Computer-assisted proofs: Packings in containers

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20/11 and 2/12/2025

1. Formalizing packings in containers
2. Bounds on objective value for square container
3. Homework I
4. Find candidate packings
5. Prove optimality by hand
6. Prove optimality by computer
7. Critical density
8. Homework II

"The Garden of Earthly Delights" Hieronymus Bosch, between 1490 and 1510

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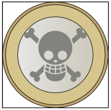
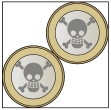
Place *n* identical coins in a smallest possible square solved for 1–33, 36 (1964–2021)

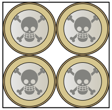
N=1



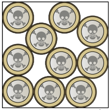
N=2



N=4

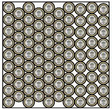


N=10

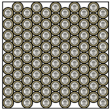


N=36

N=87



N=99



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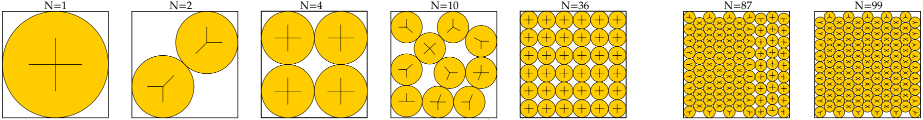

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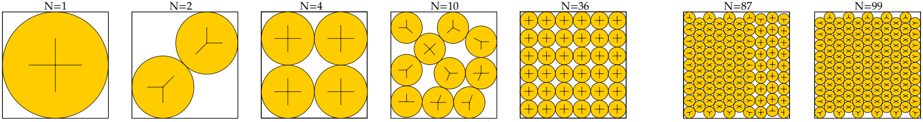
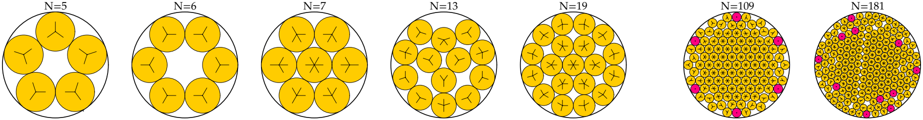


. . . circle solved for 1–13, 19 (1967–2003)



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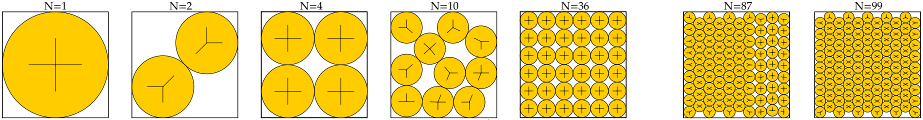

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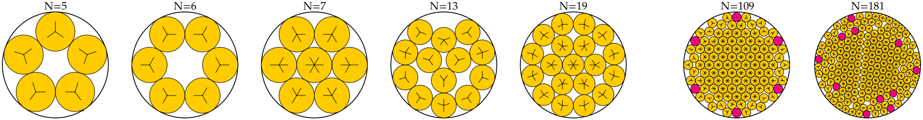

Find candidates: by hand for small n, billiard simulation, perturbation method

Prove optimality: by hand for small n and circles, interval analisys, branch-and-bound

Geometrical models: circular container

$P_n(r, R)$: the set of packings of n circles of radius r in a circle of radius R.

$$P_n(r, R) := \{\{c_i = (x_i, y_i)\}_{i=1}^n \text{ s.t. } |c_i| \leq R - r \text{ and } |c_i - c_j| \geq 2r \ \forall i, j\}$$

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$$r_n := \max_{P_n(r,1) \neq \emptyset} r$$

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$A_n(d, R)$: the set of arrangement of n points with pairwise distance at least d in a circle of radius R.

$$A_n(d, R) := \{\{p_i = (x_i, y_i)\}_{i=1}^n \text{ s.t. } |p_i| \leq R \text{ and } |p_i - p_j| \geq d \ \forall i, j\}$$

$\mathbf{\Pi_1'}$: $d = 1$ find the smallest circular containers such that n points with pairwise distance at least 1 fit inside.

$$R_n' := \min_{A_n(1,R') \neq \emptyset} R'$$

$\mathbf{\Pi_2'}$: $R = 1$ find the biggest d such that n with pairwise distance at least d fit inside unit circular container.

$$d_n := \max_{A_n(d,1) \neq \emptyset} d$$

Equivalence of geometrical models: $\Pi_1 \sim \Pi_2$

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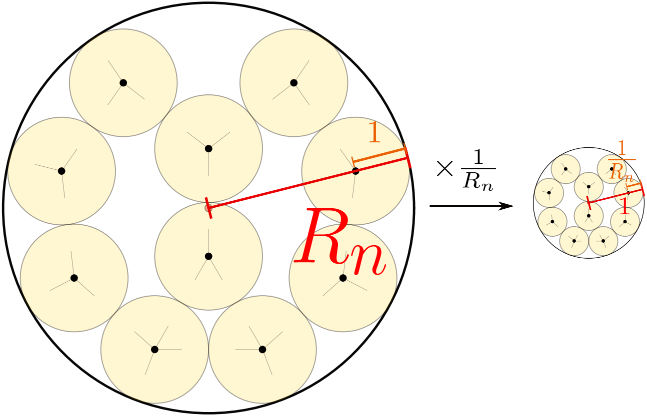
If $P \in P_n(1, R_n)$ then $\frac{1}{R_n} \times P \in P(r_n, 1)$, i.e., $r_n = \frac{1}{R_n}$.

If P is an optimal packing of n unit circles, then P deflated by R_n is an optimal packing of n circles in unit circular container.



Equivalence of geometrical models: $\Pi'_1 \sim \Pi'_2$

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If $A \in A_n(1, R'_n)$ then $\frac{1}{R'_n} \times A \in A(d_n, 1)$, i.e., $d_n = \frac{1}{R'_n}$.

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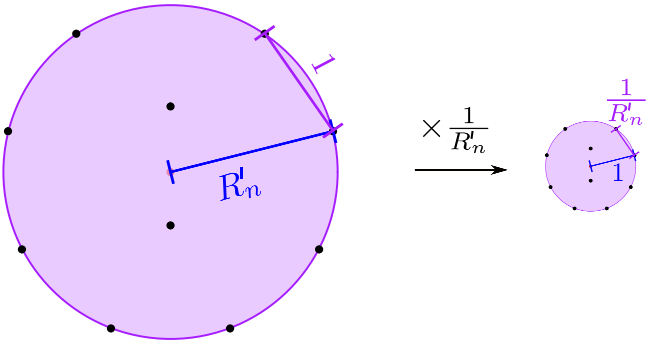

Equivalence of geometrical models: $\Pi_1 \sim \Pi_2'$

$\Pi_1' \sim \Pi_2'$

If $P \in P_n(1, R_n)$ then centers $\left(\frac{1}{R_n-1} \times P\right) \in A(d_n, 1)$, i.e., $d_n = \frac{2}{R_n-1}$.

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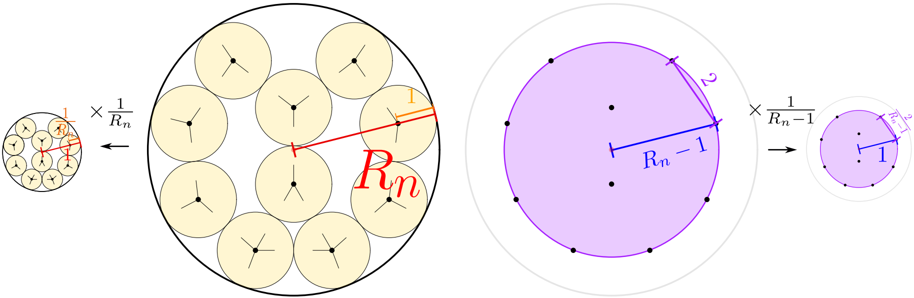

Geometrical models : circular container

Π_1 Place n unit discs in a circle of radius R_n minimize R_n .

Π_2 Place n equal discs of radius r_n in a unit circle maximize r_n.

$$r_n = \frac{1}{R_n}$$

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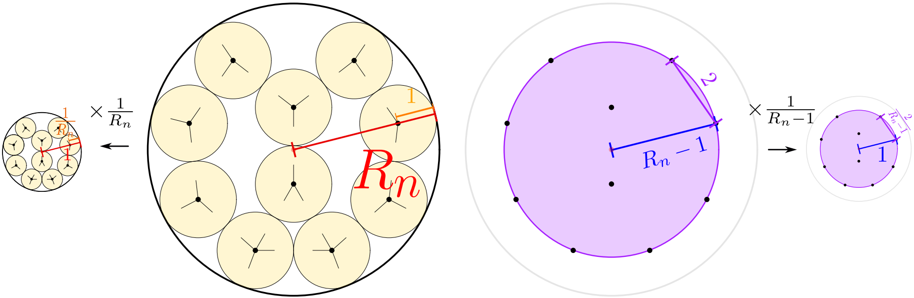


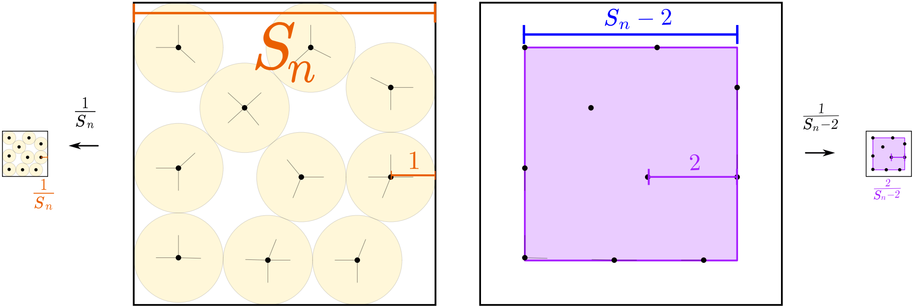
Geometrical models : circular or square container

Π_1 Place n unit discs in a circle (square) of radius R_n (of side S_n) minimize R_n (S_n).

Π_2 Place n equal discs of radius r_n in a unit circle (square) maximize r_n.

Π_2' Place n points in a unit circle (square) to maximize the min distance between points d_n.

$$r_n = \frac{1}{R_n}, \quad d_n = \frac{2}{R_n - 1} \quad \left(r_n = \frac{1}{S_n}, \quad d_n = \frac{2}{S_n - 2} \right)$$



Mathematical programming models

Maximize $d_n := \min_{1 \le i < j \le n} \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$

$0 \le x_i, x_j, y_i, y_j \le 1$

$0 \le x_i^2 + y_i^2,\ x_j^2 + y_j^2 \le 1$

max-min

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Maximize t

$t \le (x_i - x_j)^2 + (y_i - y_j)^2$ $\frac{n(n-1)}{2}$ non-convex constraints

$0 \le x_i, y_i \le 1$ $2n$ box constraints $\qquad$ $0 \le x_i^2 + y_i^2 \le 1$ n convex constraints

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What is a “solution”?

Numerical candidate: might be unfeasible (not a packing), “good” objective value

Candidate packing: feasible, good objective value but not proved optimal

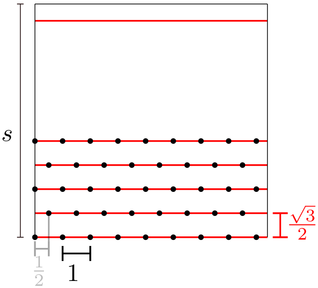
Validated enclosure of the optimum: all feasible, contains the optimum

Unique optimal packing: feasible, proved optimal

Lower bound on the maximal distance d_n

Lower bound on the optimal objective value: objective value of any feasible solution.

How to fit at least $\frac{2s^2}{\sqrt{3}}$ points at distance at least 1 in the square of side s for all $s \in \mathbb{R}^+$:



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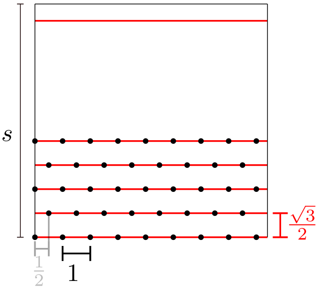

$N = \left\lfloor \frac{2s}{\sqrt{3}} \right\rfloor + 1$ red segments

$\lfloor s \rfloor + 1$ points on each odd segment

$\left\lfloor s - \frac{1}{2} \right\rfloor + 1$ points on each even segment

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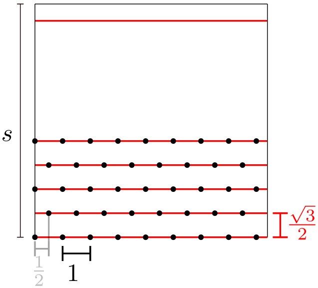

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number of points in the square:

if N is even, $\frac{N}{2}\left(\lfloor s \rfloor + 1 + \left\lfloor s - \frac{1}{2} \right\rfloor + 1\right)$

if N is odd, $\frac{N-1}{2}\left(\lfloor s \rfloor + 1 + \left\lfloor s - \frac{1}{2} \right\rfloor + 1\right) + \lfloor s \rfloor + 1$

in both cases, $\geq N\, s \geq \frac{2s^2}{\sqrt{3}}$

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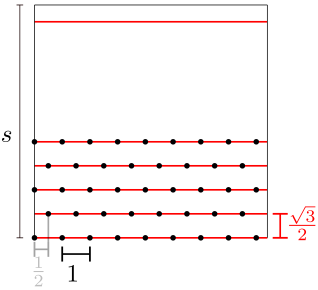

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$\times \frac{1}{s}$ $\Rightarrow$ fit at least $\frac{2}{d^2\sqrt{3}}$ points at distance at least d in the unit square for all d $(= \frac{1}{s})$

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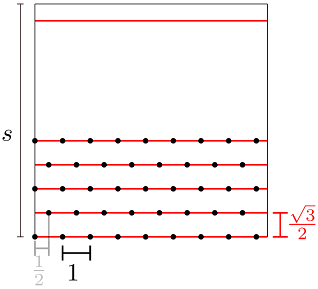

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$d = \sqrt{\frac{2}{n\sqrt{3}}}$ $\Rightarrow$ fit at least n points at distance at least $\sqrt{\frac{2}{n\sqrt{3}}}$ in the unit square for all n

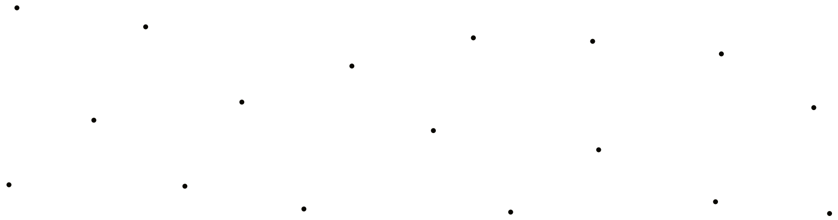
$$\Rightarrow \quad d_n \geq \sqrt{\frac{2}{n\sqrt{3}}}$$

Voronoi diagrams

Given $S \subset \mathbb{R}^2$ set of points,

Voronoi cell of point $p \in S$: $\mathrm{Vor}(p) := \{q \in \mathbb{R}^2 \mid \mathrm{dist}(q, p') > \mathrm{dist}(q, p)\ \forall p' \in S \setminus \{p\}\}$

Voronoi cell is **convex** polygonal domain (possibly unbounded)



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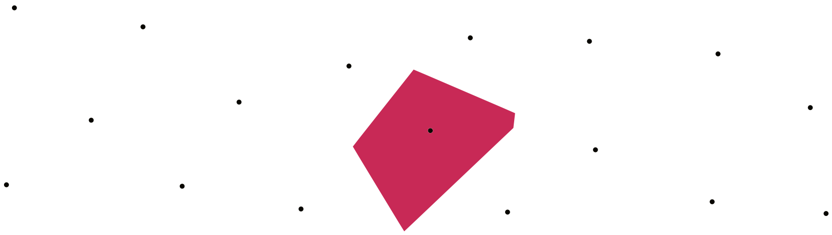

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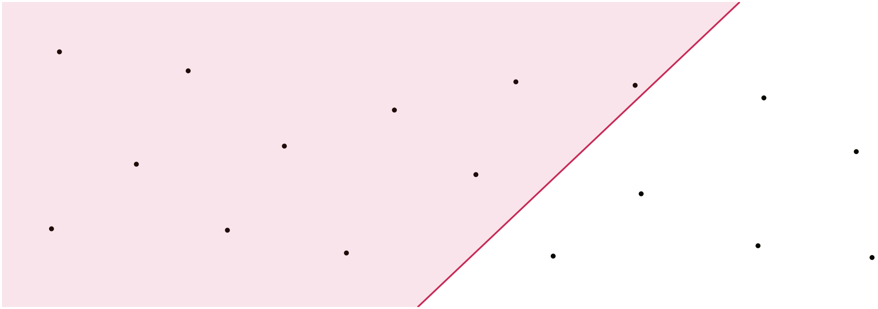

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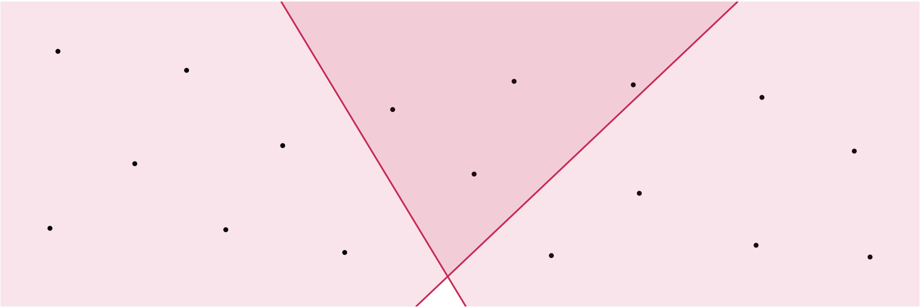

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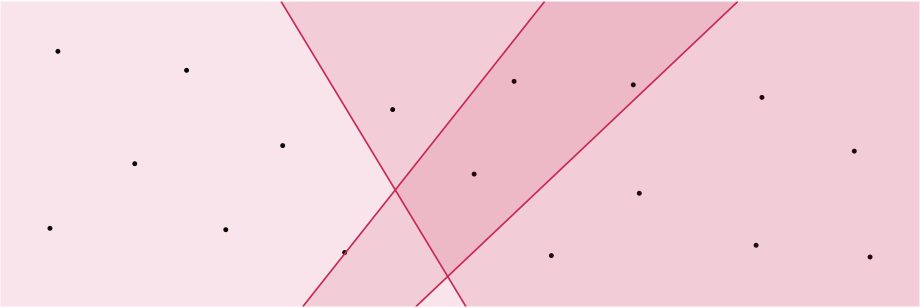

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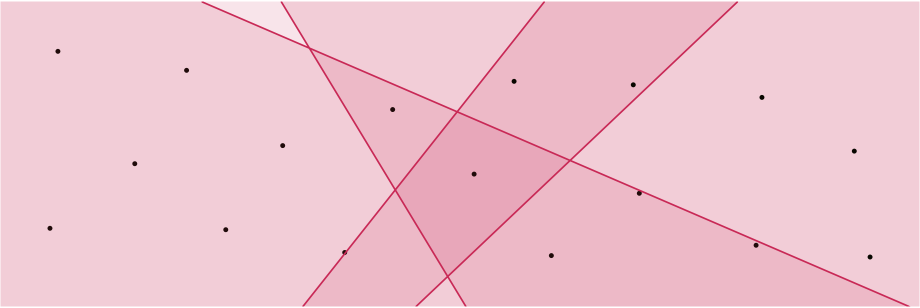

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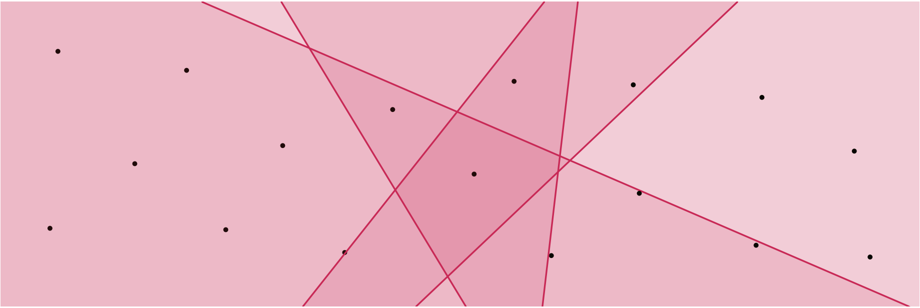

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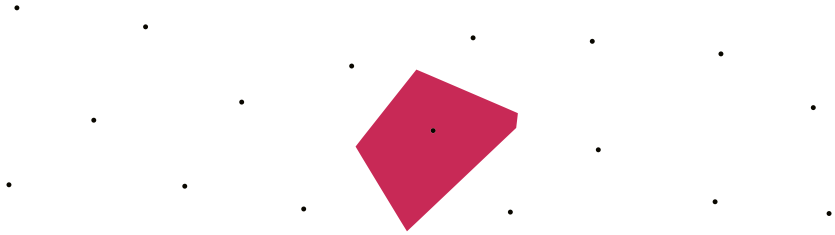

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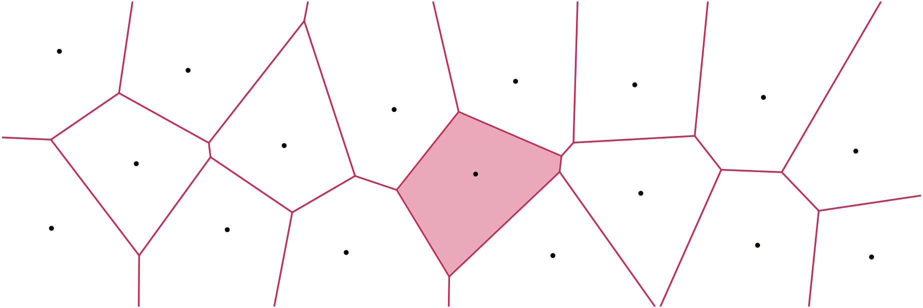

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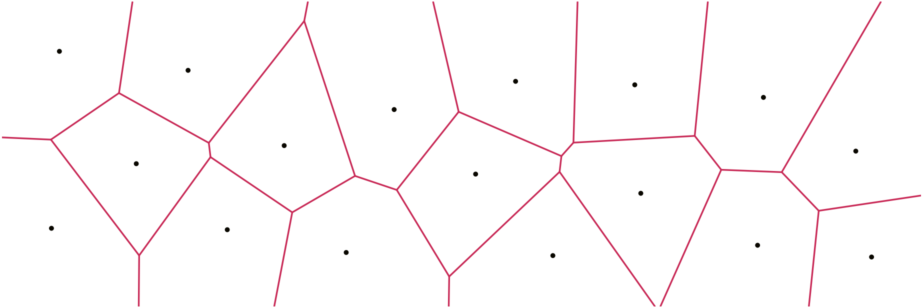

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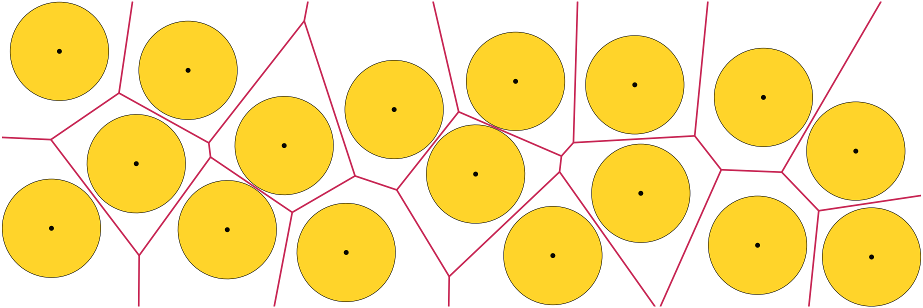
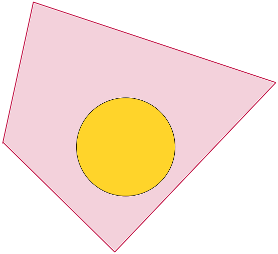


Voronoi diagram of a circle packing: Voronoi diagram of the circle centers

Smallest Voronoi cells in a circle packing

What is the Voronoi cell of smallest area in a packing of unit circles?



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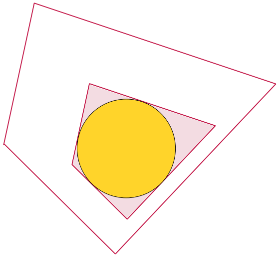

- circumscribed

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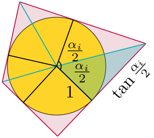

- circumscribed $\Rightarrow$ area $= \frac{\text{perimeter}}{2} = \sum_i \tan(\frac{\alpha_i}{2})$, $\sum_i \alpha_i = 2\pi$, $\quad tan\frac{x}{2}$ is convex $\Rightarrow$

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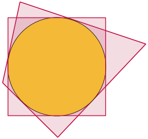

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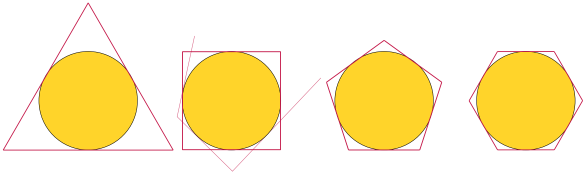

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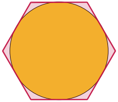
$H_1 :=$ 

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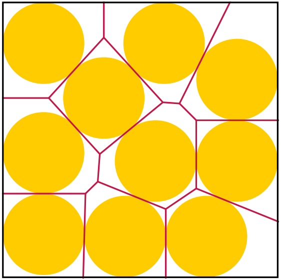
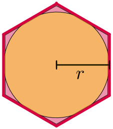
Upper bound on the maximal radius r_n

Voronoi cell of minimal area in a packing of r-circles: circumscribed regular hexagon H_r.



$H_r =$ 

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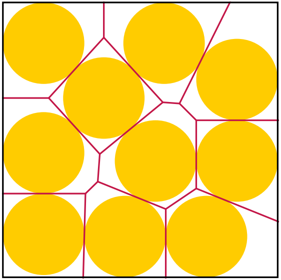

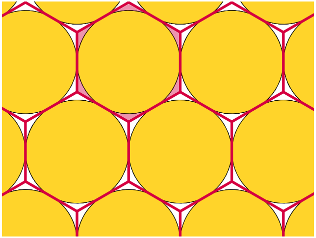

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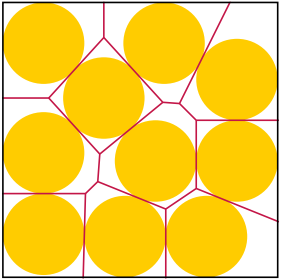
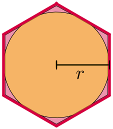


$H_r =$ 

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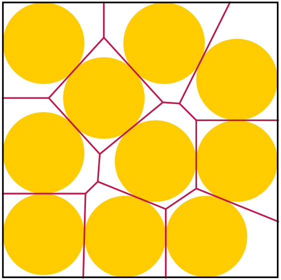
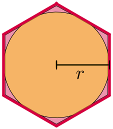


$H_r =$ 

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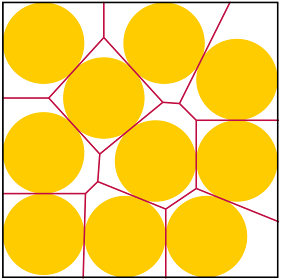
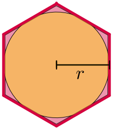


$H_r =$ 

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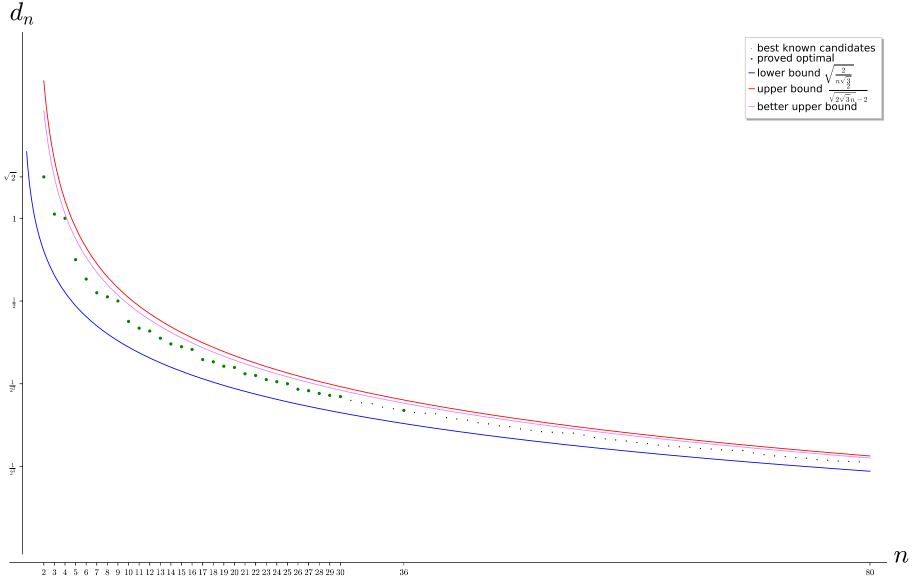
Bounds on d_n vs best known



20/11–25/11

1. Improve the upper bound on d_n in square container $\left(\frac{2}{\sqrt{2\sqrt{3}n-2}}\right)$.

2. * What is the best way to put discs of radii 1 and $\sqrt{2}-1$ in a 4×4 square? (best = cover most surface)

To be submitted by email to: daria.pchelina@ens-lyon.fr

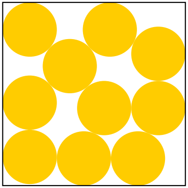
Deadline: beginning of next lecture (25/11, 15h45)

Perturbation method

Ball et al 2000: "new" candidates up to 200

- random *n* points in unit square, $\epsilon = \frac{1}{4}$
- for each point, perturb by ϵ to increase distance to the nearest neighbor
  repeat until no points to move
- $\epsilon = \frac{2\epsilon}{3}$
- stop when ϵ small

what it looks like



$d_{10} \approx 0.4212795439839, \quad r_{10} = 0.1482043225652$

Stuck in local optima $\Rightarrow$ need MANY iterations
what it looks like with 100 iterations

Billiard simulation

Graham and Lubachevsky 1996: "new" candidates up to 50
Start with an arrangement of n identic circles, of some initial radius, and random velocity vector.
Gradually inflate circles, until they can not move anymore.
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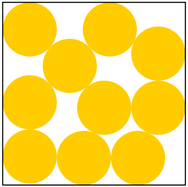

Modified Billiard Simulation or Pulsating Disk Shaking algorithm 2007
no initial velocities $\Rightarrow$ only store local interactions (circle-circle and circle-wall contacts)
improved $\approx$ 100 cases up to 200

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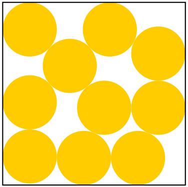

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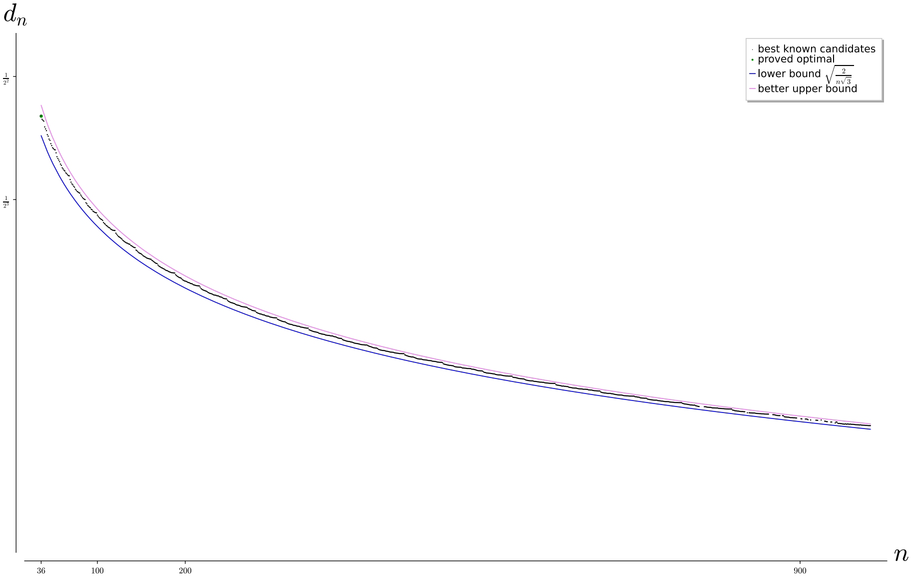
Modified Billiard Simulation or Pulsating Disk Shaking algorithm 2007
no initial velocities $\Rightarrow$ only store local interactions (circle-circle and circle-wall contacts)
improved ≈ 100 cases up to 200

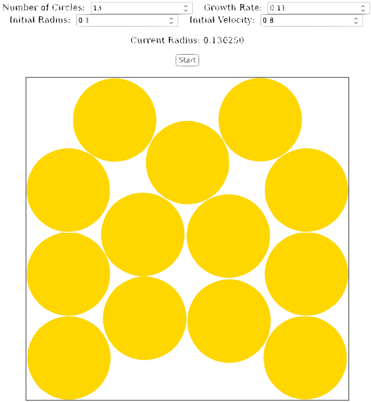
numerical candidate $\rightarrow$ feasible candidate: **interval arithmetic** in the ▶ Next Lecture

Known candidates: square container http://www.packomania.com/



From numerical candidate to feasible packing

Numerical candidate packing might be unfeasible due to rounding errors



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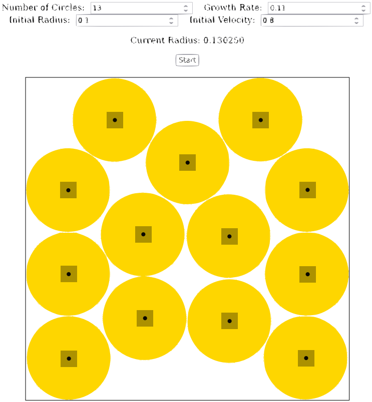

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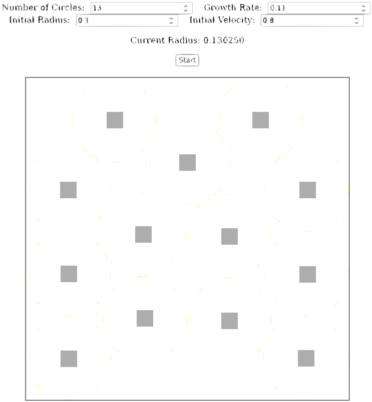

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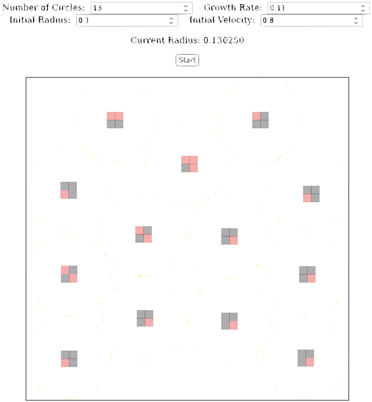

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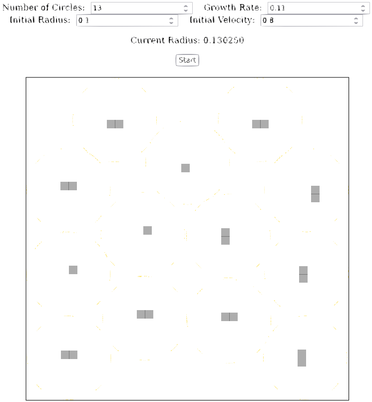
4. we got an enclosure of feasible packings



Circular container: $n \leq 7$

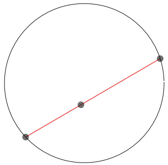
Lemma

If $n > 2$ points $a_1, \ldots, a_n$ lie in a unit disk then some pair points is at distance at most

$$\max(1, 2\sin(\frac{\pi}{n})).$$

Proof.

If point $x \in$ convex hull$(a_1, \ldots, a_k)$, then $d(x, a_j) < 1$ for some j.



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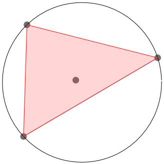

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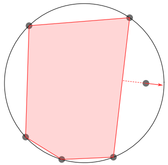

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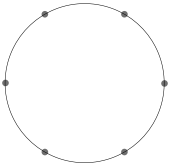

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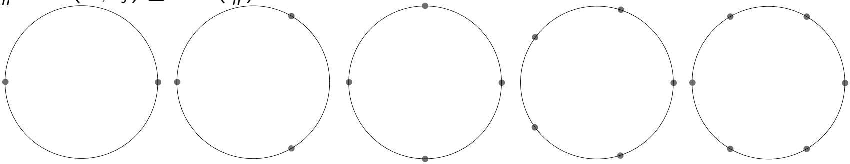

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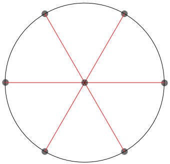

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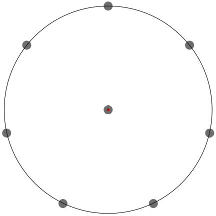
$n = 7$: 6 points on the boundary, 7th point in the center $d_7 = d_6 = 1$.

Circular container: $n = 8$ (rough idea)

Pirl 1969

Suppose we can do better than $d_8 = 2\sin\left(\frac{\pi}{7}\right)$ with < 7 points on the boundary.



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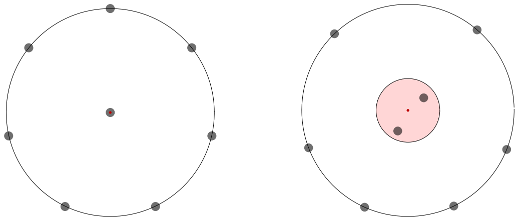
If 6 points on the boundary, then each pair of points at distance at least d_8, each arc is at least $\frac{2\pi}{7}$, then the maximal arc is at most $2\pi - 5\frac{2\pi}{7} = \frac{4\pi}{7}$ $\frac{2\pi}{7} \leq \phi \leq \frac{4\pi}{7}$



Circular container: $n = 8$ (rough idea)

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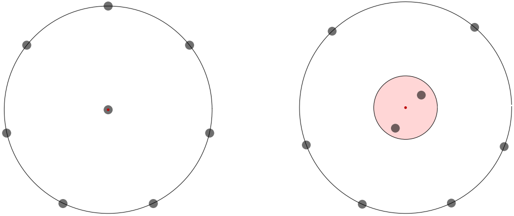
Each point not on the boundary should be at distance at most $1 - d_n^2$ from the center.
So, $d(O, x) \leq 1 - d_8^2 = 1 - 4\sin^2\frac{\pi}{7} < 1 - 4\sin^2\frac{\pi}{8} = \sqrt{2} - 1 < \sin\left(\frac{\pi}{7}\right)$

Thus, $d(x_1, x_2) < 2\sin(\frac{\pi}{7}) = d_8$: contradiction.



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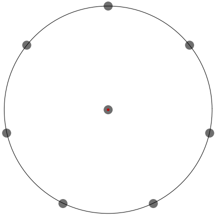
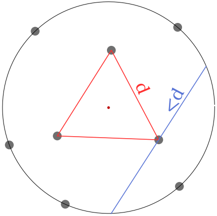
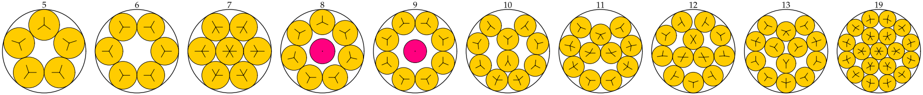
If < 6 points on the boundary, ≥ 3 points inside, separated by at least d_8.





Circular container: optimal packings

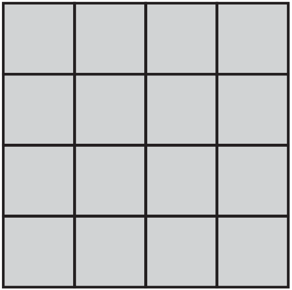
1–13,19



- Pirl 1969: 1–10
- Mellisen 1994: 11
- Fodor 2000: 12, 2003: 13, 1999: 19

Find certified enclosure of the optima: method of active cells

1. find a good lower bound $\underline{d}$ on d_n — $n = 10 : 0.42$
2. decompose the square into tiles of diameter $\leq \underline{d}$ — 16 squares $\frac{1}{4} \times \frac{1}{4}$
   at most one point in each tile



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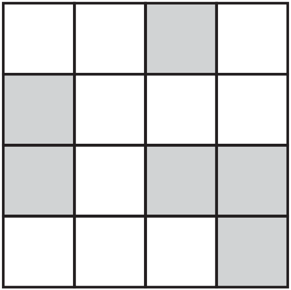

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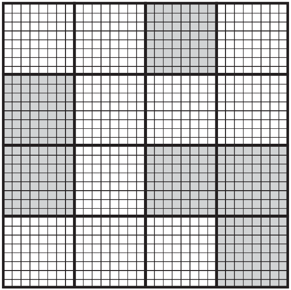

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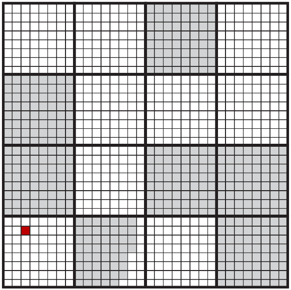

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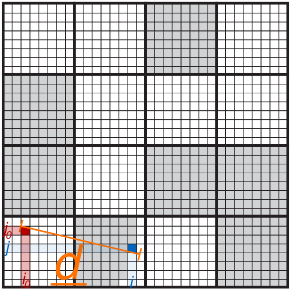

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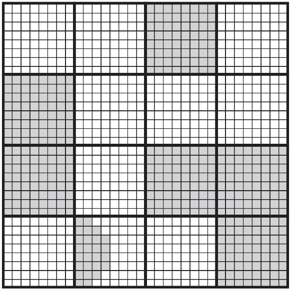

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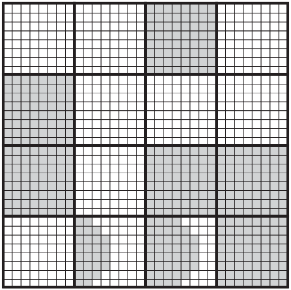

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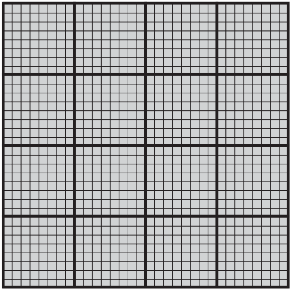

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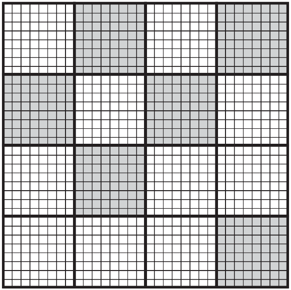

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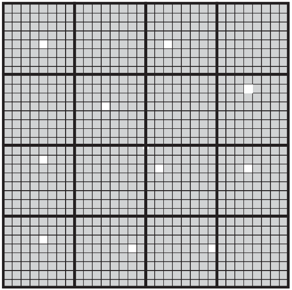
6. if active cells remain in all tiles, refine the grid: — cell $\rightarrow$ 4 cells



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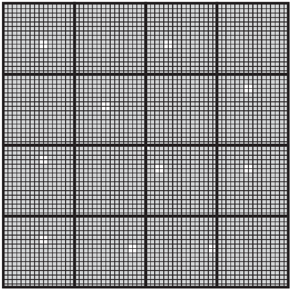

Prove optimality by computer

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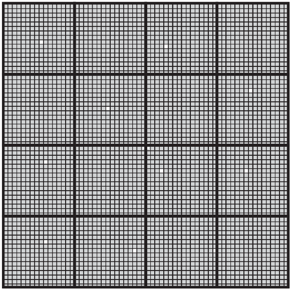
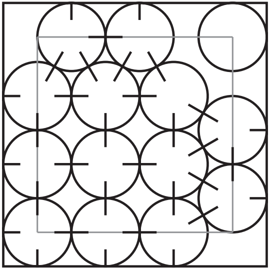
We got a validated enclosure of the optimum.



Proof of uniqueness (sketch): shrinking regions

Point arrangement → disk packing

1. "guess" tangencies of the optimal packing → get centers



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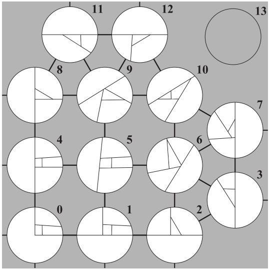

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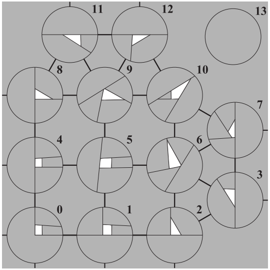

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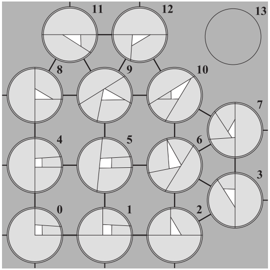

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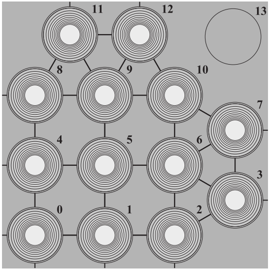

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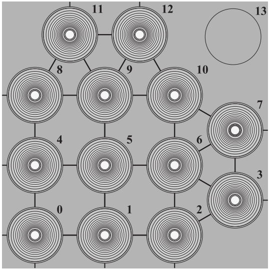
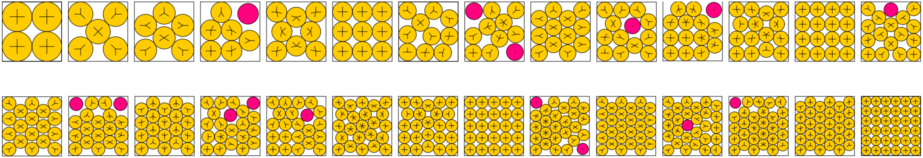
6. each sequence of concetric error-disks converges to the guessed center
7. the optimum is unique and coressponds to the guessed structure



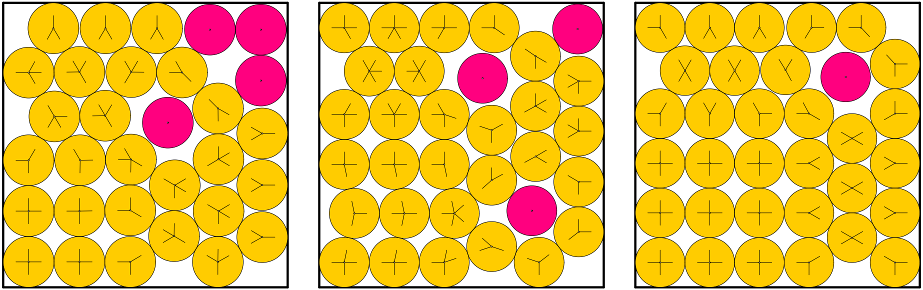
Square container: optimal packings

1–30, 36



- 1–9 by hand Schaer and Meir 1965, Schwartz 1970
- 14, 16, 25, 36 by hand Kirchner, Wengerodt 1983, 1987
- 10–20 computer-assisted Peikert, Wurtz, Monagan, de Groot 1990, 1992,
- 21–27 computer-assisted Nurmela, Östergård 1999
- 28–30 computer-assisted Markót, Csendes 2007
  28,29 — combinatorial structure, uniqueness in enclosures but no symbolic solution for coordinates

Square container: certified enclosures of the optimum



- 31–33 computer-assisted Markót 2022

tangencies might not all be present in the optimum

Circle Packing: given a set of n circles, can they be packed into a unit square?

Circle Placement: given a set of n circles, place their centers into a unit square.

Demaine, Fekete, Lang 2010

Circle Placement is NP-hard. $\Rightarrow$ Circle Packing is NP-hard.

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`3-Partition`: given a multiset of $3m$ integers, can it be partitioned into m triplets that all have the same sum?

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Restricted 3-Partition: $\frac{T}{4} < x_i < \frac{T}{2}$ where $\sum_{i=1}^{3m} x_i = mT$

Examples: $\{1, 2, 15, 15, 15, 42\}$:

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Restricted 3-Partition Problem is NP-hard. 1975

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Restricted 3-Partition: $\frac{1}{4} < x_i < \frac{1}{2}$ $\sum_{i=1}^{3m} x_i = m$ $\sum_{j=1}^{3} x_{i_j} = 1$

Examples: $\{1, 2, 15, 15, 15, 42\}$:Yes $\{\frac{4}{15}, \frac{4}{15}, \frac{4}{15}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}\}$(restricted):No

Restricted 3-Partition Problem is NP-hard. 1975

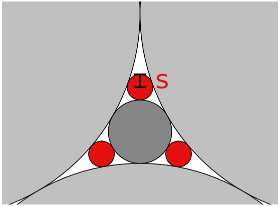
encoding 3-Partition into Circle Placement:

feasible partition iff $\forall(i_1, i_2, i_3)$ is feesible: $\sum_{j=1}^{3} x_{i_j} = 1$

$r_i := s - (\frac{1}{3} - x_i)\varepsilon^2$

circles of radii $(r_{i_1}, r_{i_2}, r_{i_3})$ can be packed into the pocket iff

(i_1, i_2, i_3) feasible



Circle Packing: given a set of n circles, can they be packed into a unit square?

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Demaine, Fekete, Lang 2010

Circle Placement is NP-hard. $\Rightarrow$ Circle Packing is NP-hard.

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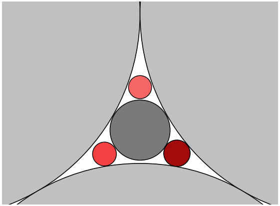

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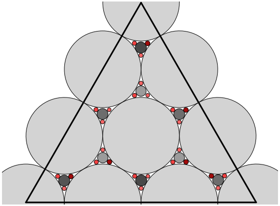

Packing disks (of different sizes) in a unit circle/square,

worst-case density D: ratio between the combined area of disks that can always be packed and the area of the container

if $\frac{\sum_{d \in S} \text{area}(d)}{\pi} \leq D$ then all disks in S will fit in the unit circle/square $\forall$ set of disks S

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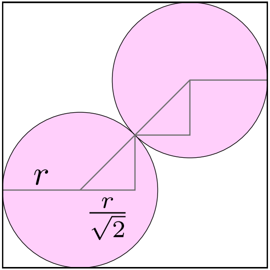
example: unit square

two disks of radius $r = \frac{1}{2+\sqrt{2}}$

density: $2\pi r^2 = \frac{2\pi}{(2+2\sqrt{2})^2} = \frac{\pi}{3+2\sqrt{2}}$

$\Rightarrow D_{\text{crit}} \geq \frac{\pi}{3+2\sqrt{2}}$



Disks in a square

Critical density for packing disks into a square is $\frac{\pi}{3+2\sqrt{2}} \approx 53.9\%$. Morr 2017

`Split Pack` algorithm sketch: divide-and-conquer

1. divide disks into two almost equal sum areas parts C_1, C_2 greedy
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3. `Split Pack` C_1 into T_1
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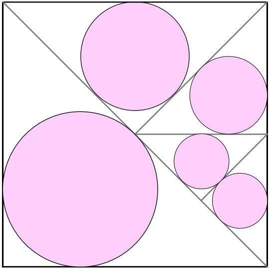

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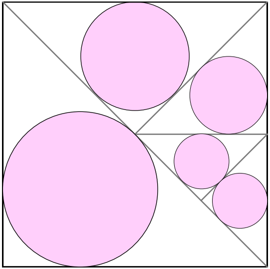

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`Split Pack` algorithm sketch: divide-and-conquer

1. divide disks into two almost equal sum areas parts C_1, C_2 greedy
2. split the region into two parts T_1, T_2 whose sizes depend on areas of C_1 and C_2
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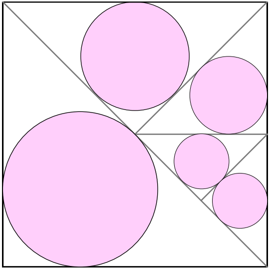
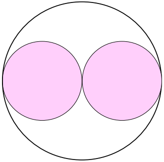


Critical density of disks in circle

two disks of radius $\frac{1}{2}$ density: $\frac{2\cdot\frac{\pi}{4}}{\pi} = \frac{1}{2} \Rightarrow D_{\text{crit}} \geq \frac{1}{2}$



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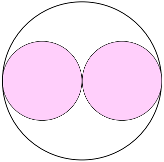

Critical density for packing disks into a circle is $\frac{1}{2}$. Fekete, Keldenich, Scheffer 2019

sketch of idea of algorithm: $r_1 \geq r_2 \geq \cdots \geq r_n$

1. boundary packing — glue disks to the interiour boundary
2. ring packing — layers of disks inside rings

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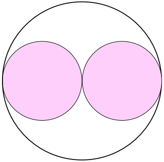

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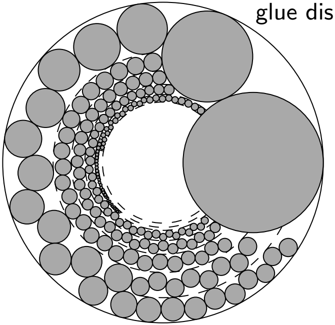

illustration from Fekete, Keldenich, Scheffer, SoCG 2019

```
rA,rB,rC = 1,1,1
ab_init = RIF(rA+rB, (rA+rB+2*rC)) # RIF(x,y)=smallest interval containing
    [x,y]
bc_init = RIF(rC+rB, (rB+rC+2*rA))

area = lambda ab, bc: ab*bc/2
cov = lambda ab, bc: RIF(pi)/4*rB**2 + arctan(ab/bc)/2*rC**2 + arctan(bc/ab
    )/2*rA**2 # RIF(x) = smallest interval containing x
density = lambda ab, bc: cov(ab,bc) / area(ab,bc)

density_init = RIF(density(ab_init,bc_init))
max_lb_dens = density_init.lower() # lower bound of the interval

boxes = [(ab_init, bc_init)]
N = 1000
while len(boxes)>0 and N>0:
    N-=1
    box = boxes.pop()
    if density(*box).upper()>max_lb_dens:
        if density(*box).lower()>max_lb_dens:
            max_lb_dens = density(*box).lower()
        for new_box in [(new_ab, new_bc) for new_ab in box[0].bisection()
    for new_bc in box[1].bisection()]: # subdivide each interval
            boxes = boxes + [new_box]

print(min([density(*b).lower() for b in boxes]))
print(max([density(*b).upper() for b in boxes]))
```

Listing 1: SageMath code for homework

2/12–9/12

For these exercises, install SageMath (or use Sage on CoCalc).

1. What does the code do? Change one line to make the result much "better" without taking longer time. How to do the same for $r_A = \sqrt{2} - 1, r_B = 1, r_C = 1$? And $r_A = 1, r_B = \frac{2}{\sqrt{3}} - 1, r_C = 1$?

2. * Write the code doing the same when $r_A = \sqrt{2} - 1, r_B = 1, r_C = 1$ without constraint on angle $\widehat{ABC}$.

3. * Formally prove that `Circle Packing` is NP-hard.

   Demaine, Fekete, Lang 2010: `https://arxiv.org/abs/1008.1224`.

LaTeX-generated pdfs, txt, anything except handwriting to be submitted by email to: daria.pchelina@ens-lyon.fr

Deadline: beginning of the lecture in one week (9/12, 15h45)