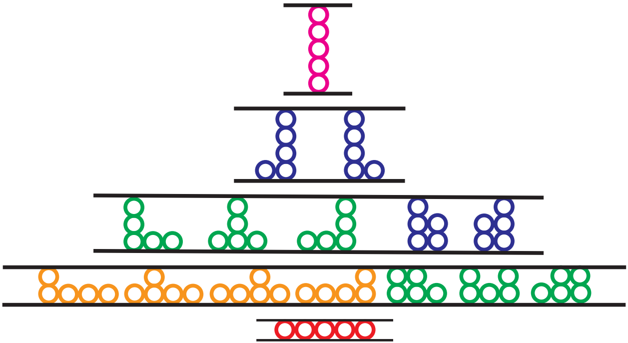
Configuration spaces: combinatorics, topology, and physics



Triangle lectures in combinatorics

Wake Forest University

Configuration space

The configuration space of n labelled points in the plane $\mathcal{C}(n)$ is defined as follows.

Definition

$$\mathcal{C}(n) = \{(x_1, x_2, \ldots, x_n) \mid x_i \in \mathbb{R}^2, x_i \neq x_j\} \subseteq \mathbb{R}^{2n}$$

Configuration space

$\mathcal{C}(n)$ is an open manifold, and its topology is well understood. For example the Poincaré polynomial is given by:

$$\beta_0 + \beta_1 t + \beta_2 t^2 + \cdots = (1+t)(1+2t)\ldots(1+(n-1)t).$$

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Here β_i denotes the dimension of ith homology — roughly speaking, β_i counts the number of i-dimensional holes.

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Let $\mathcal{C}(n, r)$ denote the configuration space of all possible arrangements of n nonoverlapping disks of radius r in some fixed bounded region $\mathcal{R} \subset \mathbb{R}^2$. I.e.

$$\mathcal{C}(n, r) = \{(x_1, x_2, \ldots, x_n) \mid d(x_i, x_j) \geq 2r, d(x_i, \partial\mathcal{R}) \geq r\}$$

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This can be thought of as the *phase space* for a hard spheres gas, so it is of intrinsic interest in physics.

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> "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. " — Persi Diaconis, 2008

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For n distinct points $\{x_1, x_2, \ldots, x_n\}$ in a region $\mathcal{R}$ let

$$F(x_1, x_2, \ldots, x_n) = \min\left(\{d(x_i, x_j)/2\} \cup \{d(x_i, \partial\mathcal{R})\}\right),$$

where $\partial\mathcal{R}$ is the boundary of $\mathcal{R}$.

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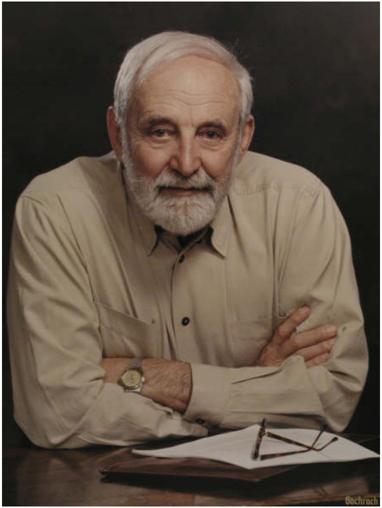
This suggests a Morse-theoretic approach.

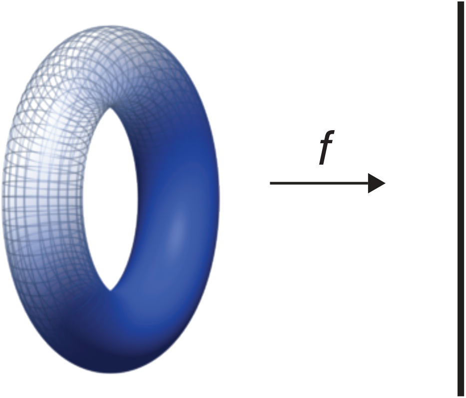
Morse theory

"Every mathematician has a secret weapon. Mine is Morse theory."

— Raoul Bott

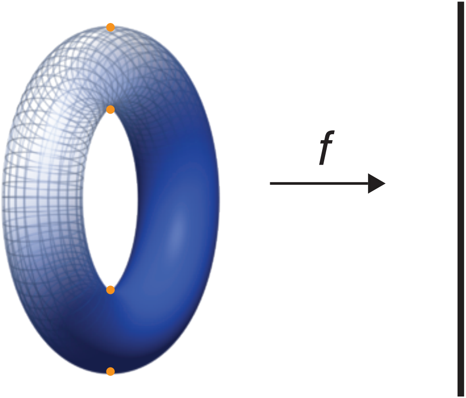


Morse theory



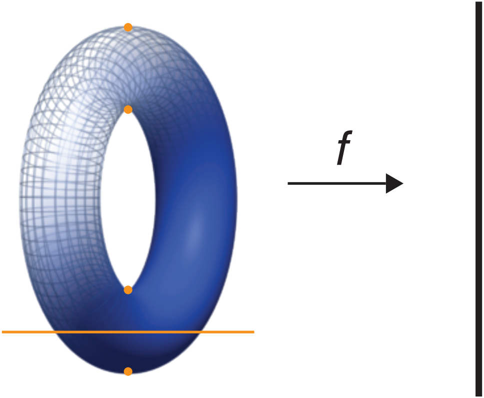
A smooth function on a torus

Morse theory



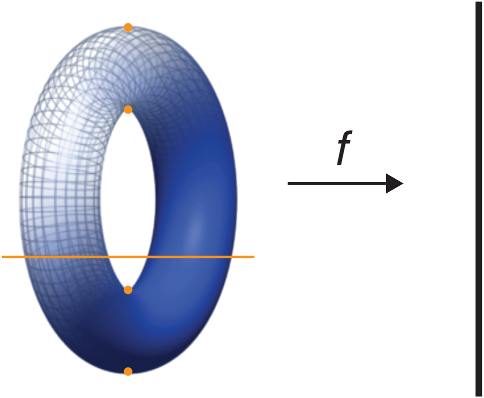
Critical points

Morse theory



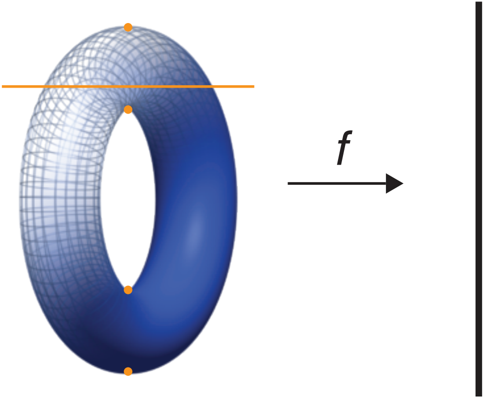
$\beta_0 = 1$

Morse theory



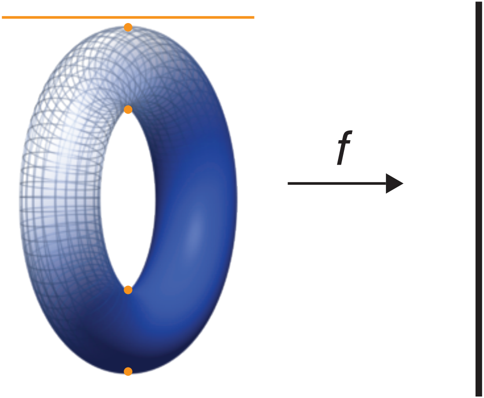
$\beta_0 = 1,\ \beta_1 = 1$

Morse theory



$\beta_0 = 1$, $\beta_1 = 2$

Morse theory



$\beta_0 = 1,\ \beta_1 = 2,\ \beta_2 = 1$

Topology only changes at critical points

Theorem (Morse?)

Let $f : M \to \mathbb{R}$ be a smooth function on a compact manifold M with isolated non-degenerate critical points. If $f^{-1}[r, r']$ contains no critical points then

$$f^{-1}(-\infty, r) \sim f^{-1}(-\infty, r').$$

(Here $\sim$ indicates homotopy equivalence.)

Mechanically-balanced configurations

We say that a configuration of disks is *mechanically-balanced* if there exist non-negative (and not all zero) weights c_{ij} on the edges of the contact graph so that

$$\sum_j c_{ij}(x_i - x_j) = 0$$

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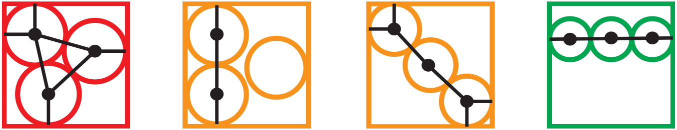

Characterization of critical points

Theorem

(Baryshnikov, Bubenik, K.) Let

$$F(x_1, x_2, \ldots, x_n) = \min\left(\{d(x_i, x_j)/2\} \cup \{d(x_i, \partial\mathcal{R})\}\right).$$

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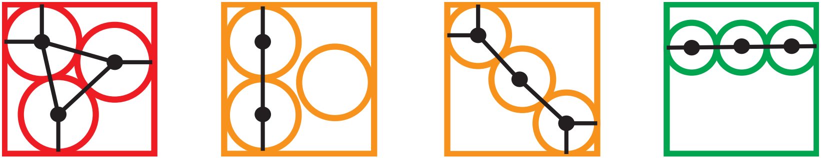
(See "Min-type Morse theory for configuration spaces of hard spheres", arXiv:1108.3061, International Mathematics Resarch Notices, 2013.)

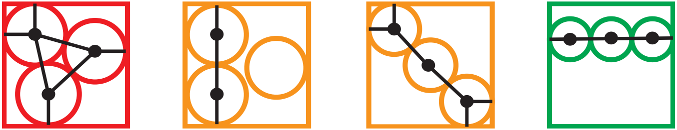
A computational approach

(See "Computational topology for configuration spaces of hard disks, *Phys. Rev. E*, Jan. 2012, joint with Gunnar Carlsson, Jackson Gorham, and Jeremy Mason.)

Three disks in a square: critical points

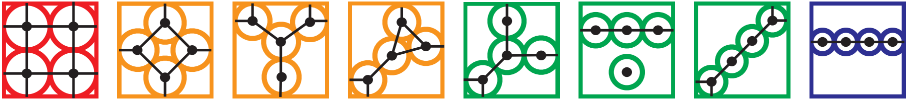


Three disks in a square: topology



disk radius r	homotopy type of $\mathcal{C}(3, r)$
$0.25433 < r$	empty
$0.25000 < r \leq 0.25433$	24 points
$0.20711 < r \leq 0.25000$	2 circles
$0.16667 < r \leq 0.20711$	wedge of 13 circles
$r \leq 0.16667$	$\mathcal{C}(3)$

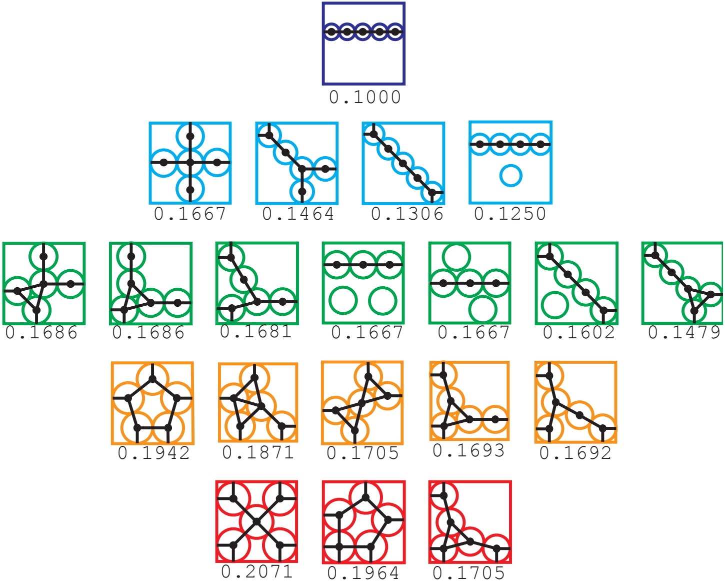
Four disks in a square: critical points



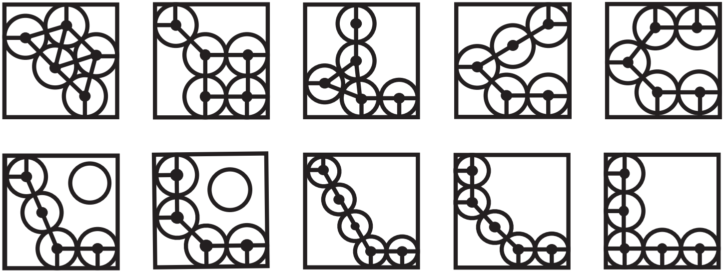
Four disks in a square: Betti numbers

radius	0.25000	0.20711	0.19231	0.18705	0.18470	0.16667	0.16019	0.12500
β_3	0	0	0	0	0	0	0	6
β_2	0	0	0	0	0	5	53	11
β_1	0	6	97	193	97	6	6	6
β_0	24	6	1	1	1	1	1	1

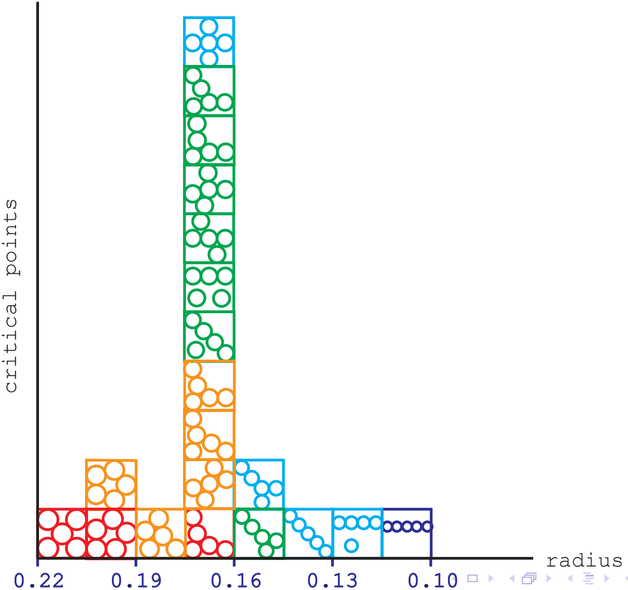
Five disks in a square: nondegenerate critical points



Five disks in a square: degenerate critical points



Five disks in a square: histogram of nondegenerate critical points



Five disks in a square: Betti numbers for $r > 0.1686$

								
radius	0.2071	0.1964	0.1942	0.1871	0.1705	0.1705	0.1693	0.1692
β_1	0	0	24	841	841	1321	1801	2761
β_0	120	600	144	1	481	481	1	1

Hard disks in a strip

(Joint work with Robert MacPherson.)

Let $\mathcal{C}(n, w)$ denote the configuration space of n disks in an infinite strip w disks wide.

Hard disks in a strip: asymptotic results for $\beta_j(n)$

Theorem (K. and MacPherson)

Fix the width $w \geq 2$ and degree $j \geq 1$, and let the number of disks $n \to \infty$.

1. *If $j < w - 2$ then β_j grows polynomially with n. In particular*

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2. *If $j \geq w - 2$ then β_j grows exponentially with n. In particular*

$$\lim_{n\to\infty} \frac{\log \beta_j}{n} = \log\left(\left\lfloor \frac{j}{w-1} \right\rfloor + 1\right).$$

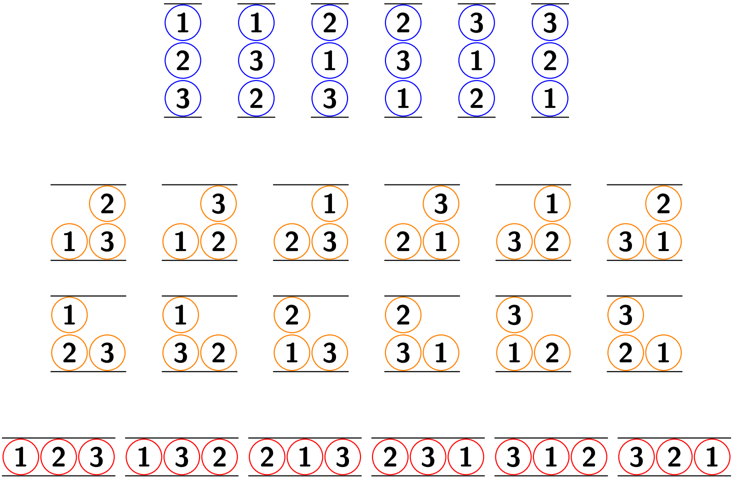
(Preprint in preparation.)

Hard disks in a strip: asymptotic results for $\beta_j(n)$

j \ w	1	2	3	4	5	6	7	8	9	10
10	0	10^n	5^n	4^n	3^n	2^n	2^n	2^n	2^n	2^n
9	0	9^n	5^n	3^n	3^n	2^n	2^n	2^n	2^n	
8	0	8^n	4^n	3^n	2^n	2^n	2^n	2^n		
7	0	7^n	4^n	3^n	2^n	2^n	2^n			
6	0	6^n	3^n	2^n	2^n	2^n				
5	0	5^n	3^n	2^n	2^n					
4	0	4^n	2^n	2^n						
3	0	3^n	2^n							
2	0	2^n								
1	$n!$									

= stable regime

Hard disks in a strip: a cell structure



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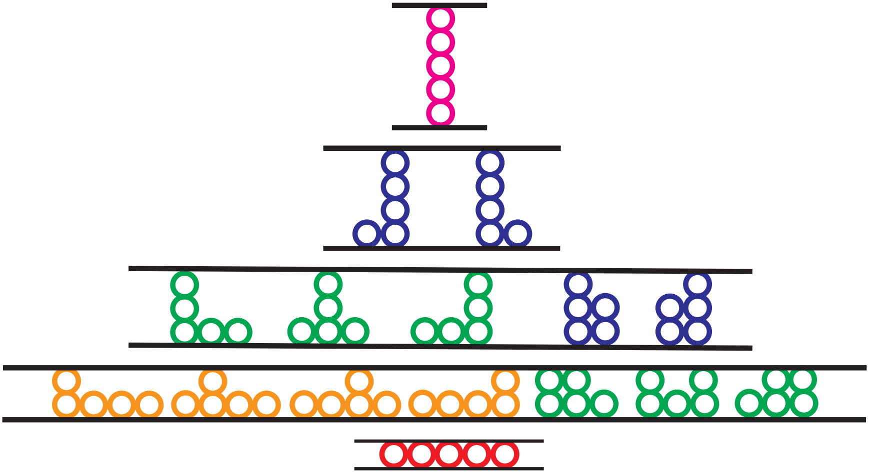

Upper bounds

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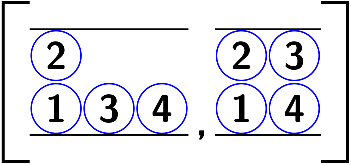
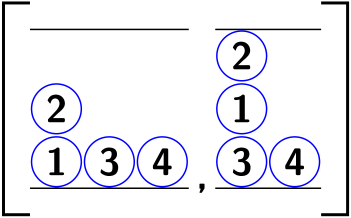
Checking that this discrete vector field is *well-defined* and *gradient* involves some delicate combinatorics...

Upper bounds

In particular which cells get matched depends the width of the strip w.



versus



Lower bounds

The essentially matching lower bounds comes from geometric arguments — namely finding submanifolds which represent nontrivial (and linearly independent) homology classes...

Open questions

1. Describe the asymptotics of the Betti numbers β_k as $n \to \infty$, for your favorite compact region $\mathcal{R}$. Statistical unimodality of Betti numbers? Concentration of homology in a small number of degrees?

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2. What is the threshold for connectivity $r = r(n)$ as $n \to \infty$?
3. Geometric questions — diameter, etc.?
4. Understanding statistical-mechanical phase transitions topologically.

Acknowledgements

Thanks to my collaborators Yuliy Baryshnikov, Peter Bubenik, Gunnar Carlsson, Jackson Gorham, Jeremy Mason, and Robert MacPherson.

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