Critical packings (in the sphere)

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Abstract

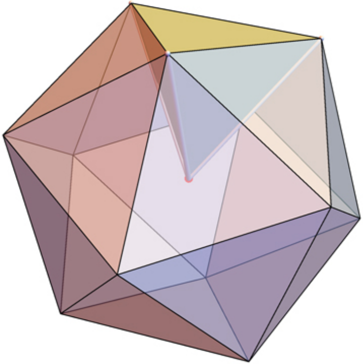
There are a number of classical problems in geometric optimization that ask for the “best” configuration of points with respect to some nice function. In particular, we are interested in the relationships between various notions of criticality and the properties of critical points for functions – like the packing/injectivity radius – on configuration spaces of points in the sphere. We will explore some of the history of and the ideas that surround this problem.

Based on work with
Robert Kusner, Jeffrey Lagarias & Senya Shlosman
arXiv 1611.10297

Aristotle: On The Heavens (c. 350 B.C.)

Question

Is the regular icosahedron made of 20 regular tetrahedra?



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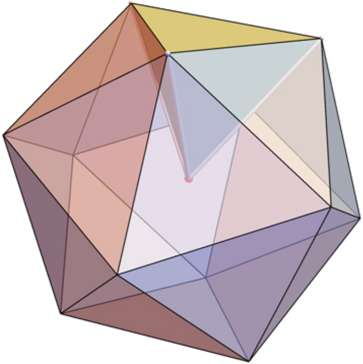
No! For circumradius 1, we can compute the edge length to be

$$\left(\frac{1}{2}\sqrt{\frac{1}{2}(5+\sqrt{5})}\right)^{-1} = 1.0514\ldots.$$



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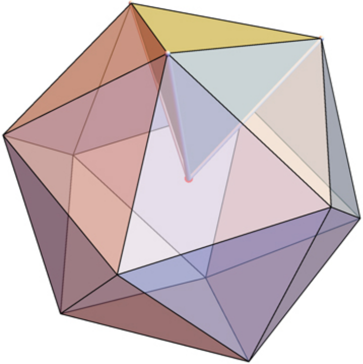
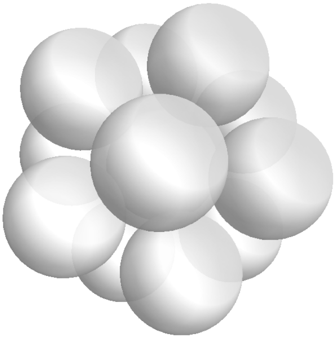


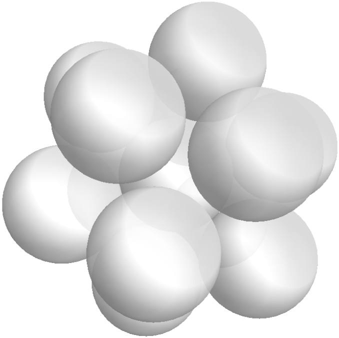
Riddle

Answer the question synthetically.

Remark

If we place unit spheres at the vertices of that regular icosahedron, there is a lot of space between them.





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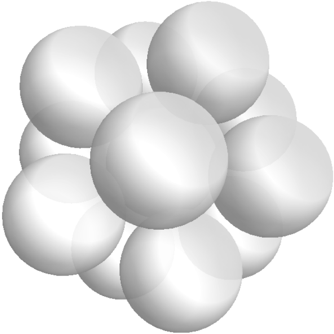
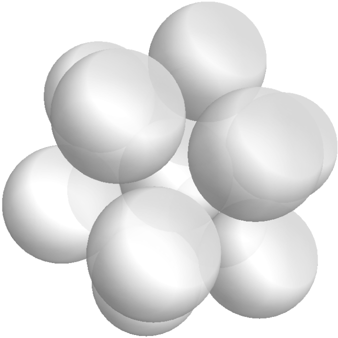
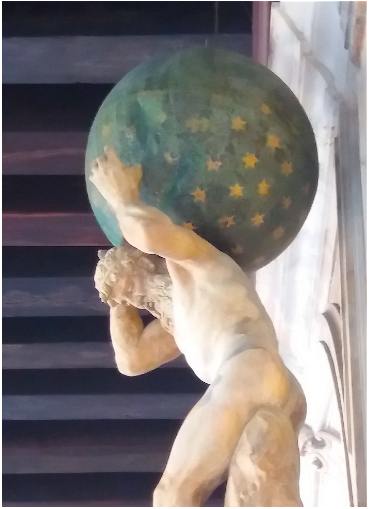




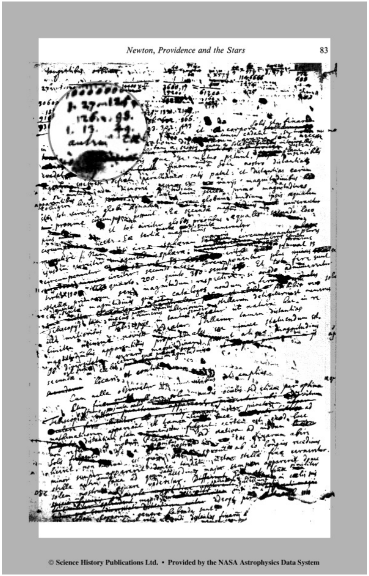
Question (Newton-Gregory)

Can we fit in a thirteenth sphere?



For Newton and Gregory, this was a problem of mechanics: Why the fixed stars don't all fall into the sun.

Newton and Gregory: Principia (revision c. 1694)


Newton, Providence and the Stars 83

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In a draft for the second edition of *Principia*, Newton considers stars of various magnitudes as modeled by arrangements of equal balls.

This method was abandoned, but history lends the names of Newton and Gregory to the problem.

Kepler: Epitome Astronomiae Copernicanae (c. 1620)

LIBER PRIMVS. 35

Si de fixis certius nihil constat, videtur illa regio infinita esse; nec Sol hic noster aliud erit, quam una ex fixis, nobis major & clarior visa, quia propior quam fixa: atq; ita circa quamlibet fixam poterit esse talis mundus, qualis circa nos est; Vel, quod eodem redit, inter innumerabiles locos in illa infinitâ fixarum congerie, Mundus hic noster cum Sole suo erit unus, nulla re diversus à locis alijs circa fixas singulares: Vt in subjecta figura litera M?

Ita quidem Brunus & veterum aliqui. At non sequitur, si centra fixarum non sunt in eadem superficie Sphaerica; propterea regionem per quam sunt dispersae fixae, esse vndiquaque sibi similem.

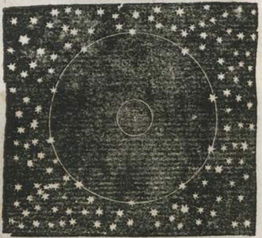
Habet enim illa omninò vacuum aliquem sinum, cavumque ingens, à fixarum agmine, confertim circumfuso,

C 2 ceu

36 EPITOMES ASTRONOMIÆ,

ceu à muro vel fornice quodam conclusum & circumscriptum: & in hujus Cavi ingentis complexu, Tellus nostra cum sole & stellis mobilibus comprehensa est.

Vide subjectam figuram.



Quod habes hujus rei Argumentum?

Si Regio fixarum vndique similiter esset consita stellis, etiam in vicinia nostri mundi mobilis sic ut situs mundi solisque nostri nullam haber[...] circumscriptionem præ situ fixæ alicujus [...] nobis paucæ aliquæ fixæ ingentes, nec ul[...] tot angulos habet Icosaedron) possent [...]dem à nobis distantiæ, & magnitudinis: [...] haud multo plures, haberent jam distantiam duplicatam proximarum; aliæ superiores triplicatam, & sic consequentes semper multipliciorem.

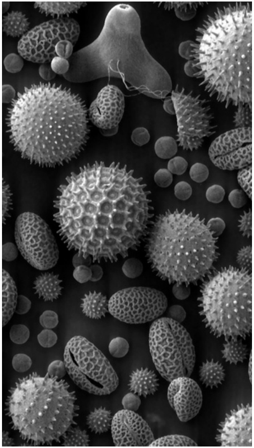
nc appare duodecim e omnes

Ac cùm omnium maximæ, tam appareant parvæ, ut vix instrumentis possint notari aut mensurari: quæ igitur duplo aut triplo &c. distarent longius, duplo & triplo apparerent minores, positis æqualibus ipsis veris magnitudinibus

Question

What is the maximal radius possible for N equal spheres, all touching a central sphere of radius 1?

The original formulation of the *Tammes problem*: How many spherical caps of angular diameter θ that can be placed without overlap?



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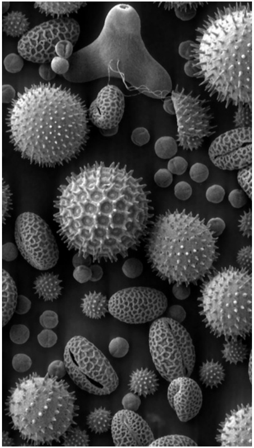
Tammes was studying pollen grains and empirically determined 6 for $\theta = \frac{2\pi}{4}$ but no more than 4 for $\theta > \frac{2\pi}{4}$.



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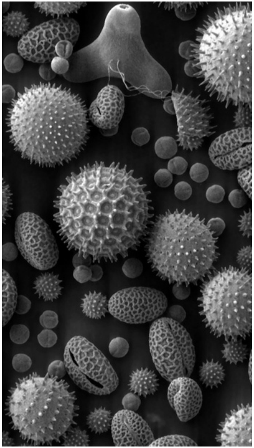
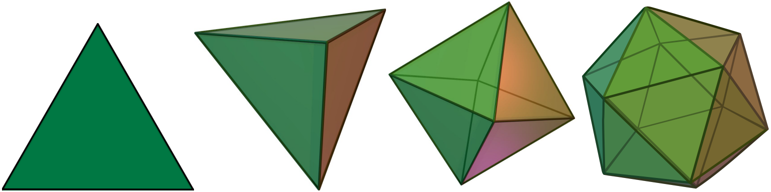


Remark

The maximizing configuration for 5 is not unique.

The Tammes problem was initially solved for $N = 3, 4, 6$ and 12, with configurations of cap centers for $N = 3$ attained by vertices of an equatorial equilateral triangle and for $N = \{4, 6, 12\}$ by vertices of regular tetrahedron, octahedron and icosahedron.



Tammes Problem: L. Fejes-Tóth (1943)

Fejes-Tóth proved the following

Theorem

for N points on the sphere, there are 2 with angular distance

$$\theta \leq \arccos\left(\frac{(\cot(\omega)^2 - 1}{2}\right), \quad \omega = \left(\frac{N}{N-2}\right)\frac{\pi}{6}.$$

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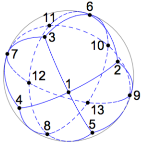
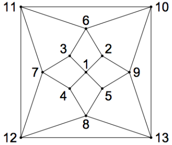
Remark

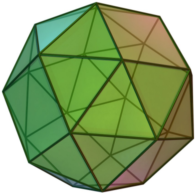
θ is the edge length of a equilateral spherical triangle with the expected area for triangle in an triangulation with N vertices.

Tammes Problem: Other N

The Tammes problem has been solved exactly for only $3 \leq N \leq 14$ and $N = 24$. It was solved for $N = \{5, 7, 8, 9\}$ by Schütte and van der Waerden in 1951, $N = \{10, 11\}$ by Danzer in his 1963 Habilitationsschrift.







The case $N = 24$ was solved by Robinson in 1961 showing the configuration of centers were the vertices of a snub cube. The cases $N = \{13, 14\}$ were solved by Musin and Tarasov, enumerating all plausible graphs by computer.

Question

We have some solutions for the global maxima for the Tammes Problem, but there could be other interesting configurations. What about other critical points? Are there local maxima?

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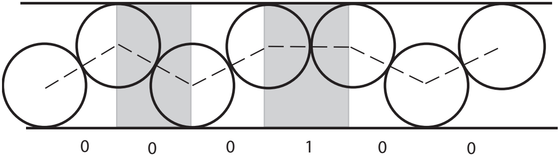

Remark

One "similar" model that can be analyzed completely is the quasi-1D packing problem. Such packings have lots of maxima.

Key Players

Definition

The classical *configuration space* $\mathrm{Conf}(N) := \mathrm{Conf}(\mathbb{S}^2, N)$ of N distinct labeled points on the unit 2-sphere $\mathbb{S}^2$.

Remark

There also is a reduced configuration space *to consider:*

$$\mathrm{Conf}(N)/SO(3).$$

Also assume $N \geq 3$ to avoid degenerate cases.

Definition

Configurations are $\mathbf{U} := (\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_N)$, where the $\mathbf{u}_j \in \mathbb{S}^2$ are distinct points.

Key Players

Definition

The *injectivity radius function* $\rho : \mathrm{Conf}(N) \to \mathbb{R}^+$ assigns a configuration $\mathbf{U} := (\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N) \in (\mathbb{S}^2)^N$ the value

$$\rho(\mathbf{U}) := \frac{1}{2}\big(\min_{i \neq j} \theta(\mathbf{u}_i, \mathbf{u}_j)\big),$$

where $\theta(\mathbf{u}_i, \mathbf{u}_j)$ is the angular distance between $\mathbf{u}_i$ and $\mathbf{u}_j$.

Remark

Since ρ is invariant under the action of $SO(3)$, it descends to a well defined function on the reduced space.

Definition

$$\mathrm{Conf}(N; \theta) := \{\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N) : \rho(\mathbf{U}) \geq \frac{\theta}{2}\}.$$

Morse Theory

Morse theory concerns how topology changes for the super level sets of a smooth real-valued function on a manifold.

Definition (super level set)

For $f : M \to \mathbb{R}$, $M^a := \{x \in M : f(x) \geq a\}$ is a superlevel set.

Theorem

Given a smooth function $f : M \to \mathbb{R}$ and an interval $[a, b]$ with compact preimage, and $[a, b]$ contains no critical values. Then M^a is diffeomorphic to M^b.

It is only at the critical values of the function that the topology of the super level *might* change.

Remark

The injectivity radius function is not Morse.

The injectivity radius function ρ on $\mathrm{Conf}(N)$ is not smooth: it is a min-function for a finite number of smooth functions. But we may still be inspired by Morse theory to pass between the topological, analytic and geometric notions of “critical”.

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To vary a configuration $\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N) \in \mathrm{Conf}(N) \subset (\mathbb{S}^2)^N$ along a tangent vector $\mathbf{V} = (\mathbf{v}_1, ..., \mathbf{v}_N)$ to $\mathrm{Conf}(N)$ at $\mathbf{U}$, use an ersatz exponential map.

Morse Theory

For sufficiently small $\mathbf{V}$, define a nearby configuration

$$\mathbf{U}\#\mathbf{V} = (\frac{\mathbf{u}_1 + \mathbf{v}_1}{|\mathbf{u}_1 + \mathbf{v}_1|}, ..., \frac{\mathbf{u}_N + \mathbf{v}_N}{|\mathbf{u}_N + \mathbf{v}_N|}) \in \mathrm{Conf}(N) \subset (\mathbb{S}^2)^N$$

by summing and projecting each factor back to $\mathbb{S}^2$.
In particular, the $\mathbf{V}$-directional derivative of a smooth function f on $\mathrm{Conf}(N)$ at $\mathbf{U}$ is $\frac{d}{dt}|_{t=0} f(\mathbf{U}\#t\mathbf{V})$.

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Definition

$\mathbf{U}$ is a critical point for smooth f provided all its $\mathbf{V}$-derivatives vanish at $\mathbf{U}$. That is, the increment $f(\mathbf{U}\#\mathbf{V}) - f(\mathbf{U}) = o(\mathbf{V})$.

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In particular, the $\mathbf{V}$-directional derivative of a smooth function f on $\mathrm{Conf}(N)$ at $\mathbf{U}$ is $\frac{d}{dt}|_{t=0} f(\mathbf{U}\#t\mathbf{V})$.

Definition

A configuration $\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N) \in \mathrm{Conf}(N)$ is *critical for maximizing* ρ provided for every sufficiently small $\mathbf{V} = (\mathbf{v}_1, ..., \mathbf{v}_N)$, we have $\max[\rho(\mathbf{U}\#\mathbf{V}) - \rho(\mathbf{U}), 0] = o(\mathbf{V})$.
That is, a configuration $\mathbf{U}$ is *critical for maximizing* if there is no variation $\mathbf{V}$ that can increase ρ to first order.

If we are not critical for maximizing, there exists a variation $\mathbf{V}$ which increases ρ to first order. By the definition of ρ as a min-function, the distance between all pairs $(\mathbf{u}_i, \mathbf{u}_j)$ realizing the minimal angular distance $\theta(\mathbf{u}_i, \mathbf{u}_j) = \theta_o$ increases to first order along $\mathbf{V}$. So there is also a notion of regular value analogous to the smooth case.

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Theorem (Topological Regularity)

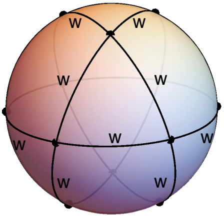
If such a variation exists for all configurations in this $\rho = \theta_o$-level set, then this level is topologically regular: *that is, the variations provide a deformation retraction from $\mathrm{Conf}(N; \theta_o - \varepsilon)$ to $\mathrm{Conf}(N; \theta_o + \varepsilon)$ for some $\varepsilon > 0$.*

Definition

For $\mathbf{U} \in \mathrm{Conf}(N;\theta)$, the *contact graph* of $\mathbf{U}$ is the graph embedded in $\mathbb{S}^2$ with vertices given by points $\mathbf{u}_i$ in $\mathbf{U}$ and edges given by the geodesic segments $[\mathbf{u}_i, \mathbf{u}_j]$ when $d(\mathbf{u}_i, \mathbf{u}_j) = \theta$.

Definition

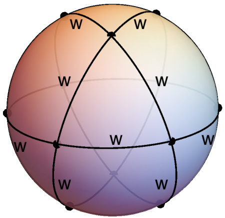
A *stress graph* for $\mathbf{U} \in \mathrm{Conf}(N;\theta)$ is a contact graph with nonnegative weights w_e on each geodesic edge $e = [\mathbf{u}_i, \mathbf{u}_j]$.



A stress graph associates a system of *tangential forces* to edges $e = [\mathbf{u}_i, \mathbf{u}_j]$ of the contact graph. The forces have magnitude w_e, are tangent to $\mathbb{S}^2$ at each point $\mathbf{u}_i$ of $\mathbf{U}$, and point outward at the ends of each edge.

Definition

A stress graph is *balanced* if the sum of the forces in $T_{\mathbf{u}_i}\mathbb{S}^2$ is zero for all points of $\mathbf{U}$. A configuration $\mathbf{U}$ is *balanced* if it has a balanced stress graph for some choice of non-negative, not everywhere zero weights on its edges.



Balanced Graphs

Theorem

For each critical value θ for the injectivity radius ρ, there exists a balanced configuration $\mathbf{U}$. The vertices of the contact graph are a subset of the points in $\mathbf{U}$ and the geodesic edges of the contact graph all have length θ.

Theorem

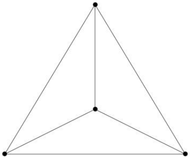
If a configuration $\mathbf{U}$ on $\mathbb{S}^2$ is balanced, then $\mathbf{U}$ is critical for maximizing the injectivity radius ρ.

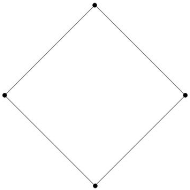
Summary

There are certain radii that are critical: The topology of the configuration space changes*.

These radii also correspond to configurations of points that are force balanced: There exists a non-trivial strut measure on the contact graph that force balances all the vertices.

Such configurations obstruct the ρ-subgradient flow, which would give a deformation retraction.





Exploring Configuration Space

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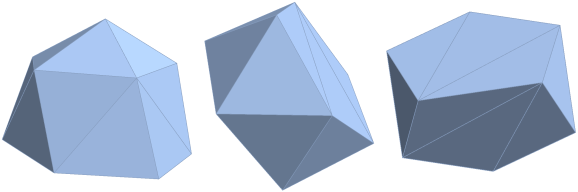
We can easily hack together an approximation of a sub-gradient descent algorithm for the injectivity radius function. With that, it is a quick step to make some conjectures about local maxima, global maxima, and the distribution of maxima just by exploring the basins of attraction randomly.



Thank you for your attention!

wkusner.github.io

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