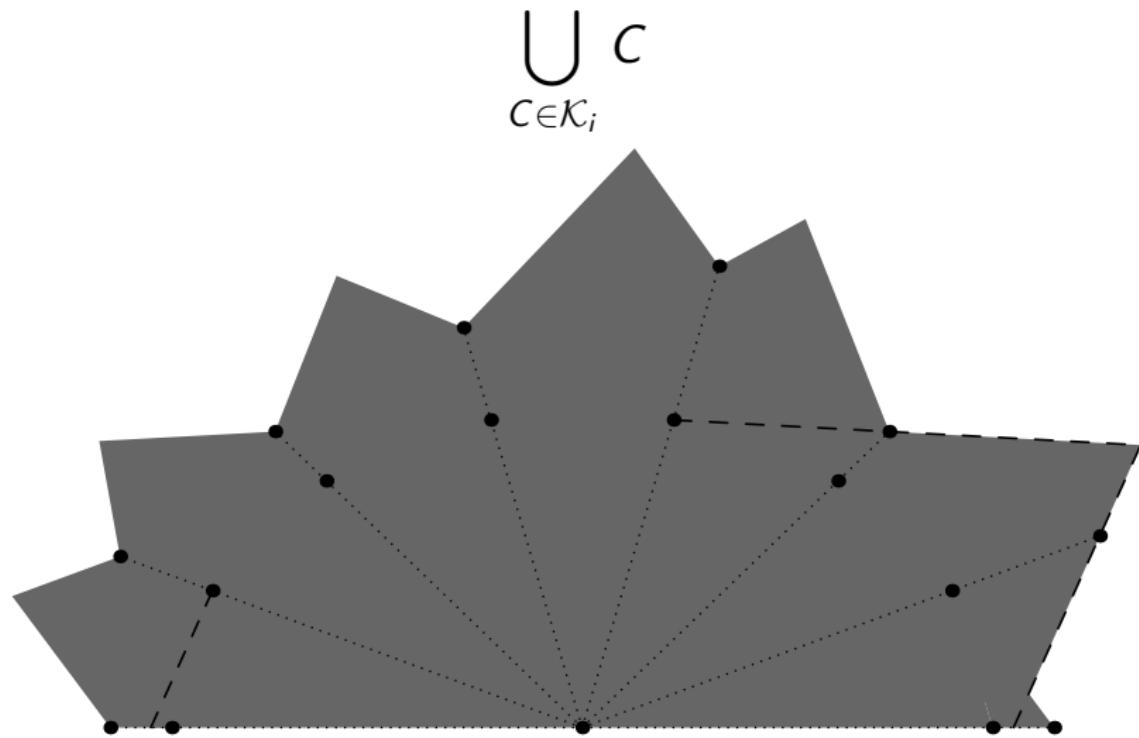


Bound setting – maximal body

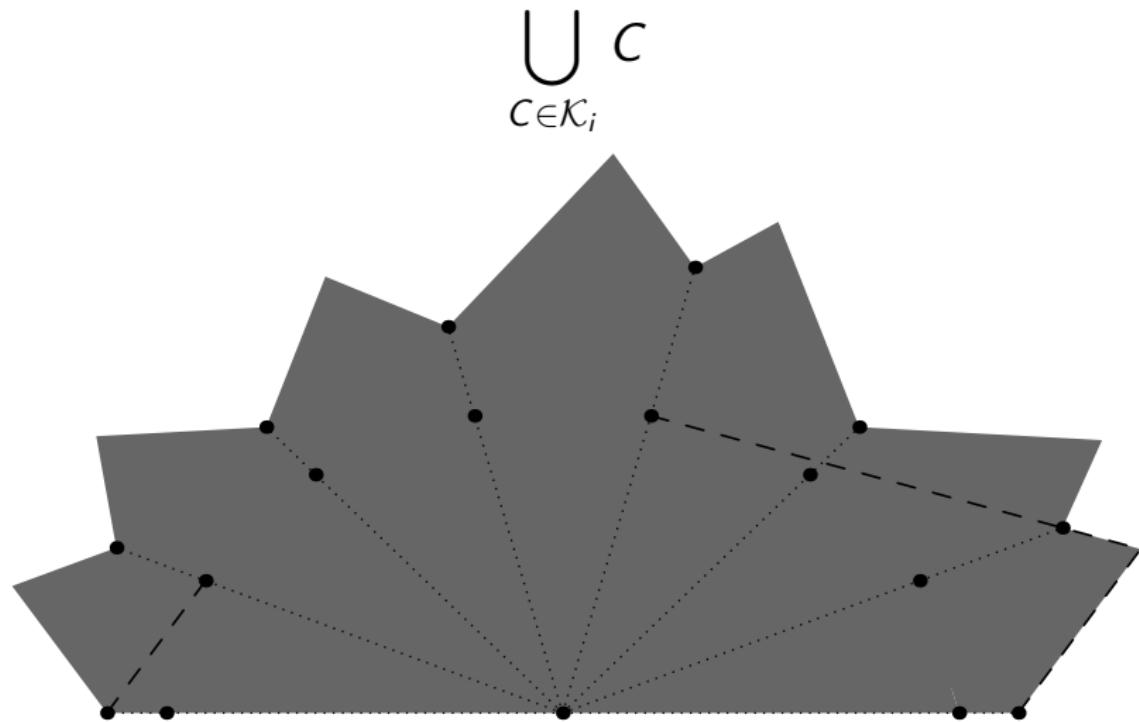
$$\bigcup_{C \in \mathcal{K}_i} C$$



Bound setting – maximal body

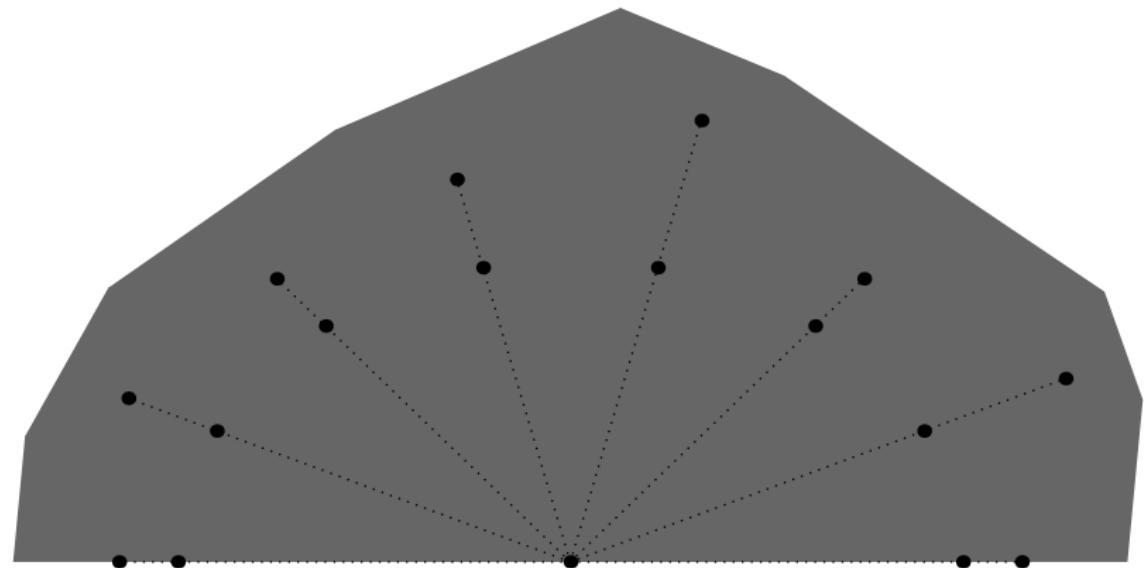


Bound setting – maximal body



Bound setting – maximal body

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



Bound setting

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

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

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

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

Bound setting

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

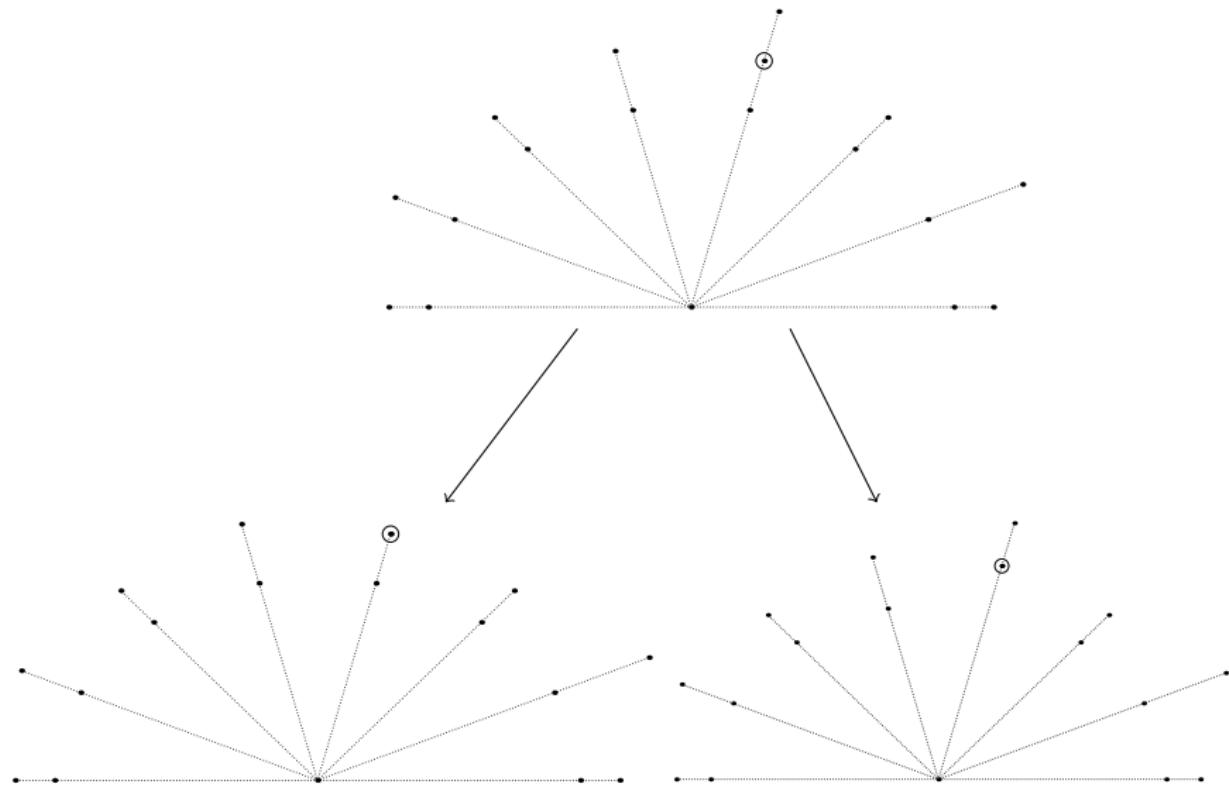
$$\phi(C) \geq \frac{\phi(C_{\max}) \text{area}(C_{\min})}{\text{area}(C_{\max})}$$

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

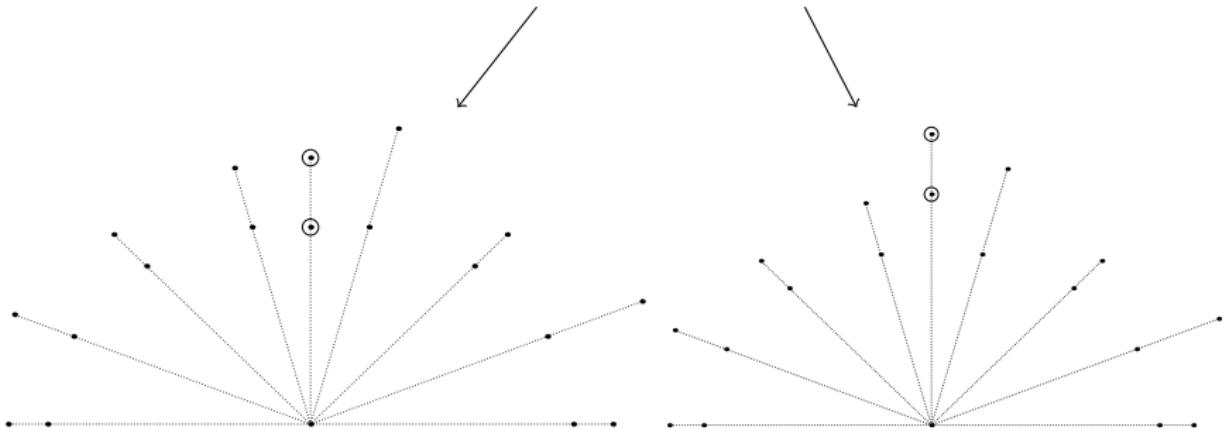
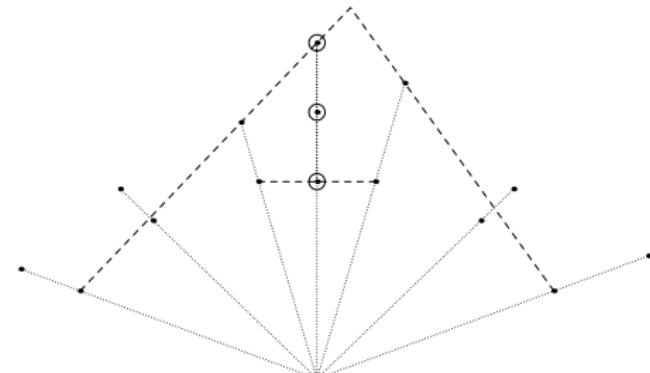
$O(n)$ algorithm to compute $\phi(C_{\max})$.

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

Splitting: no new radii



Splitting: adding a radius



Results

Disks: $\phi(B) = 0.9069$.

Conjecture: $\phi(C) \geq 0.9024$ for all C .

Ennola (1961): $\phi(C) \geq 0.8813$ for all C .

Tammela (1970): $\phi(C) \geq 0.8926$ for all C .

ϕ_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
ϕ_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}