topology of hard disks in a box

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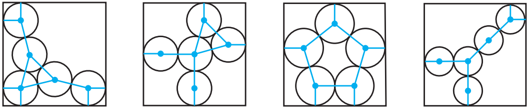
supported by ONR

June 13, 2011



setup

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In statistical mechanics these balls are often called "hard spheres," or in the two-dimensional setting "hard disks".

One might expect that the configuration space $\mathtt{Conf}(n,r)$ for small r to be homotopy equivalent to the configuration space $\mathtt{Conf}(n)$ of n distinct points in $\mathcal{B}$. On the other hand, for r sufficiently large the space $\mathtt{Conf}(n,r)$ is empty; indeed finding the largest r such that $\mathtt{Conf}(n,r) \neq \emptyset$ is the *sphere packing problem*. Sphere packing in bounded regions is a well studied problem — for example in the works of Graham et al and Melissen.

algorithmic roots

There are several situations where the configuration spaces $\texttt{Conf}(n, r)$ appear:

- Packing problems are an important example. One often looks for a dense (or stable, in some sense) packing by slowly expanding the radii of the disks. To understand how the configuration space changes is a natural question.
- Sampling from the configuration space of hard balls is one of the critical tools in computational statistical physics.
- In robotics, the complexity of algorithms of motion planning for swarms of round robots depends on the topology of the corresponding configuration spaces.

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Studying these kinds of configuration spaces topologically is a natural problem. In a recent survey article Persi Diaconis wrote,

> *"We know very, very little about the topology of the set of configurations: for fixed n, what are useful bounds on r for the space to be connected? What are the Betti numbers? Of course, for r small this set is connected but very little else is known."*

questions

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- What is the largest r_* such that $\mathtt{Conf}(n, r)$ is homotopy equivalent to $\mathtt{Conf}(n)$ for $r \in (0, r_*)$, and what happens at r_*?

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- What is the largest r_* such that $\texttt{Conf}(n, r)$ is homotopy equivalent to $\texttt{Conf}(n)$ for $r \in (0, r_*)$, and what happens at r_*?
- What is the topology of $\texttt{Conf}(n, r)$ for various asymptotic regimes?

We are mostly interested in the planar situation, $\mathcal{B} \subset \mathbb{R}^2$, but a big chunk of general story is valid for all dimensions.

tautological function

Fix n, and define $\texttt{Conf}(n)$ to be the set of ordered n-tuples of distinct points in the domain $\mathcal{B} \subset \mathbb{R}^d$:

$$\texttt{Conf}(n) = \{\vec{x} = (x_1, \ldots, x_n) \mid x_i \in \mathcal{B}, x_i \neq x_j\}.$$

As an open subset of $\mathbb{R}^{dn}$, $\texttt{Conf}(n)$ is a smooth manifold.

Let $\tau : \texttt{Conf}(n) \to \mathbb{R}$ be defined by

$$\tau(\vec{x}) := \min\left(\frac{1}{2}\min_{i \neq j} d(x_i, x_j), \min_i d(x_i, \partial\mathcal{B})\right), \tag{1}$$

where $\partial\mathcal{B}$ denotes the boundary of $\mathcal{B}$.

topology of connectivity space

Then by definition the configuration space of n balls of radius r in $\mathcal{B}$ is given by

$$\mathtt{Conf}(n, r) = \tau^{-1}[r, \infty).$$

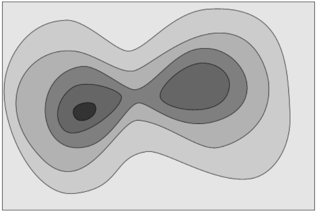
This observation suggests using a 'Morse'-type theory of τ to study the topology of $\mathtt{Conf}(n, r)$ and the topology changes as r varies, and this is our approach.

One obvious trouble on that route is the fact that τ typically is not smooth, so that we need to discuss a general framework which allows us to work with non-smooth functions.

how Morse theory works

The power of Morse theory lies in its ability to localize the changes in topology, as one considers the whole family of sets $\{\tau \geq r\}$.

For the classical Morse theory, where the functions are smooth, and the points are non-degenerate, one can argue that the topology of $\tau^{-1}[r, \infty)$ does not change on an interval $a < r < b$, *if there are no critical points of* τ *with critical values between* a *and* b.



Moreover, one can say what happens near a critical value corresponding to a critical point of index k, as one increases r: a small disk of dimension k is cut off.

configuration spaces

If we implement this approach for our tautological function τ, we need first to understand the "initial condition", the topology of

$$\{\tau \geq \epsilon\}$$

for some small enough ϵ.

This space is easy to see to be (homotopy equivalent to) the "classical" configuration space of n points in $\mathbb{R}^d$, denoted $\texttt{Conf}_\circ(n)$.

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This is already a very interesting space; luckily a lot is known about it. For example, on the plane, one has

$$\sum \beta_i(\mathtt{Conf}_\circ(n))t^i = (1+t)(1+2t)\cdots(1+(n-1)t).$$

(Here β_i is the rank of the i-th homology group, roughly measuring the number of holes of dimension i.)

min-type functions

The tautological function τ is a *min*-type functions, that is the functions on a manifold M given as the minimum of a parametric family

$$\tau(x) := \min_p f(p,x), x \in M, p \in P,$$

where P is a compact, and f is continuously differentiable in x.

Indeed, we can take P to be the disjoint union of the discrete set corresponding to pairs $(i,j), 1 \leq i < j \leq n$ and of the boundary $\partial\mathcal{B}$.

Such functions are typically not smooth, yet one can create a pretty good version of Morse theory for them.

regular and critical values

For a *min*-type function τ, the set $N \subset P \times M$ defined by

$$N := \{(p, x) : f(p, x) = \tau(x)\}.$$

It is compact, and the slices

$$N_x := \{p \in P : (p, x) \in N\}$$

are *upper semi-continuous*: for any $x \in M$ there exist open neighborhood $Ux \ni x$ and an open neighborhood $UN_x \supset N_x$ such that for $x' \in Ux$, $N_{x'} \subset UN_x$.

For $x \in M$ consider the intersection of the open half-spaces

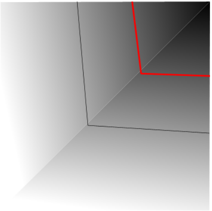
$$H_x(p) := \{v : \langle df_p|_x, v\rangle > 0\}$$

over all $p \in N_x$. This is an open convex cone

$$C_x^o := \cap_{p \in N_x} H_x(p).$$

context: configuration spaces

Theorem 1 *If the cones* C_x^o *are non-empty over the level set* $\tau^{-1}(c)$*, then* c *is topologically regular.*



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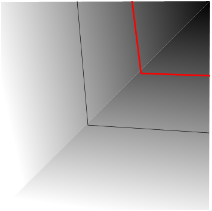


For general *min*-type functions this is essentially the best possible condition for the regularity of the critical values. If the functions f_p are *quasi-convex*, i.e. have convex lower excursion sets $\{f_p \leq c\}$, then 1 can be considerable strengthened.

stress graphs

Corollary 1 implies that unless the level set of the tautological function $\{\tau = r\}$ contains a point x with $C_x^o =$, the homotopy type of $\texttt{Conf}(n, r)$ is locally constant at r.

By Farkas lemma, the fact that $C_x^o =$ implies that there exists a finite collection of points $p_i \in N_x, i = 1, \ldots, I \leq \dim M + 1$, and positive weights $w_i > 0$ such that

$$\sum_i w_i df_{p_i}|_x = 0. \tag{2}$$

In our situation, the convex combination 2 has a clear geometric interpretation.

stress graphs, cont'd

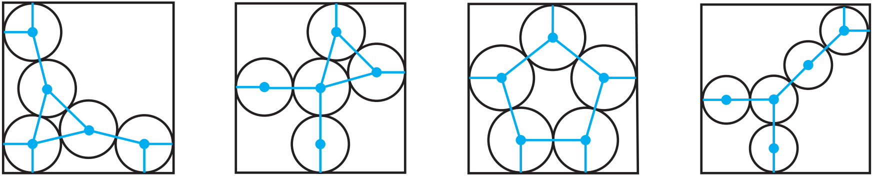
In the construction above, the points p_i correspond either to the pairs of points x_{a_i}, x_{b_i} at distance $2r$, or to the pairs of points $x_{c_i}, y_i, b_i \in \partial\mathcal{B}$, such the distance from x_{c_i} to the boundary is r and is realized at y_i. (Here $r = \tau(x)$, the critical value at the critical point x.)

To such system of weights $w = \{w_i\}$ we associate a *graph* $\Gamma(w)$ embedded into $\mathbb{R}^d$ whose vertices are the points $x_1, \ldots, x_n$, and the boundary points b_l. The edge connects the pairs x_{a_i}, x_{b_i} or x_{c_i}, y_i and has the positive weight w_i.

We interpret this graph as a system of *mechanical stresses*. The points x_i are referred to as the *internal points* of the graph; the points b_i as the *boundary points*.

stress graphs, cont'd

Proposition 1 *For any internal vertex x_i, the sum of the stresses acting on it vanishes.*



Corollary 1 *The sum of unit normals to the boundary components at boundary points belonging to a connected component of $\Gamma(w)$ weighted by w_I vanishes.*

first hit

From now on we will restrict to the case of hard spheres in a rectangular box with sides $L := L_1 \leq \ldots \leq L_d$.

Lemma 1 *The total length of any connected component of the stress graph is at least* L*.*

Corollary 2 *The the rectangular box* $\mathcal{B}$*, there are no critical values of* τ *in* $(0, L)$*, and therefore,*

$$\texttt{Conf}(n, r) \cong \texttt{Conf}_{\circ}$$

for $0 < r < r_* = L/n$*.*

what happens at r_*?

We can in fact very precisely describe what happens at r_*.

Let $i = (n-1)(d-1)$. Then for sufficiently small $\epsilon > 0$,

$$\beta_i(\texttt{Conf}(n, r-\epsilon), \texttt{Conf}(n, r+\epsilon)) = (n-1)!,$$

and for all other $k \neq i$, $\beta_i(\texttt{Conf}(n, r-\epsilon), \texttt{Conf}(n, r+\epsilon)) = 0$. In other words, one acquires $n!$ new 'holes' in dimension i.

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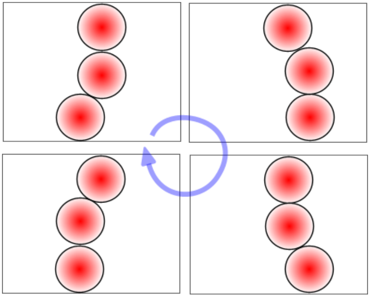
One can even visualize these new cycles.



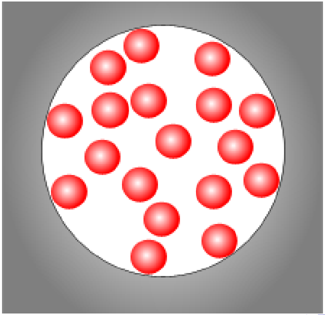
asymptotic regimes

- sparse regime: $rn = O(1)$
- intermediate: $r^k n \to \infty, r^{k+1} n \to 0$.
- dense: $r^d n = O(1)$.

Most interesting for physicists regime is dense regime (phase transition to solid).

For us, intermediate regimes are most interesting.

On the plane, the intermediate regime is $rn \to \infty, r^2 n \to 0$. Is the configuration space connected? Far from obvious!



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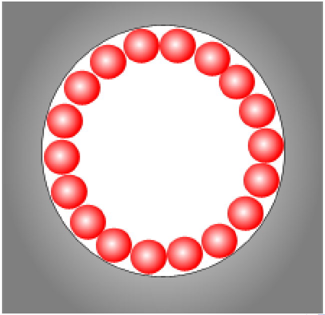

topological complexity

In the context of this talk, the *topological complexity* a space is the logarithm of its total Betti number *normalized by* $n!$:

For a field $\mathbb{F}$, define by

$$\beta_k(\texttt{Conf}(n, r)) = rank\, H^k(\texttt{Conf}(n, r), \mathbb{F}),$$

the rank of k-th homology group of $\texttt{Conf}(n, r)$.

Definition 1 *The topological complexity of* $\texttt{Conf}(n, r)$ *is the*

$$\beta_*(n) = \log \frac{\sum_k \beta_k}{n!}.$$

For example, for $0 < r < r_*$, $\beta_* = 0$.

asymptotics in the sparse regime

For planar configurations in a not too complicated box, the topological complexity behaves pretty reasonably on the intermediate regime:

Theorem 2 *For $d = 2$, let $nr \to \infty$, $nr^2 \to 0$. If the box $\mathcal{B}$ has semi-algebraic boundary, then*

$$\beta_*(n) = \Theta(n).$$

In other words, the total Betti number (up to $n!$ factor) behaves "thermodynamically".

This should be compared with the "topological conjecture" in statistical physics.

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There are many further questions to explore, about `Conf` and related spaces - stay tuned.

The End