A nonsmooth program for jamming hard spheres

Peter Hinow

Department of Mathematical Sciences, University of Wisconsin - Milwaukee, P.O. Box 413, Milwaukee, WI 53201-0413, USA; email: hinow@uwm.edu

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Luke 6:38

Give, and it will be given to you. A good measure, **pressed down, shaken together** and running over, will be poured into your lap. For with the measure you use, it will be measured to you.

Experiments: Bernal (1960), Scott (1960)

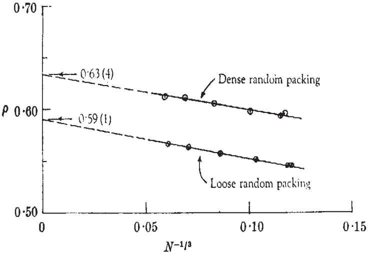


Fig. 1. Packing density for steel balls in glass flasks. Packing density (ρ) versus $N^{-1/3}$. N is the number to fill the flask

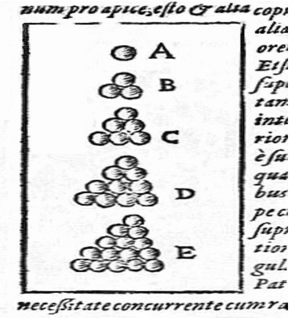
Fig. 5. Portion of random close packed ball assembly showing marks of further contacts

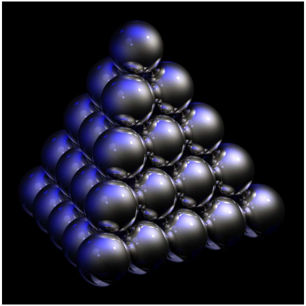
There exists a "universal" volume packing fraction of

$$\phi = \frac{vol(\text{spheres})}{vol(\text{container})} \approx 0.64$$

for random dense packings of large numbers of spheres.

The end of the spectrum



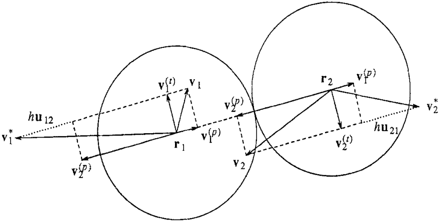


Johannes Kepler (1611) conjectured and Thomas Hales (1998, 2005) proved that the optimal density of a sphere packing in $\mathbb{R}^3$ is

$$\phi_{max} = \frac{\pi}{\sqrt{18}} \approx 0.74048.$$

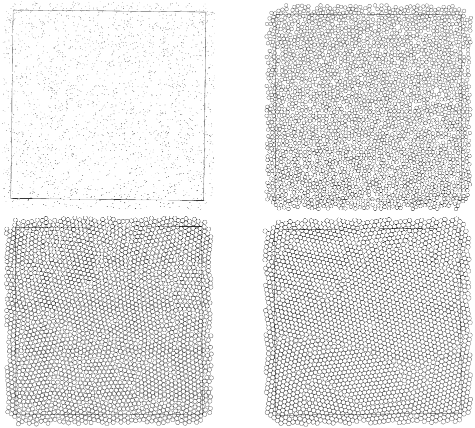
Simulation method: Lubachevsky & Stillinger (1990)

The "stochastic billiard" method



Growing spheres of radius $r(t) = at$ collide with each other and the walls until the collision frequency exceeds a threshold.

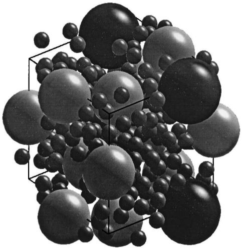
Results

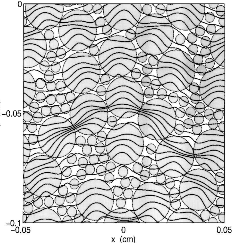


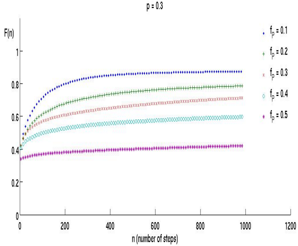
J. Stat. Phys. **60**:561 (1990)

Disadvantage: this is a parameter dependent protocol. A small growth rate *a* produces crystalline, regular substructures.

Applications of random dense sphere packings



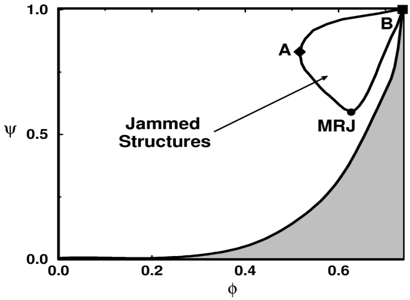




Buckmaster *et al.* (2001): Combustion of solid rocket propellant,
Baeumer *et al.* (2009): Release kinetics of matrix tablets,
Diaconis *et al.* (2009): Phase transitions in statistical mechanics.

Maximally random jammed states: Torquato *et al.* (2000)

Density and randomness are at variance with each other and an increase in one must come at the cost of a decrease of the other.



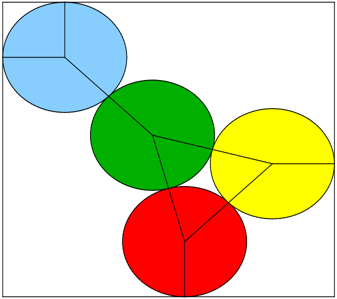
Phys. Rev. Lett. **84**:2064 (2000)

Torquato *et al.* suggest to minimize an "order parameter" ψ among all jammed packings.

Jammed sphere packings

A packing of finitely many spheres in a container is *(collectively) jammed* if no subfamily of spheres can be displaced continuously while fixing the positions of all other spheres.

Is that easy to see?



Jammed sphere packings

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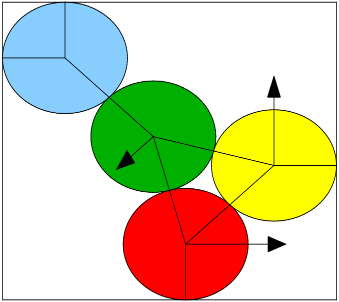
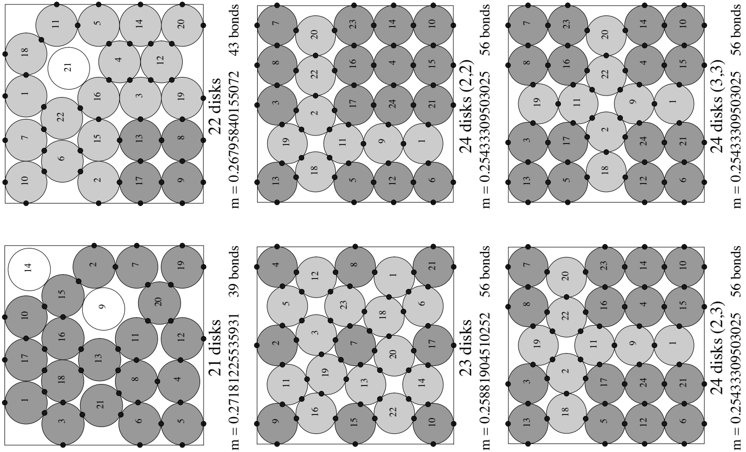


This packing is **not** collectively jammed.

Densest known (!) disk packings up to $n \approx 100$



Lubachevsky & Graham. *Electron. J. Combin.* **3**:R16 (1996)

In some cases, optimality has been proved using computers.

The optimization approach

Minimize the smooth discrete *Riesz s-energy* of a configuration $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ of sphere centers

$$E_s(\mathbf{x}) = \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^s}$$

in the limit $s \to \infty$, when this energy approaches the nearest neighbor distances.

We will work instead with a nonsmooth objective function and try to find as many local extrema as possible.

r-admissible configurations

Let n be the number of spheres and

$$\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n) = (x_{11}, \ldots, x_{1d}, \ldots, x_{n1}, \ldots, x_{nd})$$

be a collection of n points $\mathbf{x}_j \in \mathbb{R}^d$, $d \geq 2$. We say that $\mathbf{x}$ is *r-admissible* for $r \geq 0$ if

$$|\mathbf{x}_i - \mathbf{x}_j| \geq 2r$$

for all $i, j = 1, \ldots, n$ with $i \neq j$ and

$$r \leq x_{ik} \leq 1 - r$$

for all $i = 1, \ldots, n$ and $k = 1, \ldots, d$.

The configuration space

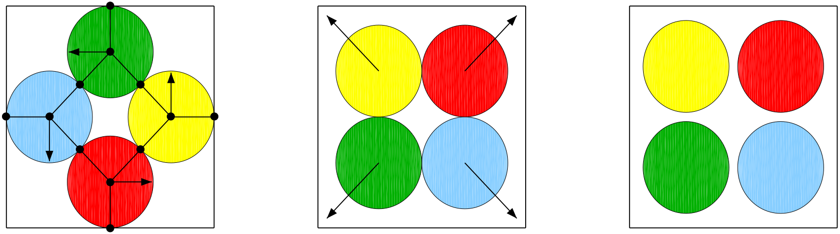
Denote by $M_n^d(r) \subset \mathbb{R}^{dn}$ the set of all r-admissible configurations of n distinct points in $[0,1]^d$. We say that r is *critical*, if there exists a $\varepsilon > 0$ such that for the numbers of connected components we have $\beta_0(M_n^d(s)) \neq \beta_0(M_n^d(t))$ for every $r - \varepsilon < s < r < t < r + \varepsilon$.
In particular, if $\beta_0(M_n^d(s)) > \beta_0(M_n^d(t))$, we speak of a *disappearance* and we call the set

$$C(r) = M_n^d(r) \setminus \overline{\bigcap_{t>r} M_n^d(t)}$$

a *critical set* (this is the union of all disappearing connected components at the critical radius r).

Disappearances

We call a point $\mathbf{x} \in C(r)$ a *partially jammed* configuration of spheres and an isolated point of $C(r)$ a *fully jammed* configuration of spheres.
Note that $int\, C(r) = \varnothing$ excludes that the spheres can be displaced continuously so that eventually they all loose contact with the walls and each other and the radius can be increased.



The maximal radius function

Let

$$\varphi_{ij}(\mathbf{x}) = \frac{|\mathbf{x}_i - \mathbf{x}_j|}{2}, \quad i = 1, \dots, n-1,\, j = i+1, \dots, n,$$
$$\psi_{ik}(\mathbf{x}) = x_{ik}\,, \quad \psi^{ik}(\mathbf{x}) = 1 - x_{ik}\,, \quad i = 1, \dots, n,\ k = 1, \dots, d,$$

and let $\mathcal{F}$ be the set of these $N(n,d) := \dfrac{n(n-1)}{2} + 2nd$ functions.
Define $G : [0,1]^{nd} \to [0,\infty)$ by the lower envelope

$$G(\mathbf{x}) = \min_{f \in \mathcal{F}} \{f(\mathbf{x})\}\,.$$

This is the maximal r such that a sphere of radius r can be centered at every entry of the n-tuple $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ without violating any of the other spheres or the walls of the unit cube.

Local maxima of G

Lemma

If $\mathbf{x}^*$ is a local maximum of G, then $\mathbf{x}^*$ is a partially jammed configuration. If $\mathbf{x}^*$ is a strict local maximum of G, then it is fully jammed.

Proof. We have that $M_n^d(r) = G^{-1}([r, \infty))$. If there exists a $\delta > 0$ such that $G(\mathbf{x}) \leq G(\mathbf{x}^*)$ for all $\mathbf{x} \neq \mathbf{x}^*$ with $|\mathbf{x} - \mathbf{x}^*| < \delta$, then none of these $\mathbf{x}$ lies in $M_n^d(G(\mathbf{x}^*) + \varepsilon)$ for any $\varepsilon > 0$. $\square$

Nonsmooth Optimization

For a function G defined by a minimum selection of functions indexed by a set $\mathcal{L}$ let

$$\mathcal{L}(\mathbf{x}) = \{l \in \mathcal{L} \ : \ f_l(\mathbf{x}) = G(\mathbf{x})\}$$

the *active indices*. Then the *Clarke subdifferential* of G at a point $\mathbf{x}$ is

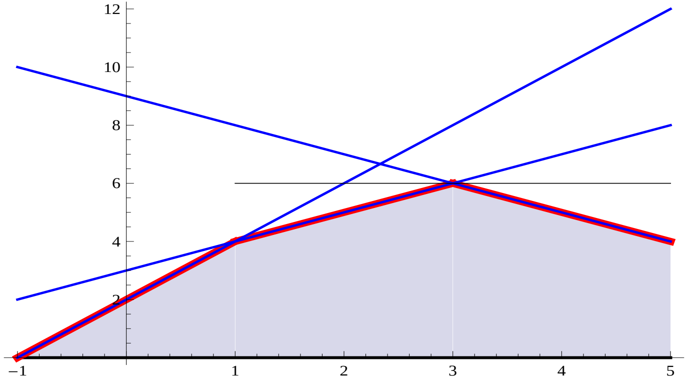
$$\partial G(\mathbf{x}) = \mathrm{conv}\{\nabla f_l(\mathbf{x}) \ : \ l \in \mathcal{L}(\mathbf{x})\}.$$

Theorem

If f has an extremum at $\mathbf{x}$, then $0 \in \partial f(\mathbf{x})$.

F. H. Clarke. *Optimization and Nonsmooth Analysis.* Wiley Interscience, New York, 1983.

Nonsmooth Optimization



Theorem

For every number of spheres n and dimension d, the function G has finitely many local maxima.

Iteration procedure

Given the iteration $\mathbf{x}^k$, let $J(\mathbf{x}^k)$ be the matrix whose rows are the active gradients $\nabla f_l(\mathbf{x}^k)$ for all $l \in \mathcal{L}(\mathbf{x}^k)$. We seek an ascent direction ξ^k in which the active functions all increase infinitesimally at the same rate, that is

$$J(\mathbf{x}^k)\xi^k = \mathbb{1},$$

where $\mathbb{1}$ is a vector with $|\mathcal{L}(\mathbf{x}^k)|$ entries 1. This is achieved by by solving the minimization problem

$$\xi^k \in \operatorname*{argmin}_{\xi} |J(\mathbf{x}^k)\xi - \mathbb{1}|^2.$$

Iteration procedure

Then we begin a line search in that direction. A triple $0 \leq t_1 < t_2 < t_3$ is a *bracket* of a directional maximum, if

$$G(\mathbf{x}^k + t_1\xi^k) \leq G(\mathbf{x}^k + t_2\xi^k) \geq G(\mathbf{x}^k + t_3\xi^k),$$

and at least one of the inequalities is strict. We successively decrease the width of the bracket $t_3 - t_1$ by testing the midpoint. When $t_3 - t_1$ is sufficiently small, we set $\mathbf{x}^{k+1} = \mathbf{x}^k + t_2\xi^k$. This is repeated until a convergence criterion is satisfied. $\square$

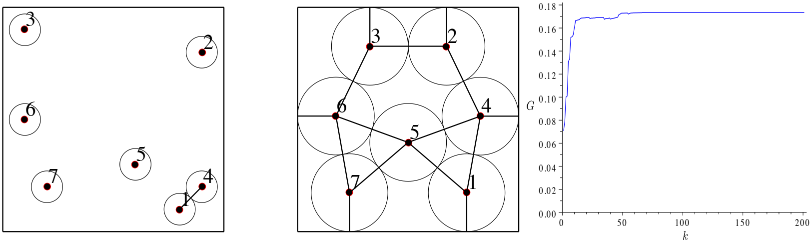
To find multiple local maxima, **repeat** with initial point $\mathbf{x}^0$ uniformly distributed in $[0, 1]^{nd}$.

Implementation issues

1. rounding errors: for $\varepsilon > 0$ define
$$\mathcal{L}_\varepsilon(\mathbf{x}) = \{l \in \mathcal{L} \, : \, f_l(\mathbf{x}) \leq G(\mathbf{x}) + \varepsilon\},$$
2. detection and treatment of saddle points: if necessary, perturb iteration state $\mathbf{x}^k$ by a random vector
3. termination: if $J(\mathbf{x}^k)\xi = \mathbb{1}$ has no more solution or a maximum number of iterations has been reached.

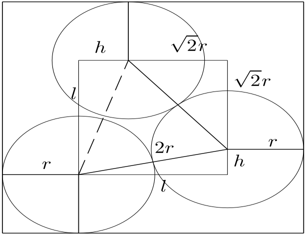
Room for improvement: recalculate only those distances that have changed.

Results



(Left) An initial configuration of seven disks in the unit square. *(Center)* The resulting local maximum of G provided by the search algorithm. *(Right)* Value of G over 200 iterations of the line search procedure.

Refinement



$$2r + l = 1$$

$$(2 + \sqrt{2})r + h = 1$$

$$h^2 + l^2 = (2r)^2$$

From a terminal configuration we construct the contact graph and a system of quadratic equations. Solving this system with MATHEMATICA gives

$$r = \frac{4 + \sqrt{2} - \sqrt{6}}{2\left(3 + 2\sqrt{2}\right)} \approx 0.254333095$$

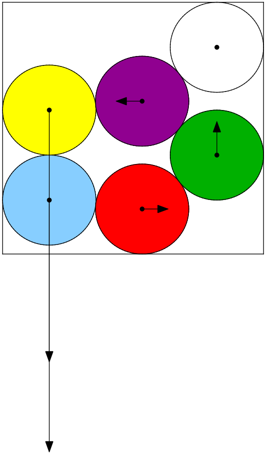
as the maximal value.

Test for full jamming: Connelly's criterion

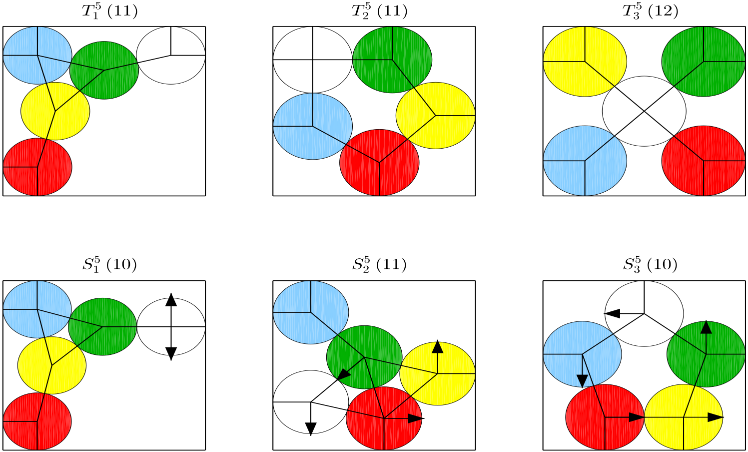
If there is an infinitesimal motion $\mathbf{x}' = (\mathbf{x}_1', \ldots, \mathbf{x}_n')$ of the configuration $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ that satisfies

$$(\mathbf{x}_i - \mathbf{x}_j) \cdot (\mathbf{x}_i' - \mathbf{x}_j') \geq 0$$

for every pair (i, j) of touching disks, then the motion must vanish for the configuration to be fully jammed, $\mathbf{x}' = 0$.
(R. Connelly, *Invent. Math.* **66**:11, 1982)

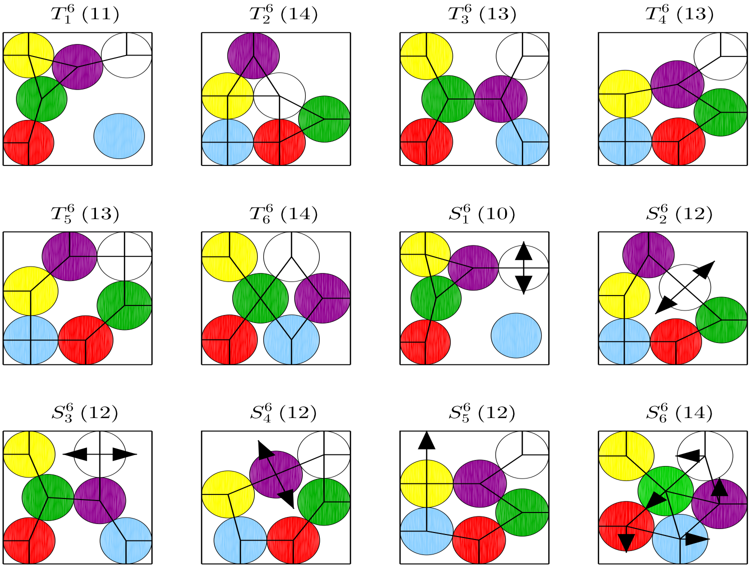


Results: five disks



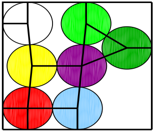
Local extrema *(top)* and critical points *(bottom)*.

Results: six disks

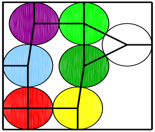


Results: seven disks

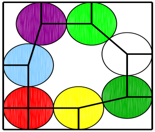
T_1^7 (15)



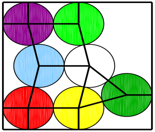
T_2^7 (15)



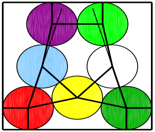
T_3^7 (15)



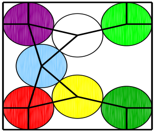
T_4^7 (16)



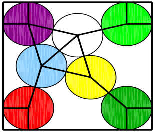
T_5^7 (15)



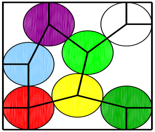
T_6^7 (16)



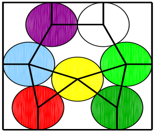
T_6^7 (16)



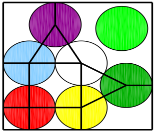
T_7^7 (15)



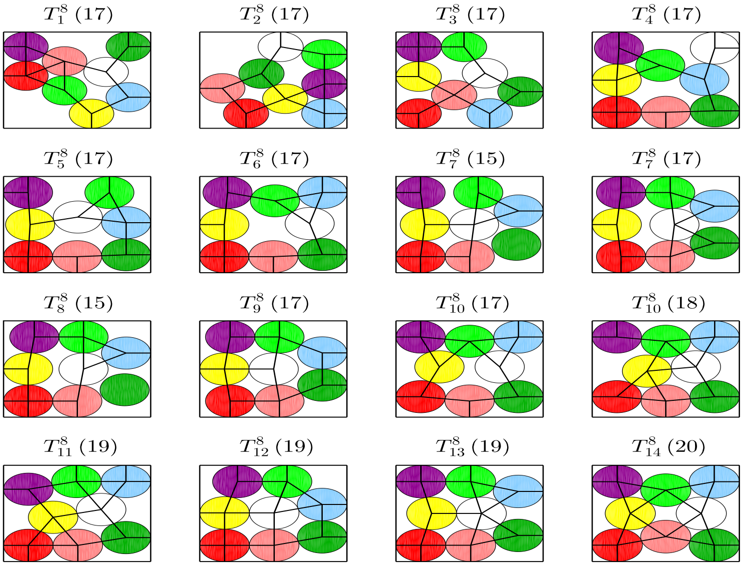
T_8^7 (15)



T_9^7 (14)

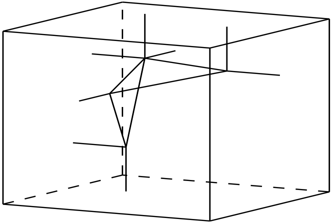


Results: eight disks

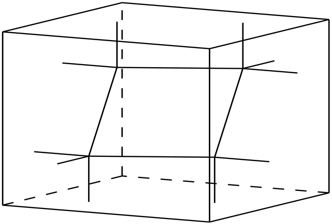


Results: four spheres

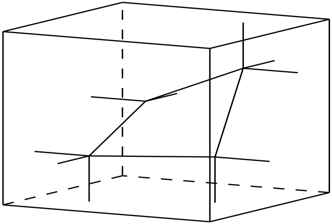
T_1^4 (13)



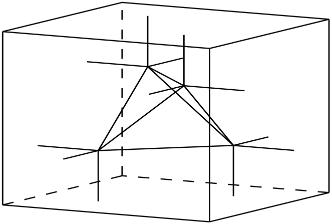
T_2^4 (14)



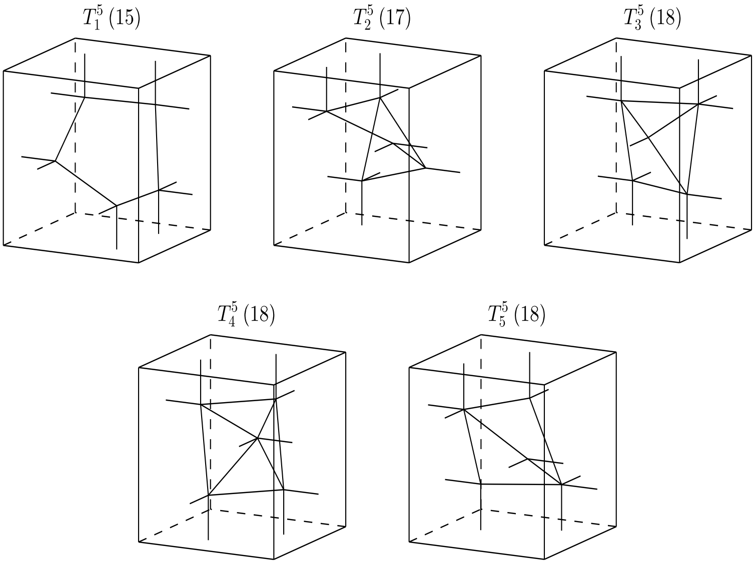
T_2^4 (14)



T_3^4 (18)

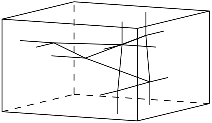


Results: five spheres

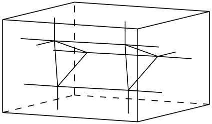


Results: six spheres

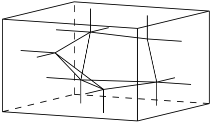
T_1^6 (19)



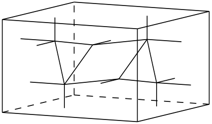
T_2^6 (21)



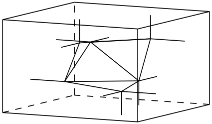
T_3^6 (22)



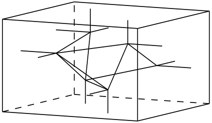
T_4^6 (20)



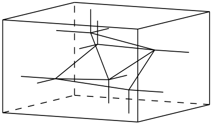
T_5^6 (21)



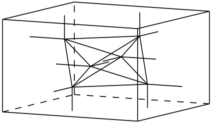
T_5^6 (21)



T_6^6 (19)



T_7^6 (24)

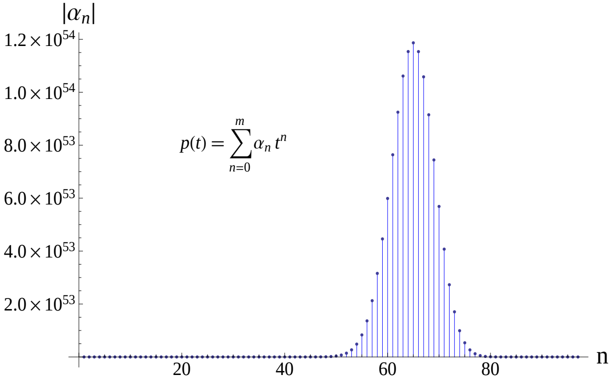


Results: minimal polynomials of radii

value	minimal polynomial
T_1^4	$1 - 16t + 104t^2 - 352t^3 + 704t^4 - 1024t^5 + 1216t^6 - 768t^7 + 64t^8$
T_2^4	$5 - 20t + 4t^2$
T_3^4	$5 - 4t + 2t^2$
T_1^5	$13 - 104t + 240t^2 - 128t^3 + t^4$
T_2^5	$1 - 8t + 20t^2 - 16t^3 + 16t^6$
T_3^5	$1 - 16t + 104t^2 - 352t^3 + 704t^4 - 1024t^5 + 1216t^6 - 768t^7 + 64t^8$
T_4^5	$9 - 36t + 4t^2$
T_5^5	$5 - 20t + 4t^2$
T_1^6	$628849 - 35215544t + 920916520t^2 - 14925909856t^3$
	$+167788673872t^4 - 1387008330496t^5 + 8720616629536t^6$
	$-42537931528576t^7 + 162698001135232t^8 - 489697674935296t^9$
	$+1156878795748352t^{10} - 2126444318666752t^{11}$
	$+2994825062826240t^{12} - 3163357034848256t^{13}$
	$+2454984222679040t^{14} - 1420158379393024t^{15}$
	$+698664367800320t^{16} - 324380948299776t^{17}$
	$+55492564615168t^{18} + 84665382207488t^{19}$
	$-46125516718080t^{20} - 14650005520384t^{21}$
	$+9630847598592t^{22} + 3387487682560t^{23} - 753326358528t^{24}$
	$-527777660928t^{25} - 87879057408t^{26} - 4697620480t^{27}$
	$+16777216t^{28}$
T_2^6	$13 - 104t + 240t^2 - 128t^3 + t^4$
T_3^6	$1 - 8t + 20t^2 - 16t^3 + t^4$
T_4^6	$1 - 16t + 96t^2 - 256t^3 + 544t^4 - 2304t^5 + 5632t^6 - 4096t^7 + 256t^8$
T_5^6	see Table 4
T_6^6	see Table 5
T_7^6	$9 - 36t + 4t^2$

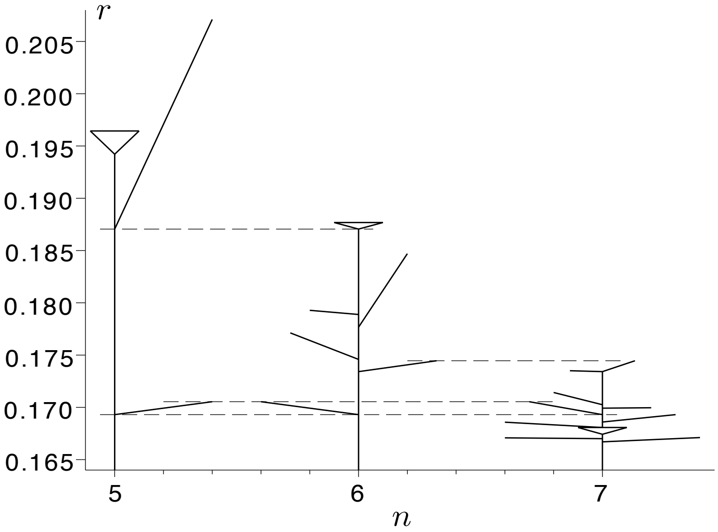
Minimal polynomials of the radii for 4 - 6 spheres (MATHEMATICA, `GroebnerBasis`).

Results: minimal polynomials of radii



Example of a distribution of polynomial coefficients ($deg = 96$).

Results: splitting trees



Simplified splitting trees of the level sets of G for n disks.

Observations

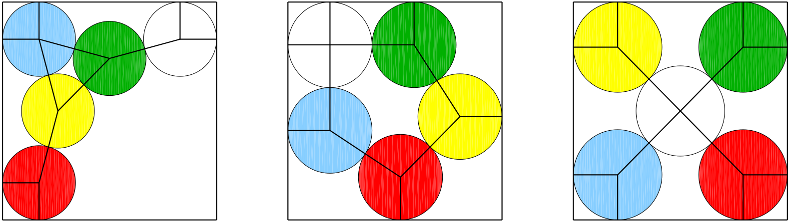
No contact graph appears at more than one critical value.

Is it possible to give upper and lower bounds on the number of (distinct) local extrema of G?

A coarse upper bound is the number of subsets of the index set $\mathcal{L}$ with $nd + 1$ and more elements. Since the functions ψ_{ik} and ψ^{ik} are complementary to each other, at most one of these can be active and so a reduced upper bound for minimally determined maxima ($nd + 1$ active functions) is

$$\binom{n(n-1)/2 + nd}{nd + 1}.$$

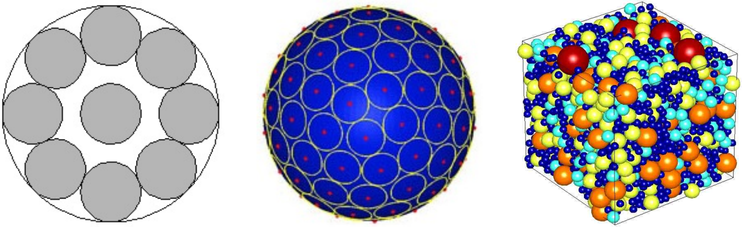
Open questions



Are there any other jammed configurations of 5 disks?

Diaconis *et al.*, *Invent. Math.* **185**:239 (2011): The configuration space of n spheres is arc-wise connected up to a radius $O\left(n^{-1}\right)$.

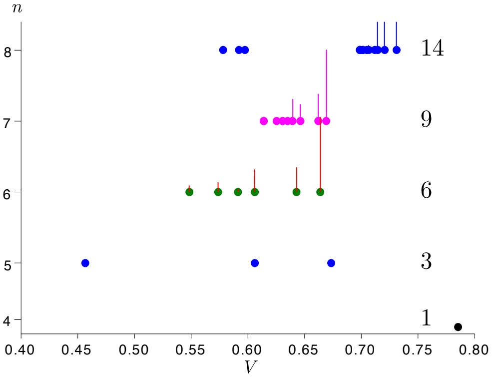
Related problems



(Left) 9 disks in a circle, *(Center)* the *Tammes* problem, packing spherical caps, and *(Right)* multidisperse mixtures.

Realizable packing fractions

For a jammed packing $\mathbf{x}^*$ of n spheres in $[0,1]^d$, the packing fraction is $n\omega_d G(\mathbf{x}^*)^d$, where ω_d is the volume of the d-dimensional unit ball.



Area fractions realized by jammed packings of 4 to 8 disks and relative frequencies.

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PH. A nonsmooth program for jamming hard spheres. *Optimization Letters* **8**:13-33, 2014. arXiv:1209.4053

Thank you for your attention