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 call upon many different areas of mathematics: topology, soft and hard analysis, linear and non-linear programming, combinatorial and algebraic methods, and 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. I have shown with Yoav Kallus that this local result extends to other polygons, and with Thomas Hales that it extends to a global result for regular pentagons, both results are the first of their kind. The potential applications of this form 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 is one that minimizes energy, density or some other function, dates to antiquity. A modern motivation is found in Hilbert's 18th, from *Mathematische Probleme* [10], 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.

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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 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 $\pi/\sqrt{12}$.

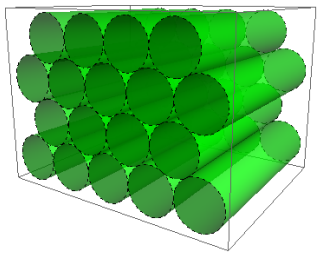

FIGURE 1. Region taken from a maximal density cylinder packing. - *Image produced in Mathematica 9.*

RESULTS

Asymptotic Bounds for Finite Cylinders. In [8], I extend the previous result of A. Bezdek and W. Kuperberg to the case of finite height cylinders.

Theorem 1 (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 4 also yields some interesting corollaries. For example,

Theorem 2. (K). *The upper density δ^+ of half-infinite cylinders is exactly $\pi/\sqrt{12}$.*

Theorem 3 (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* and bounding their area. 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. The density bound the becomes a problem of approximating an integral of slices over a discrete set of lines in $\mathbb{R}^3$ yielding

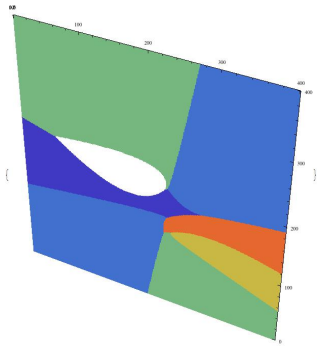

FIGURE 2. A slice of the Dirichlet-Voronoi decomposition for a random packing by bi-infinite cylinders. - *Image produced in Mathematica 9.*

Theorem 4. (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

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

Sharp Bounds in High Dimensions. Using results in affine algebra, the result for bi-infinite cylinders is also sufficient to prove higher dimensional packing density bounds for poly-cylinders [9].

Theorem 5. (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.

Global Optimality for 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. It seems that the first reasonable upper bounds were produced in 2013, where pentagons serve as an archetype for non-centrally-symmetric figures [11].

Work with Thomas Hales [5] proves that the best known lower bound for the density of pentagon packings, shown in Figure 3, is in fact the global maximizer for density.

Theorem 6 (Hales, K)**.** *The maximum density of a packing of regular pentagons in the plane is* $(5-\sqrt{5})/3 = 0.902\ldots$.

Local Optimality of the Double Lattice. I had previous proved that the then conjectured optimal configuration was 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 7 (K)**.** *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* $(5-\sqrt{5})/3 = 0.902\ldots$.

This result was extended in recent work with Yoav Kallus [7] reformulating the local result to apply to a general/generic convex polygon.

Theorem 8 (Kallus, K)**.** *There is a open set in the configuration space of a generic polygon in the plane, in which the maximum density with respect to its finite Delaunay triangles is given by the optimal double lattice packing.*

Numerical Results. Although the initial numerical results are superseded by the theorems of the previous sections, I want to mention that this project started by generating sufficient evidence that the conjectured optimal configuration is a local maximum for density. Starting with a Delaunay decomposition on four pentagons, local density results appeared to match with conjecture.

This was 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

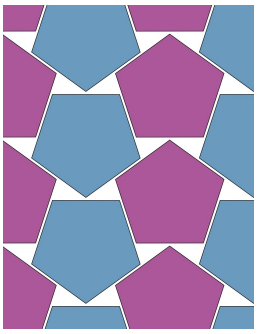

FIGURE 3. Pentagons in a densest packing arrangement.
- *Image courtesy of Toby Hudson (Wikimedia Commons).*

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.

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 (K)**.** *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.

Current Work

In addition to continuing work on projects related to the previous section, I have several other areas of active research.

Computing Spherical Cap Discrepancy. Given a 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 of order n^4. At some cost in memory, it is possible to reduce the runtime to order $n^3 \log n$.

By implementing this algorithm in work with Alden Walker, 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 still 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.

Critical Configurations. 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 define 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, we would like to 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 described. 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.

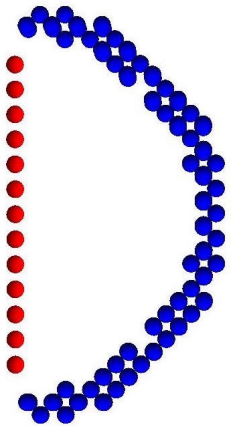

FIGURE 4. A cluster not discoverable by existing algorithms. - *Image produced in Mathematica 10.*

Clusters of Sticky Spheres. Recent work in materials science has led to interest in the enumeration of clusters of rigid sticky sphere clusters (e.g. [6]). These are essentially rigid bar frameworks with an integrality condition on the edge lengths. For clusters containing a small number of spheres, there are algorithmic approaches to generating and checking the allowed configurations. I am currently using a mechanical approach to construct examples of medium size clusters that are poorly behaved with respect to the rules used for current enumeration algorithms. See Figure 4.

Hyperuniform Structures. Consider points $(X_i)_i$ generated by a point process on a space, such that $\mu_n := \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}$, the empirical measure, converges weakly to the uniform measure on the space.

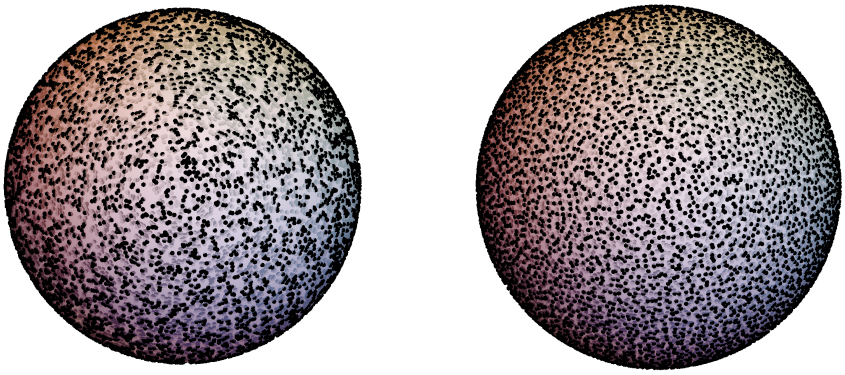

FIGURE 5. Left: 10000 uniform random points. Right: 10000 determinantal points. - *Image produced in Mathematica 10.*

For test sets B in this space, $\mu_n(B)$ is the random variable counting how many points the process at time n has placed in B. Low variance of $\mu_n(B)$ suggests that there is extra order in the point set. Torquato and Stillinger identified this extra order in the context of thermodynamical ensembles in Euclidean space and called it *hyperuniformity*.

When we consider a process that places an increasing number of points in shrinking test sets, heuristically, *hyperuniformity in the compact setting* should mean that the variance $\mathrm{Var}\,[N_R]$ is smaller than in the i.i.d. case. This becomes more precise in the following.

A point process on a manifold M with joint densities $(\rho^{(n)})_{n\in\mathbb{N}}$ is called **determinantal with kernel** $K^{(n)}$, if

$$\rho^{(n)}(x_1,\dots,x_n) = \det(K^{(n)}(x_i,x_j))_{i,j=1}^n \quad \text{for all } n\in\mathbb{N},\ x_i\in M.$$

In particular, there is a determinantal point process on $\mathbb{S}^2$ with density

$$\rho^{(n)}(p_1,\dots,p_n) = const.\prod_{i<j}\|p_i-p_j\|_{\mathbb{R}^3}^2,$$

with respect to the normalized Lebesgue measure σ on $\mathbb{S}^2$. Configurations where points are close together have low probability according to this density. Processes with joint densities

$$\rho^{(n)}(x_1,\dots,x_n) = const.\prod_{i<j}\|x_i-x_j\|^2$$

on compact $M\subseteq\mathbb{R}^d$ exhibit repulsion of points. It is apparent that such point sets are good in that they are "uniformly distributed more uniformly" than random points. See Figure 5.

FUTURE WORK

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.

Construct various linkages related to critical configurations. Such configurations define frameworks with some degrees of freedom. For example, the jitterbug framework that appears when considering configurations of 12 points on a sphere has 6 degrees of freedom in space corresponding to the Euclidean group of motions. This means that there is a very simple linkage that transforms 6 linear motions into rotations and translations.

Use high quality point sets for integration and motion planning can increase efficiency. Currently, one of the best ways to plan motion or to integrate is to randomly sample (Monte Carlo) configuration space. Using sampling schemes coming from deterministic or determinantal processes (Quasi-Monte Carlo) can reduce the time it takes to explore large portions of configuration space.

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