RESEARCH STATEMENT

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Introduction

My research interests are in geometric optimization and frustration, primarily dealing with discrete packing density and configuration problems. This area has the distinction of having nice problems combined with non-obvious, counter-intuitive, or nonexistent solutions. Because of the general nature of these problems, I must call upon many different areas of mathematics: topology, soft and hard analysis, linear and non-linear programming, combinatorial and algebraic methods, and, of course, various sub-disciplines of geometry. Using a broad array of techniques, I have found the best known packing density bound for long cylinders and the first sharp non-trivial packing density bounds in high dimension. The potential applications of this area are appealingly interdisciplinary. Notably, one encounters questions about geometric optimization and frustration in chemistry, condensed matter physics and materials science.

Motivation

The study of *best* configurations, where a *best* configuration could result in minimized energy, density or other function, has a long and ancient history. A modern motivation is found in Hilbert's 18th, from *Mathematische Probleme* [5], regarding *dense* configurations:

> I point out the following question, related to the preceding one, and important to number theory and perhaps sometimes useful to physics and chemistry: How can one arrange most densely in space an infinite number of equal solids of given form, e. g., spheres with given radii or regular tetrahedra with given edges (or in prescribed position), that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?

Conway, Goodman-Strauss and Sloane [2] point out that the density of Hilbert's question is too malleable a notion to use in uniquely defining a *best* configuration, but is still natural to consider. Even then, there is an implicit assumption in Hilbert's question, that the behavior of planar configurations with respect to density is well understood. This is not the case.

Packings and Density. The prototypical packing problem is that of maximizing the density of a collection of disjoint bodies in some ambient space. For example, a collection $\mathscr{C}$ of congruent bodies in Euclidean n-space, with the density defined with respect to $B^n(r)$: expanding n-balls of radius r. This gives a modestly well-behaved notion of packing density:

$$\delta^+(\mathcal{C}) = \limsup_{r\to\infty} \frac{\mathrm{Vol}(\mathscr{C} \cap B^n(r))}{\mathrm{Vol}(B^n(r))}.$$

Then, for the particular body that constitutes a packing $\mathscr{C}$, one considers the least upper bound of density over all possible packings. In this way, we might gain some insight in to

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large-scale behavior of large configurations of a particular body, as one might find in a crystal or glass.

Structure and Jamming. Any rigidity to the structure of a *best* configuration is also of interest. In two dimensions, some cases of packings are well enough understood that the choice of a *good* structure is fairly straightforward. For example, L. Fejes Tóth [3] showed that the maximal packing density of a convex centrally-symmetric body is always attained by a lattice packing. In three dimensions, things are much harder to pin down. A. Bezdek and W. Kuperberg [1] provided one the first sharp results for the packing density of an object in $\mathbb{R}^3$, by showing that a maximal density packing of $D^2 \times \mathbb{R}$, the bi-infinite right circular cylinder, was very ridged, forcing it to have packing density $\pi/\sqrt{12}$.

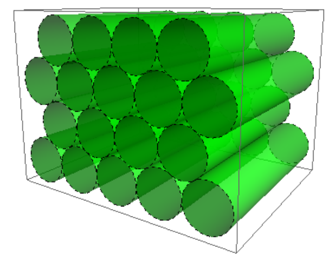

FIGURE 1. Region taken from a maximal density cylinder packing. - *Image produced in Mathematica 9.*

RESULTS

Asymptotic Bounds for Finite Cylinders. In [4], I extend the previous result of A. Bezdek and W. Kuperberg to the case of finite height cylinders.

Theorem 1. (K). *Fix $t \geq t_0 := \frac{8}{3}(\frac{4}{\sqrt{3}}+1)^3$. The upper density δ^+ of a packing $\mathscr{C}$ of $\mathbb{R}^3$ by capped cylinders of height t satisfies the inequality*

$$\delta^+(\mathscr{C}) \leq \frac{t+\frac{4}{3}}{\frac{\sqrt{12}}{\pi}(t-2t_0)+(2t_0)+\frac{4}{3}}.$$

Theorem 2. (K). *The upper density δ^+ of a packing $\mathscr{C}$ of $\mathbb{R}^3$ by cylinders of height t satisfies*

$$\delta^+(\mathscr{C}) \leq \frac{\pi}{\sqrt{12}} + \frac{10}{t}.$$

This new result is one of very few non-trivial upper bounds for packings of bounded domains in $\mathbb{R}^3$. It is of significance in that it gives bounds for a useful class of objects, cylinders, which are already used for volume estimates in polygonal curves and hyperbolic manifolds. Furthermore, it is the only known bound that is asymptoticly sharp, improving a result of W. Kuperberg and G. Fejes Tóth [7].

The asymptotic result in Theorem 1 also yields some interesting corollaries. For example,

Theorem 3. (K). *The upper density δ^+ of half-infinite cylinders is exactly $\pi/\sqrt{12}$.*

Theorem 4. (K). *Given a packing $\mathscr{C} = \{C_i\}_{i\in I}$ by non-congruent capped unit cylinders with lengths constrained to be between $\frac{8}{3}(\frac{4}{\sqrt{3}}+1)^3$ and some uniform upper bound M, the density satisfies the inequality*

$$\delta^+(\mathscr{C}) \leq \frac{t+\frac{4}{3}}{\frac{\sqrt{12}}{\pi}(t-2t_0)+(2t_0)+\frac{4}{3}}$$

where t is the infimum of cylinder length.

Methods. Results for circular cylinders do not follow from planar results for circles, and the finite height case is not a simple corollary to the infinite height case. To illustrate this, I ask you to consider one of the primary objects of study, the Dirichlet-Voronoi decomposition of a packing. This is a decomposition of the ambient space into cells, where each cell is the set of points closer to a particular object than to any other. In the case of circles in the plane, one may consider only the centers and find that it is exactly a Voronoi tessellation. The cells are convex with polygonal boundaries. For bi-infinite cylinders, it is also possible to consider the axes. Then, the cells are bounded by regions of hyperbolic paraboloids. Finally, in the case of finite height cylinders, the cells become even more degenerate. It is no longer possible to consider only the arrangement of axes, and the cells are bounded by even more degenerate surfaces.

These problems are addressed using various approximation methods from geometry, combinatorics and hard analysis. The pathological nature of the cells is resolved by considering special two-dimensional slices, the *Dirichlet slices.* These are associated with points on the axes of cylinders, and are defined to be the intersection of the Dirichlet-Voronoi cell with the plane normal to an axis and containing the associated point on that axis. Finite height cylinders can be approximated by finite height cylinders with hemispherical caps, which again have cells equivalent to the cells of their axis. Then the philosophy is that the error between packings by finite and bi-infinite cylinders occurs near the ends of axes. This error is captured by:

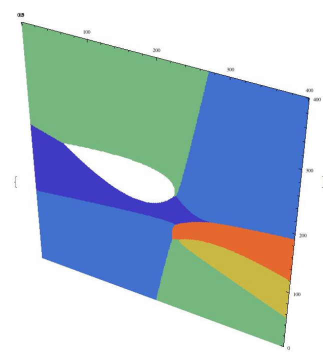

FIGURE 2. A slice of the Dirichlet-Voronoi decomposition for a random packing by bi-infinite cylinders. - *Image produced in Mathematica 9.*

Proposition 5. *Fix a packing of $\mathbb{R}^3$ by capped cylinders. Let x be a point on the axis of a cylinder. If $B_x(4/\sqrt{3})$ contains no end points of cylindrical axes, the Dirichlet slice at x has area no less than $\pi/\sqrt{12}$.*

This is a highly modified version of a result for bi-infinite cylinders. By generalizing a series of technical lemmas, it is possible to show that Dirichlet slices of the type described in the previous proposition can be truncated and rearranged, all while not increasing area, into a simple type of parabola-sided polygon, the area of which is well understood.

The density bound the becomes a problem of approximating an integral of slices over a discrete set of lines in $\mathbb{R}^3$. It is possible to reduce this to an estimate for a packing of n cylinders in $B(R)$, a finite ball of radius R, and modify the definition of density to be

$$\delta(\mathscr{C}, R) = \sum_{C_i \subseteq B(R-2/\sqrt{3})} \frac{\mathrm{Vol}(C_i)}{\mathrm{Vol}(B(R))}.$$

This can be rewritten as

$$\delta(\mathscr{C}, R) \leq \frac{\sum_{I^*} nt\pi + +n\frac{4}{3}\pi}{\sum_{I^*} \mathrm{Vol}(D_i) + n\frac{4}{3}\pi}$$

where C_i is a capped cylinder of height t, D_i is the union of the Dirichlet slices associated to the axis of C_i intersected with the finite ball of radius R, and I^* indexes the cylinders in the ball of radius $R - 2/\sqrt{3}$, chosen to avoid boundary error. Then, by are consideration of inequalities of integrals on subsets of the set of axes with respect to the Hausdorff measure, I show that

Lemma 6. *For $t \geq \frac{8}{3}(\frac{4}{\sqrt{3}} + 1)^3$,*

$$\sum_{I^*} \mathrm{Vol}(D_i) \geq n(\sqrt{12}(t - 2t_0) + \pi(2t_0)).$$

When the density functions limit behavior in R is analyzed, it gives the desired bound on the upper density of the packing $\mathcal{C}$ of $\mathbb{R}^3$.

Dimensional Reduction and Stability. Using results in affine algebra, the result for bi-infinite cylinders is also sufficient to prove higher dimensional packing density bounds for poly-cylinders.

Theorem 7. (K). *$\delta^+(D^2 \times \mathbb{R}^n) = \delta^+(D^2)$ for all natural numbers n.*

This appears to be the first non-trivial exact bound for higher dimensional objects.

Methods. While the three-dimensional density results for cylinder packings do not follow from the two-dimensional ones, in higher dimensions, transversality type results come into play. Once the core of the poly-cylinder is middle-dimensional or higher, non-intersection conditions force the cores to have a pairwise common parallel. This turns out to be sufficient to apply cylinder packing results to poly-cylinders by careful consideration of how various quotient operations behave with respect to the Voronoi-Dirichlet cells of the packing, allowing the lower-dimensional density estimates to apply.

Current Work

Pentagons. In recent years, there has been significant attention focused on the other body explicitly mentioned in Hilbert's 18th, the regular tetrahedron. I suggest that packings of regular pentagons are a reasonable toy model for tetrahedra packing, exhibiting some of the same issues of geometrical frustration. Furthermore, the packing of regular pentagons in the plane is still an open area. The "best" arrangement of pentagons in the plane is not known. The best known lower bound for the density of pentagon packings and the conjectured maximal density configuration is shown in Figure 3. It seems that only recently (2013!) have reasonable upper bounds been produced, where pentagons serve as an archetype for non-centrally-symmetric figures [8]. I expect to prove that this conjectured optimal configuration is locally optimal, in that it gives a local maximum of density in the configuration space of four pentagons with respect to a Delaunay triangulation. This is stated approximately as

Conjecture 8. *There is a open set in the configuration space of four regular pentagons in the plane, in which the maximum density with respect to its finite Delaunay triangles is* $(5 - \sqrt{5})/3 = 0.902\ldots$.

Numerical Results. I have generated numerical evidence that the conjectured optimal configuration is a local maximum for density. Starting with a Delaunay decomposition on four pentagons, local density results appear to match with conjecture. This is not the case for a three-pentagon configuration. In fact, the desired configuration is not critical, nor even near critical. There is a one-parameter family of configurations with maximally forced contact between pentagons which has an interval of higher density than the conjectured global minimum. This issue is removed by using local symmetry in a Delaunay decomposition on four pentagons, but produces a constrained non-linear program in nine variables. Using the geometric properties of the packing, it is possible to reduce locally to a more constrained linear programming problem, but with some degeneracy. The numerical solution indicates that the desired configuration is indeed a local maximum for density.

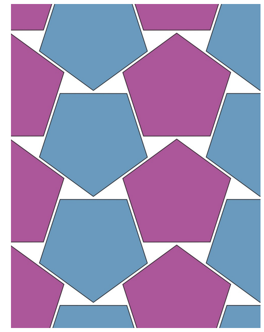

FIGURE 3. Is this a packing by regular pentagons with maximal density? - *Image courtesy of Toby Hudson (Wikimedia Commons).*

Interval Arithmetic. It remains to be shown that the reduction to a further constrained linear program is sound, and that numerical error can be overcome. My analysis indicates that the potentially unstable parts of the program can be resolved geometrically, and that the more stable parts can be resolved using some form of interval arithmetic. I am currently working on two methods to show the stability of the program: one based an approach in [6] used to prove geometric inequalities via duality, and one based on a related conical program's geometric stability under perturbation.

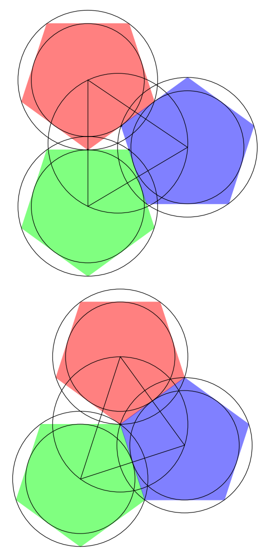

FIGURE 4. The conjectured optimal, and a configuration with locally higher density. - *Image produced in Mathematica 9.*

FUTURE WORK

From my previous work, there are several natural extensions.

Cylinders. Reduce the poly-cylinder and cylinder height requirements. In the case of poly-cylinders, where the reduction is from an infinite core to a finite one, a method similar to that used in previously-described work may be sufficient. In the case of cylinders, this would be an attempt to resolve the difficult Wilker's conjecture: that the packing density of a cylinder of arbitrary height has packs with density at most $\pi/\sqrt{12}$. There are also several other more tractable conjectures of a similar spirit in the literature.

Pentagons. Extend the local program to the whole configuration space of pentagons. This would resolve the pentagon packing question. The techniques used in this analysis are not special to pentagons, but rather use geometry common to all $(2n+1)$-gons. As it stands, the numerical results could be retooled, potentially giving local numerical results for any regular odd polygon.

Local-Global Transitions. Explore the large-scale behavior of packings. Even when dealing with density, there are configurations which are locally denser than the configurations with optimal global density. It is worthwhile to consider the behavior of large systems. This emergence of phenomena from purely geometric or topological considerations can be seen in several areas already mentioned: in the case of poly-cylinders, it is a geometrical frustration from middle-dimensional linear manifolds; in the case of pentagons, the behavior emerges from the incommensurability of the interior angle. This can be extended further by asking how small- and large-scale behaviors interact. Packing density is only one function: a hard shell energy which is fairly local. Other functions used commonly correspond to other energies with larger scale interactions, with the best configuration being the energy minimizer. How the optimal configurations vary for different functions is of interest, especially the transition where the small- and large-scale behaviors interact.

Interdisciplinary Work. Fabricate some of the special structures that appear in the literature. There are ellipsoids and elliptical cylinders, the structures of which have potential for creating geometrically doped quasi-crystals. Various other known or conjectured critical domains and configurations present attractive experimental opportunities. In the fabrication of microstructures, the methods we use to analyze packings may prove fruitful in the construction of materials by taking advantage of the obstruction to, and emergence of, large-scale properties and defects.

References

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