

Min-Type Morse Theory for Configuration Spaces of Hard Spheres

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In this paper we study configuration spaces of hard spheres in a bounded region. We develop a general Morse-theoretic framework and show that mechanically balanced configurations play the role of critical points. As an application, we find the precise threshold radius for a configuration space to be homotopy equivalent to the configuration space of points.

1 Introduction

Configuration spaces of n points in \mathbb{R}^d are well studied [4]. In this article we are interested in a natural generalization, configuration spaces of nonoverlapping balls in a bounded region in \mathbb{R}^d .

Besides their intrinsic mathematical interest, the study of these spaces is motivated by physical considerations. For example, in statistical mechanics "hard spheres" (or in two dimensions "hard disks") are among the most well-studied models of matter. Computer simulations suggest a solid–liquid phase transition for hard spheres [17], but this is not well understood mathematically.

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We dedicate this paper to the memory of Boris Lubachevsky

A number of papers in statistical mechanics have explored the hypothesis that underpinning phase transitions are changes in the topology of the underlying configuration space or equipotential submanifolds [1, 9, 16, 24]. Franzosi et al. [10, 11] show that under fairly general conditions (smooth, finite-range, confining potentials), the Helmholtz free energy cannot pass through a phase transition unless there is a change in the topology of the underlying configuration space. This theorem unfortunately does not apply to configuration spaces of hard spheres, since the potential function is not smooth—but the Morse-theoretic methods developed here may be a step in the direction of extending it to include hard spheres.

Several other papers have investigated configuration spaces as models of motion planning for robots [8, 13]. For example, Farber’s “topological complexity” can be thought of as measuring the difficulty of designing an algorithm for navigating the space. As Deeley [6] recently pointed out when he studied “thick particles” on metric graphs, the assumption that robots are points is not physically realistic, and giving the points thickness wildly complicates the topology of the underlying configuration space.

Let \mathcal{B} be a bounded region in \mathbb{R}^d . Define $\text{Conf}(n, r)$ to be the configuration space of n nonoverlapping balls of radius r in \mathcal{B} . We are especially interested here in understanding when the topology changes if n is fixed and r is varying. First we consider the extreme cases. For r sufficiently small, one expects that $\text{Conf}(n, r)$ is homotopy equivalent to the configuration space $\text{Conf}(n)$ of n distinct points in \mathcal{B} —for a survey of configuration spaces of points, see Cohen [4]. On the other hand for r sufficiently large, $\text{Conf}(n, r)$ is empty. Indeed, finding the smallest such r is the sphere packing problem in a bounded region—see, for example, Graham et al. [2, 15, 18, 19] and Melissen [21, 22].

In this note we develop a Morse-theoretic framework which provides a necessary condition for the topology to change—mechanically balanced configurations play the role of critical points (and submanifolds). As an illustration of the method, we find the precise threshold radius below which $\text{Conf}(n, r)$ is homotopy equivalent to $\text{Conf}(n)$.

2 Tautological Morse Function

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

$$\text{Conf}(n) = \{\vec{x} = (x_1, \dots, x_n) \mid x_i \in \mathcal{B}, x_i \neq x_j \text{ for } i \neq j\}.$$

As an open subset of \mathbb{R}^{dn} , $\text{Conf}(n)$ has the structure of a smooth manifold. Let $\tau : \text{Conf}(n) \rightarrow \mathbb{R}$ be defined by

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

where $\partial \mathcal{B}$ denotes the boundary of \mathcal{B} . We call τ the tautological function. Then, by definition, the configuration space of n balls of radius r in \mathcal{B} is given by

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

This observation suggests using a ‘‘Morse’’-type theory of τ to study the topology of $\text{Conf}(n, r)$ and especially how the topology changes as r varies. One obvious trouble on that route is the fact that τ typically is not smooth, so that we need a general framework that allows us to work with nonsmooth functions.

In the next section we will discuss the properties of min-type functions, that is functions on a manifold M given as the minimum of a parametric family of real-valued functions

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

where P is a compact parameter space and f is continuously differentiable in x for every fixed $p \in P$. We note that the function given by (1) falls within this category, if one considers as P the disjoint union of the discrete set corresponding to pairs (i, j) , $1 \leq i < j \leq n$ and of n copies of the boundary, formed by the pairs (i, p) , $1 \leq i \leq n$, $p \in \partial \mathcal{B}$.

It should be remarked that the Morse-type theory of the min (or even min–max) type functions has appeared in the literature (cf. [3, 12, 20]), but in a much more restrictive context (with essentially finite parameter space).

3 Min-Type Morse Theory

Let us start with some notation and definitions.

For a manifold M and function $f : M \rightarrow \mathbb{R}$, let M^c denote the superlevel set at c , that is, $M^c = f^{-1}[c, \infty)$.

We say that a function $h : (s, t) \rightarrow \mathbb{R}$ is *increasing with speed at least $v > 0$* if $h(t') - h(s') \geq v(t' - s')$ for any $s' < t'$ in the interval (s, t) . We note that such a function does not have to be even continuous.

We record for later use the following (immediate) result.

Lemma 3.1. Let $f: M \times \mathbb{R} \rightarrow \mathbb{R}$ be a continuous proper function, (strictly) increasing along each fiber $\{x\} \times \mathbb{R}$. Then the fiber-wise inverse $\phi: (x, c) \mapsto \inf\{t: f(x, t) = c\}$ is continuous on $M \times [c_1, c_2]$ for any interval $[c_1, c_2]$ which belongs to the ranges of all the functions $f_x(\cdot) := f(x, \cdot)$. \square

For a smooth vector field V on M , we shall denote the time t shift along the trajectories of V as S_t^V . We will say that the function f *increases along the trajectories of V with nonzero speed*, if, for some common $v > 0$, and for all $x \in M$, $h_x: t \mapsto f(S_t^V x)$ increases with speed at least v .

Lemma 3.2. Let M be a smooth manifold and $f: M \rightarrow \mathbb{R}$ be a continuous function, such that M^a is compact. Suppose that M admits a smooth vector field V nonvanishing on $f^{-1}[a, b]$, and such that f is increasing along the trajectories of V on the set $f^{-1}[a, b]$ with nonzero speed. Then M^b is a deformation retract of M^a . \square

Lemma 3.2 can be seen as a generalization of [23, Theorem 3.1] for nonsmooth functions f . We remark here that one can drop here the nonzero speed condition, requiring only that f be increasing along the trajectories of V , but we do not need this strengthened form in this paper.

Proof. For $x \in M^a$ set a partially defined function on $M^a \times \mathbb{R}$ by $g(x, t) := f(S_t^V x)$. The nonzero speed condition implies that $[a, b]$ is in the range of $g(x, \cdot)$ for any $x \in f^{-1}([a, b])$, and together with the compactness of M^a implies that g is proper. Hence, by Lemma 3.1, $\tilde{\phi}(x, c) = \inf\{t: f(S_t^V x) \geq c\}$ is well defined and continuous, as well as $\phi(x, c) = \max(\tilde{\phi}(x, c), 0)$. As for any $c \leq f(x)$, $\phi(x, c) = 0$, ϕ vanishes on $M^b \times [a, b]$.

Now define the homotopy

$$H: M^a \times [0, 1] \rightarrow M^a$$

as

$$H: (x, \tau) \mapsto S_{\phi(x, (1-\tau)a + \tau b)}^V x.$$

The continuity of ϕ implies the continuity of H ; the facts that $H(x, 0) = id_{M^a}$, $H(x, \tau)|_{M^b} = id_{M^b}$ for $0 \leq \tau \leq 1$ and $H(x, 1) \in M^b$ are immediate. \blacksquare

3.1 Regular values of min-type functions

Next, we will use the fact that the tautological function τ is the minimum of a compact family of smooth functions. We want to establish conditions when a value c is *topologically regular*, that is for which there exists some $\epsilon > 0$ such that $M^{c+\epsilon}$ is a deformation retract of $M^{c-\epsilon}$.

We give a general condition for topological regularity, as follows.

Let P be a compact metric space, M be a compact smooth manifold with boundary and

$$f : P \times M \rightarrow \mathbb{R}$$

be a continuous function such that the x -derivative of f (i.e., the gradient of f_p , where $f_p(x) = f(p, x)$) is continuous on $P \times M$. We consider P to be the *parameter space*.

We denote by $\tau := \min_{p \in P} f_p$ the min-function of the family f . The set $N \subset P \times M$ defined by

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

is compact, and the slices

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

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

Next we show that if one can perturb each x to increase τ , then we can do so globally with a minimum speed.

Lemma 3.3. Assume that, for any $x \in M$, there exists a tangent vector $V_x \in T_x M$ such that $L_{V_x} f_p > 0$ for all $p \in N_x$. Then

- for some positive v there exists a smooth vector field V on M such that $L_V f_p \geq v > 0$ in some open neighborhood of N and
- along the trajectories of V , the min-function τ increases with speed at least v . □

Proof. For any $x \in M$, we can extend the vector $V_x \in T_x M$ to a smooth vector field on M (which we still denote as V_x), such that $L_{V_x} f > 0$ in some open neighborhood $UN_x \times Ux$ of $N_x \times \{x\}$. By compactness, there exists a finite collection of points $\{x_i\}$ in M such that the open sets $U_i := UN_{x_i} \times Ux_i$ cover N (and the open sets Ux_i cover M), and $v > 0$ such that

$L_{V_i} f_p \geq v$ on U_i (here $V_i := V_{x_i}$). Using a partition of unity, we arrive at the first conclusion. The second conclusion is immediate. ■

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

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

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

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

in $T_x M$.

The upper semicontinuity of N_x implies the lower semicontinuity of $C_{x'}^o$ for any $x \in M$ and any open set $V \subset TM$ intersecting C_x^o , there exists an open neighborhood $U_x \ni x$ such that, for $x' \in U_x$, $C_{x'}^o$ intersects V . In particular, if C_x^o is nonempty, it remains such in a neighborhood of x .

Combining Lemmata 3.2 and 3.3, we obtain the following corollary.

Corollary 3.4. If the cones C_x^o are nonempty over the level set $\tau^{-1}(c)$, then c is topologically regular. □

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*, that is, have convex lower excursion sets $\{f_p \leq c\}$, then Corollary 3.4 can be considerably strengthened. Thus, one can show (we will do it in a follow-up paper) that a critical value is topologically regular, if, for all points at the level set, the intersection of the *closed* half-spaces is a cone over a contractible base. This observation relies on stratified Morse theory due to Goresky and MacPherson [14], but is in a nutshell close to the elementary result used by Connelly in his work on the existence of continuous “unlocking” deformations of hard ball configurations, see [5].

Corollary 3.4 implies that unless the level set of the tautological function $\tau^{-1}(r)$ contains a point x with $C_x^o = \emptyset$, the homotopy type of $\text{Conf}(n, r)$ is locally constant at r .

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

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

4 Critical Points and Stress Graphs

In our hard spheres setting, the vanishing of the convex combination (2) has a clear geometric interpretation.

For $\vec{x} \in \text{Conf}(n, r)$, define a *stress graph* of \vec{x} to be a graph embedded in \mathbb{R}^d whose vertices are the points x_1, \dots, x_n and boundary points $y \in \partial\mathcal{B}$ where $d(x_i, y) = r$ for some i . The edges are the pairs $\{x_i, x_j\}$ where $d(x_i, x_j) = 2r$ and $\{x_i, y\}$ where $d(x_i, y) = r$. Each edge k is assigned a positive weight w_k . The points x_i are referred to as *internal points* and the points y are referred to as *boundary points*. We interpret this graph as a system of *mechanical stresses*, with (repulsive) forces acting on the endpoints of a segment k equal to w_k times the unit vector in the direction of k . Call the mechanical stresses acting on boundary points *boundary mechanical stresses*. Call a connected component *trivial* if it consists of a single point. Call \vec{x} trivial if $\Gamma(\vec{x})$ has no edges.

A stress graph is said to be *balanced* if it satisfies the following condition.

- The mechanical stresses at each internal point sum to zero. (This result is similar to the necessary conditions for “locking”, see, e.g. [5].)
- The boundary mechanical stresses on each connected component sum to zero.

Say that the configuration is \vec{x} is *balanced* if it has a balanced stress graph.

Call an internal point *isolated* if it is not in the boundary of any edges. For each point x_i call the intersection of the stress graph with the points on the sphere $d(x_i, x) = r$ *kissing points* of x_i . Call a kissing point that is also a boundary point a *boundary kissing point*.

Lemma 4.1. Assume that $\vec{x} \in \text{Conf}(n, r)$ is balanced. Then, for the stress graph of \vec{x} ,

- (1) each nonisolated internal point is in the convex hull of its kissing points and
- (2) each nontrivial connected component is contained in the convex hull of its boundary points. □

Proof. Let x_i be a nonisolated internal point. Let $Z = \{z_1, \dots, z_m\}$ be its kissing points, where $m \geq 1$ since x_i is nonisolated. For $1 \leq j \leq m$, let $w_j > 0$ be the weight of the edge $x_i z_j$ and let v_j be the unit vector pointing from z_j to x_i . Since the stress graph of \vec{x} is balanced,

$$\sum_{j=1}^m w_j v_j = 0. \tag{3}$$

Assume that x_i is not in the convex hull of Z . That is, there exists a hyperplane Π containing x_i so that Z is contained in one of the two open half-spaces of Π . Let n be a normal vector of Π in the direction of Z . Then, for each $1 \leq j \leq m$, $\langle n, v_j \rangle < 0$, so $\langle n, \sum_{j=1}^m w_j v_j \rangle = \sum_{j=1}^m w_j \langle n, v_j \rangle < 0$, contradicting (3).

Let C be a nontrivial connected component of the stress graph of \vec{x} . Let Y denote the boundary points in C . Assume that there exists an $x_i \in C$ that is not in the convex hull of Y . That is, there is a hyperplane Π containing x_i such that Y is contained in one of the two open halfspaces of Π . Let n be a normal vector of Π pointing toward Y . Let D be the full subgraph of C containing the vertices z such that $\langle z, n \rangle$ is minimal. Then, D contains only internal points. The convex hull of D is a polytope, each of whose vertices is a nonisolated internal point of the stress graph of \vec{x} that is not in the convex hull of its kissing points, contradicting statement 1. ■

Now, consider $\vec{x} \in \text{Conf}(n)$ that is a critical point of τ with critical value r . In (2), the parameters p_i correspond either to the pairs of touching hard spheres, $d(x_{a_i}, x_{b_i}) = 2r$, or to the hard sphere x_{c_i} touching the boundary, $d(x_{c_i}, y_i) = r$, at a point $y_i \in \partial\mathcal{B}$. Let $\Gamma(\vec{x})$ be the corresponding stress graph for \vec{x} with weights given by the coefficients w_i in (2).

Theorem 4.2. If $\vec{x} \in \text{Conf}(n)$ is a critical point of τ with critical value r , then \vec{x} is balanced and nontrivial as a point in $\text{Conf}(n, r)$. □

Proof. Consider $\vec{x} \in \text{Conf}(n, r)$ and consider $\Gamma(\vec{x})$. From (2) it follows that the mechanical stresses at each internal point sum to zero.

The sum of mechanical stresses in each connected component equals the sum of mechanical stresses on internal points and the sum of external mechanical stresses. From (2) and the first observation it follows that the boundary mechanical stresses on each connected component sum to zero.

Finally, since the sum in (2) is nontrivial, \vec{x} is nontrivial. ■

5 Hard Spheres in a Box

Consider now in more detail the case of hard spheres in a rectangular box with sides $L := L_1 \leq \dots \leq L_d$, given, for definitiveness sake, by

$$\mathcal{B} = \{0 \leq f_m \leq L_m, m = 1, \dots, d\}.$$

(Here $\{f_m\}$ is the orthonormal coordinate system on \mathbb{R}^d .)

5.1 Initial interval

We show that Theorem 4.2 implies a lower bound on the length of the initial interval of values of r , where the homotopy type of $\text{Conf}(n, r)$ remains constant.

Theorem 5.1. For the rectangular box \mathcal{B} , there are no critical values of τ in $(0, L/2n)$, and, therefore,

$$\text{Conf}(n, r) \simeq \text{Conf}(n)$$

for $r < L/2n$. □

Proof. Assume that $\vec{x} \in \text{Conf}(n)$ is a critical value for τ with critical value r . Then, by Theorem 4.2, \vec{x} is balanced and nontrivial. Since the internal points of $\Gamma(\vec{x})$ are the points $x_i, 1 \leq i \leq n$, a connected component of $\Gamma(\vec{x})$ contains at most n internal points. Since the edges of $\Gamma(\vec{x})$ between internal points have length $2r$ and the edges between internal points and boundary points have length r , a connected component of $\Gamma(\vec{x})$ has diameter at most $2nr$.

Since \vec{x} is nontrivial, it has at least one nontrivial connected component. By Lemma 4.1, it is contained in the convex hull of its boundary points, so it contains at least one boundary point. Since $\Gamma(\vec{x})$ is balanced, the boundary mechanical stresses of this connected component sum to zero. Since the weights are (strictly) positive and the unit vectors corresponding to the edges between internal points and boundary points are parallel to the coordinate vectors, this connected component must contain a pair of boundary points from opposing faces. Thus, the diameter of this connected component is at least L . Therefore $r \geq L/2n$. ■

We remark that the balanced stress graph of minimal diameter is not necessarily a segment, for nonrectangular boxes. For example, for the “concave triangle”, it is a cone over three points (see Figure 1).

5.2 First perestroika

A natural question now to ask is, whether there is a topology change as nr goes above the minimal length of the stress graph. We concentrate in the rest of the note on the case of the rectangular box with the shortest side of length L , and will investigate whether

$$i : \text{Conf}(n, r') \rightarrow \text{Conf}(n, r), \quad r' = L/2n + \epsilon, \quad r = L/2n - \epsilon$$

is a homotopy equivalence for small enough ϵ .

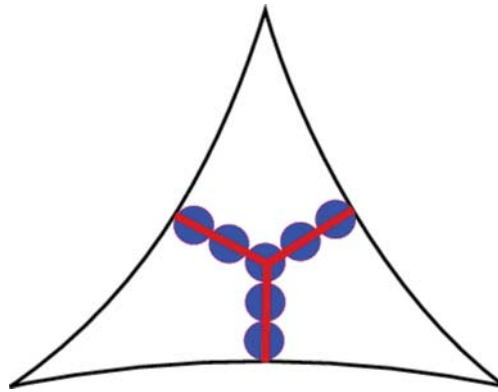


Fig. 1. Minimal length stress graph.

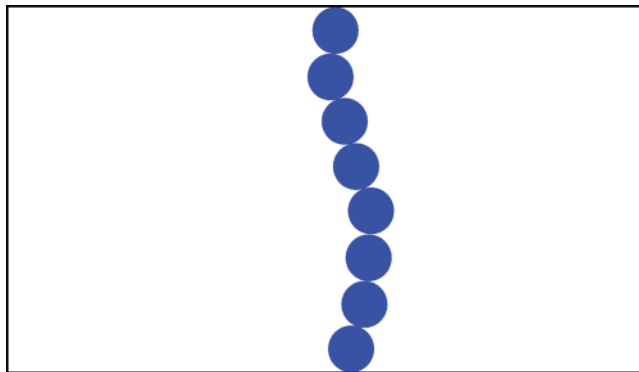


Fig. 2. A configuration in S_ϵ .

We argue that it is not, by presenting explicit nontrivial $(dn - n - d)$ -cycles in $\ker(Hi) \subset H_{dn-n-d}(\text{Conf}(n, r'), \mathbb{Z})$.

Indeed, let $0 < \epsilon < L/2n(n - 1)$. Then $L/2n < r' < L/2(n - 1)$, and thus $(n - 1)$ disks of radius r' would fit within the box when arranged in a vertical column, and n would not. Now, consider the set S_ϵ of n -point configurations in \mathcal{B} given by the following conditions:

- x_1 fixed is at distance r' from the center of the face $\{f_1 = 0\}$;
- $|x_{i+1} - x_i| = 2r'$ for $i = 1, \dots, n - 1$;
- x_n is at distance r' from the face $\{f_1 = L_1\}$.

In other words, we consider the configurations for which the n disks touch each other and the opposite horizontal faces, forming a chain (see Figure 2).

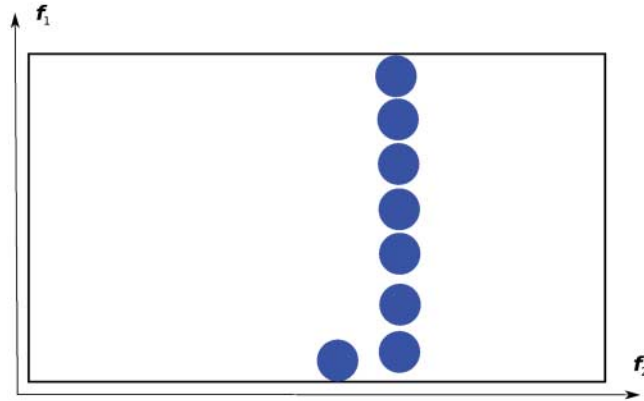


Fig. 3. A configuration in Σ .

An immediate computation shows that S_ϵ is diffeomorphic to an $(nd - n - d)$ -dimensional sphere. Orient it in some way, obtaining a class $s \in H_{nd-n-d}(\text{Conf}(n, r'))$.

Next, we show that s is nontrivial by constructing a cohomology class with which it has a nontrivial pairing.

Consider now the set Σ of configurations in \mathcal{B}^n given by the following conditions:

- all points x_1, \dots, x_n have the same coordinates f_3, \dots, f_d ;
- all points x_2, \dots, x_n have the same coordinates f_2, \dots, f_d ;
- the f_1 coordinates of x_2, \dots, x_n satisfy

$$f_1(x_1) \geq r; \quad f_1(x_{i+1}) - f_1(x_i) \geq 2r, \text{ for } i = 2, \dots, n - 1; \quad f_1(x_n) \leq L - r;$$

- $f_2(x_1) \leq f_2(x_2)$.

In other words, the configuration consists of $n - 1$ vertically aligned nonoverlapping r -disks constrained to have the same (f_1, f_2) -plane (with the same f_3, \dots, f_d coordinates as the disk x_1) (see Figure 3).

The conditions above are given by a finite collection of linear equalities and inequalities, and therefore define a convex polyhedron of dimension $d + n$. The boundary of this polyhedron is in $\mathcal{B}^n - \text{Conf}(n, r')$, whence, upon orientation it defines a relative class $\sigma \in H_{n+d}(\mathcal{B}^n, \mathcal{B}^n - \text{Conf}(n, r'))$.

We note that the space \mathcal{B}^n of n -tuples of points in \mathcal{B} can be embedded into the nd -dimensional sphere S^{nd} (consider a large ball containing \mathcal{B}^n and contract its boundary to a point). By excision and the long exact sequence for a pair, $H_{n+d}(\mathcal{B}^n, \mathcal{B}^n - \text{Conf}(n, r')) \cong$

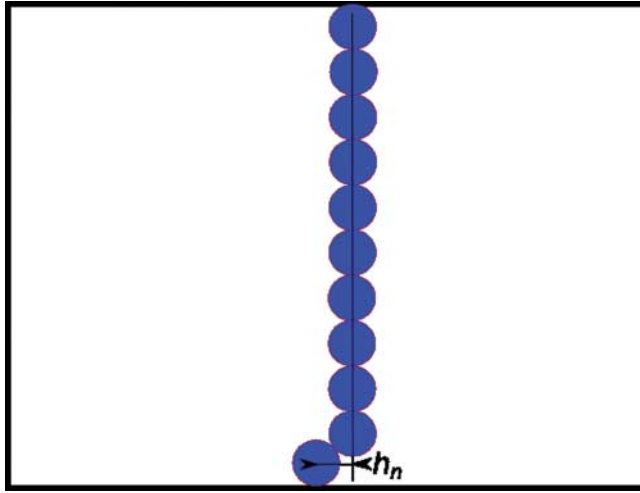


Fig. 4. Configuration corresponding to $x = S_\epsilon \cap \Sigma$.

$H_{n+d}(S^{nd}, S^{nd} - \text{Conf}(n, r')) \cong H_{n+d-1}(S^{nd} - \text{Conf}(n, r'))$. By Alexander duality the class σ can be identified with a class (which we still denote by σ) in $H^{nd-n-d}(\text{Conf}(n, r'))$.

Lemma 5.2. The pairing between the classes s and σ is nontrivial: $s \cdot \sigma = \pm 1$. □

Proof. Indeed, the manifolds S_ϵ and Σ intersect transversely at a single point. This point $x = S_\epsilon \cap \Sigma$ corresponds to the configuration where all n balls touch each other, and $(n - 1)$ of them are aligned in a vertical column, touching on one side the box boundary, and on the other side the last, n th ball (see Figure 4).

The transversality is quite immediate. Indeed, introduce as coordinates $\{h_k\}_{k=1}^n$ in the submanifold S_ϵ the vertical coordinates $h_k, k = 1, \dots, n - 1$, of the points forming the centers of the disks in the column, bottom-to-top, and the displacement h_n of the column away from the bottom disk (as shown in Figure 4). The differentials dh_k at the point

$$h_k = L - (2n - 2k - 1)r, \quad k = 1, \dots, n - 1, \quad h_n = \sqrt{(2r)^2 - (h_1 - r)^2}$$

corresponding to x form, obviously, a nondegenerate frame at the tangent space $T_x \Sigma$. ■

As one can observe, there exists a retraction of S_ϵ to a point staying within $\text{Conf}(n, r)$, implying that the class s is in the kernel of Hi . Indeed, we first can reduce all the distances between by shrinking the differences between the adjacent chain centers

so that

$$x_{i+1} - x_i \mapsto \frac{tr - (1-t)r'}{r'}(x_{i+1} - x_i), \quad t = [0, 1]; \quad i = 1, \dots, n-1$$

and x_1 remains fixed (clearly, this homotopy keeps the configuration in $\text{Conf}(n, r)$). Then one can pull all the vectors $(x_{i+1} - x_i)$ so that they point vertically upward (We think of f_1 as height.) (as not one was initially pointing downward).

For each permutation π of indices $1, \dots, n$, one obtains different classes s_π , and one can easily see that the pairing with the corresponding $n!$ classes σ_π is nondegenerate (because corresponding S_ϵ and Σ 's are all geometrically distinct). Hence, the rank of the kernel of Hi is at least $n!$.

We note that the sphericity of the set S_ϵ does not depend on the fact that the stress graph is a chain. For the configuration on Figure 1, the corresponding set is diffeomorphic to a sphere as well: it is just the corollary of the first critical value coming from a *topologically Morse* critical point; cf. [20].

5.3 Betti numbers

We can also compute how the Betti numbers change across the first threshold. Set $r_* = L/2n$, and note that, as the tautological function is semialgebraic for semialgebraic regions, its critical values are isolated. As the only balanced stress graphs in the case of a rectangular domain are the chains spanning the shortest dimension, for some small ϵ there are no other critical values in $(r_* - \epsilon, r_* + \epsilon)$.

It is well known [4] that the configuration space $\text{Conf}(n)$ of n (labeled) points in \mathbb{R}^d has Poincaré polynomial

$$\begin{aligned} P(t) &:= \sum_{i \geq 0} \beta_i t^i \\ &= \prod_{i=1}^{n-1} (1 + it^{d-1}) \\ &= 1 + \dots + (n-1)! H_{n-1} t^{(n-2)(d-1)} + (n-1)! t^{(n-1)(d-1)}, \end{aligned}$$

where

$$H_{n-1} = \sum_{i=1}^{n-1} 1/i.$$

This tells us the Betti numbers of $\text{Conf}(n, r_* - \epsilon)$, since we have already shown that $\text{Conf}(n, r_* - \epsilon)$ is homotopy equivalent to $\text{Conf}(n)$. We wish to compute the Betti numbers of $\text{Conf}(n, r_* + \epsilon)$.

Let $N = (n - 1)(d - 1)$. As we shrink the disks across the critical value $r_* = L/2n$, to the configuration space, we attach $kn!$ cells of dimension N , where k is the largest number such that $L_k = L$, whose boundaries are representatives for the homology classes s defined in Section 5.2. Each of these cells either increments β_N or decrements β_{N-1} .

The first observation is that

$$\beta_i[\text{Conf}(n, r_* + \epsilon)] = \beta_i[\text{Conf}(n, r_* - \epsilon)]$$

for $i \leq N - 2$. As (the proof to appear in a follow-up paper) one can show that $\beta_i(\text{Conf}(n, r)) = 0$ for $i \geq N$ and $r > r_*$, so in particular

$$\beta_i[\text{Conf}(n, r_* + \epsilon)] = 0$$

for $i \geq N$. Thus $(n - 1)!$ of the N -cells increase β_N . This leaves only β_{N-1} to compute.

Every N -cell that does not contribute to β_N decreases β_{N-1} . Since we know that $kn!$ cells are added, $(n - 1)!$ of them contributing to β_N , we have

$$\beta_{N-1}[\text{Conf}(n, r_* + \epsilon)] = \beta_{N-1}[\text{Conf}(n, r_* - \epsilon)] + kn! - (n - 1)!,$$

and since

$$\beta_{N-1}[\text{Conf}(n, r_* - \epsilon)] = \begin{cases} (n - 1)!H_{n-1} & : d = 2, \\ 0 & : d \geq 3, \end{cases}$$

we have

$$\beta_{N-1}[\text{Conf}(n, r_* + \epsilon)] = \begin{cases} (H_{n-1} + kn - 1)(n - 1)! & : d = 2, \\ (kn - 1)(n - 1)! & : d \geq 3. \end{cases}$$

6 Concluding Remarks

In a future article we will discuss nondegeneracy of critical points, which is closely related to the question of making our necessary condition for a change in the topology

sufficient. We also discuss defining and computing the index of critical points, and especially investigate more of the asymptotic properties of $\text{Conf}(n, r)$ as $n \rightarrow \infty$. In particular, we obtain bounds on the rate of growth of Betti numbers.

An important special case for which little seems known is: What is the threshold radius $r = r(n)$ for the connectivity of $\text{Conf}(n, r)$? This is an important question physically, since, for example, ergodicity of any Markov process hinges on the connectivity of the state space. Diaconis, Lebeau, and Michel noted that $r \leq c/n$ is sufficient to guarantee the connectivity of $\text{Conf}(n, r)$ [7] and this is best possible for certain regions. It would be interesting to know if the connectivity of the configuration space ever extends into the thermodynamic limit, i.e. are there any bounding regions so that $\text{Conf}(n, r)$ is connected for $r \leq Cn^{-1/d}$ and some constant $C > 0$?

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