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 addressing 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 all dimensions greater than 3. I have also shown that the conjectured densest configuration of regular pentagons in the plane is a local minimum. The potential applications of optimal geometry 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, dates to antiquity. A modern motivation is found in Hilbert's 18th, from *Mathematische Probleme* [8], 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] note that the definition of density in 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:

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

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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 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 [4] 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 $\pi/\sqrt{12}$.

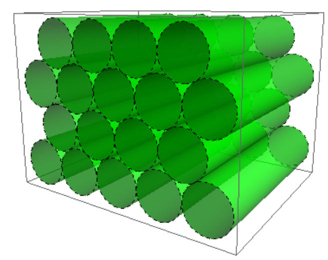

FIGURE 1. Region taken from a maximal density cylinder packing. - *Image produced in Mathematica 9.*

Results

Asymptotic Bounds for Finite Cylinders. In [7], 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 [3].

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:

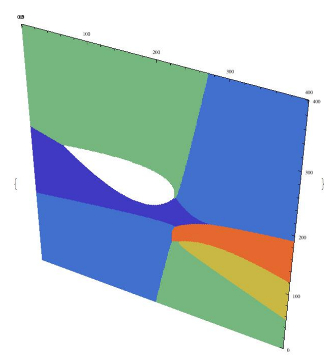

Figure 2. A slice of the Dirichlet-Voronoi decomposition for a random packing by bi-infinite cylinders. - *Image produced in Mathematica 9.*

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 [6].

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.

Pentagons. In the early 2000s, 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 [9].

I have proved that this conjectured optimal configuration is locally optimal, in that it gives a local maximum of density in the configuration space of four pentagons. This extends to packings with respect to a particularly useful topology; one that considers local separation only, thus allowing for stretching and rescaling. This is stated approximately as

Theorem 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 initially 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.

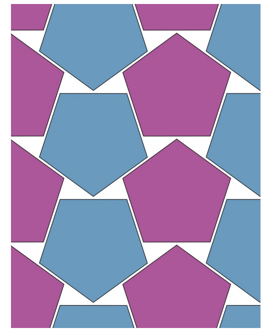

FIGURE 3. Is this a packing by regular pentagons with maximal density? - *Image courtesy of Toby Hudson (Wikimedia Commons).*

Interval Arithmetic. Further analysis of the constrained non-linear programming problem show that it can be made to satisfy a number of special conditions based on a related conical program's geometric stability under perturbation.

Theorem 9. *A nonlinear program satisfying such conditions has an isolated local maximum at 0.*

Furthermore, any numerical error from previous results can be overcome.The potentially unstable parts of the program can be resolved geometrically, and the more stable parts can be resolved using interval arithmetic.

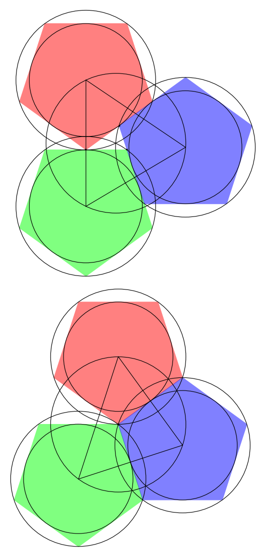

FIGURE 4. The conjectured optimal, and a configuration with locally higher density. - *Image produced in Mathematica 9.*

0.0.1. *Double lattices.* This project has been subsumed into a larger project, [5]. Working with Yoav Kallus, we were able to reformulate the previous results to apply to a general/generic convex polygon.

Current Work

Spherical cap discrepancy. given an geometric sphere $\mathbb{S}^d$ with radius 1 and normalized uniform measure σ and a spherical cap C embedded in $\mathbb{R}^{d+1}$, the *local spherical cap discrepancy* of a set X_N of N distinct points in the d-sphere is given by

$$\mathrm{D}_C[X_N] := |[\mathrm{Vol}(C) - \frac{1}{N}\#|X_N \cap C|]|$$

and the *spherical cap discrepancy* is given as

$$\mathrm{D}(X_N) := \sup_C \mathrm{D}_C[X_N].$$

which describes the largest deviation of the point measure from the uniform measure with respect to spherical caps.

I discovered that there is indeed a polynomial time algorithm to compute the discrepancy. This turns out to be the spherical version Niederreiter's algorithm for star discrepancy. This may have been neglected, as Niederreiter's algorithm is described as exponential and it is know that the discrepancy problem is NP-Hard in that setting. However, the runtime statements are with respect to dimension, and in the context of very high dimensional approximation, this is reasonable. In the context of spherical discrepancy, it is reasonable to fix the dimension $d = 2$ and consider the runtime in n, the size of the point set. Then the algorithm described is potentially of order n^4.

By implementing this algorithm, it is possible to compute the discrepancy of point sets and generate a large experimental database. Proof of concept tests give expected results in convergence, but the algorithm is not implemented in an efficient manner. For example, it could be massively parallelized.

It is also possible to use this algorithm to find a minimal discrepancy set of four points, perhaps the first explicitly constructed non-trivial set of minimal discrepancy on the sphere. It is still open if this can be used to find larger sets of points with low or minimal discrepancy. (bound given by Josef Dick on rate of convergence).

Morse theory for configuration spaces. A configuration space of a collection of spheres in a container is a subspace of the configuration space of the centers of those spheres. As the the radius of the spheres changes, the topology and geometry of the configuration space changes. These changes are characterized critical points. For certain classes of potential functions there are explicit characterizations of criticality, which equate criticality to the existence of a strut measure. Such characterizations suggest that one can use a Morse-theoretic approach to describe families of configuration spaces, building up the handlebody structure of such families as one classifies the critical configurations. This process inspires the study of critical configurations not only as special optimizers with respect to a fixed potential or class of potentials, but as transition points for the geometry and topology of families of configuration spaces.

To determine which configurations are critical, this project will develop and refine various tools from combinatorial and computational optimization. Configurations need to be certified as critical, and how they affect the structure of configuration space must also be characterized. The criticality of a configuration might be characterized via balance or rigidity criteria. Determining criticality in this manner involves generating and sorting combinatorial objects such as contact graphs. A major difficulty in the analysis of critical points comes from the inherent constraints. As with any constrained optimization problem, there may be critical configurations that arise from boundary conditions. In this context, analysis may become highly nontrivial as the Morse index of a critical point interacts with the boundary. For example, criticality may no longer be completely characterized by stationarity. When the packing radius of a critical kissing configuration is varied, there may be linear variations that contribute to the index but are associated with quadratic variations in the co-index. However, there are computational approaches to certify a constrained configuration as critical and characterize it from a parametrization of configuration space based on work developed in previous sections.

Global pentagons. Initial computations indicate that it is possible to extend the local program to the whole configuration space of pentagons. This would resolve the packing question for regular pentagons. The techniques used in this analysis are not special to pentagons, but rather use geometry common to all $(2n+1)$-gons.

Future Work

Due to the evolving of the previous projects, it is difficult to separate specific future projects from the ongoing ones. From previous work completed, there are several natural extensions that seem worth mentioning in a more speculative setting.

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.

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.

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