Centroidal Voronoi Tessellations And Gersho's Conjecture In 3D And On The Sphere

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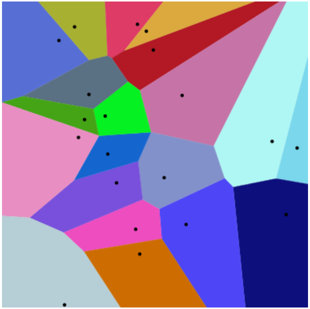
(Joint work with Rustum Choksi)

Question: given a continuous distribution of mass, which we want to approximate with only N points, how to place them so to minimize the approximation error?

Voronoi diagrams, Euclidean distance:



Given a collection if points $\{y_k\}$ (the black dots), the Voronoi cell of a point y_k is the set

$$V := \{x \in Q : |x - y_k| \leq |x - y_j| \text{ for all } j \neq k\}.$$

We associate to $\{y_k\}_{k=1}^n$ the second moment energy:

$$E(Y) := \int_Q \mathrm{dist}^2(x, Y)\mathrm{d}x = \sum_{k=1}^n E(V_k),$$

$$E(V_k) := \int_{V_k} |x - y_k|^2 \mathrm{d}x, \qquad k = 1, \cdots, n$$

where $Q = [0,1]^d$ and V_k denotes the Voronoi cell of y_k.

Centroid of a set: given a set Ω, a centroid is a point $y \in \Omega$ such that

$$\int_\Omega (x - y)\mathrm{d}x = 0 \Longrightarrow y = \frac{1}{|\Omega|}\int_\Omega x\mathrm{d}x.$$

Observation: optimal Voronoi tessellations are also centroidal Voronoi tessellation (CVT).

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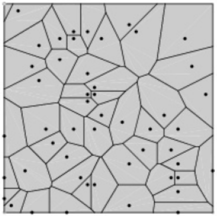
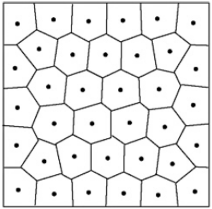
Voronoi tessellations:





Left: a Voronoi diagram   Right: a centroidal Voronoi tessellation (CVT)

Voronoi tessellations are all around us: some examples and applications

Centroidal Voronoi tessellation (CVT) in nature:

[b]0.5  [b]0.4 

Left: SEM of the corneal endothelium of a dog.

Right: Honeycomb

Giant's causeway

Voronoi tessellations are useful in a wide array of applications:

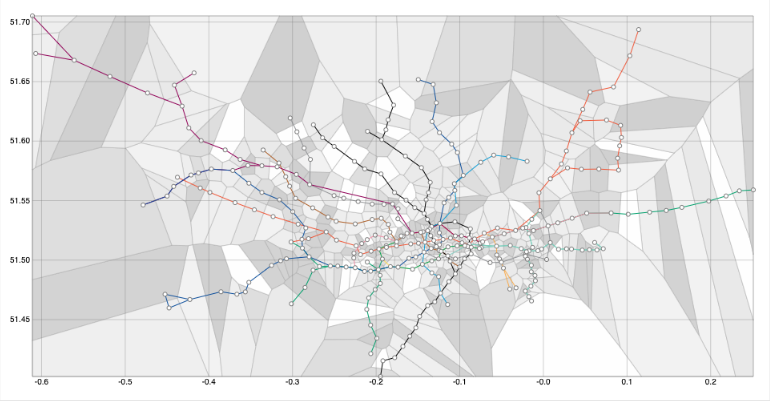


Figure: London's tube network, with Voronoi cells of its stations.

The Voronoi cells of a stations represents the region closest to that particular station.

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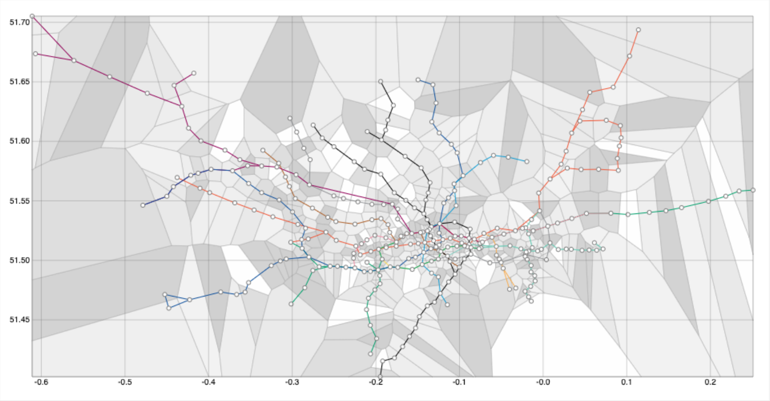

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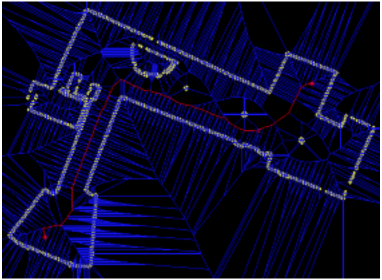

Figure: Driving path (red), and obstacles detected (white).

By driving on edges of Voronoi cells of the obstacles, the car keeps a maximal distance from these...

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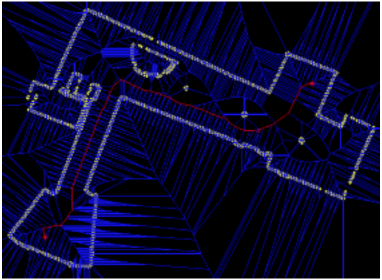

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The idea of Voronoi tessellations is quite *not* new...

Figure: "Boundary of equal distance between Broad Street Pump and other Pumps", J. Snow's report on the cholera outbreak in the Parish of St. James, Westminster 1854.

Voronoi cell of Broad Street Pump, i.e. the region where people collected (infected) water from this pump.

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Gersho's conjecture (1979)

There exists a polytope V with $|V| = 1$ which tiles the space with congruent copies such that the following holds: let $(Y_n)_n$ be a sequence of minimizers, with Y_n minimizer with n points, then the Voronoi cells of points Y_n are asymptotically congruent to $n^{\alpha(d)}V$ as $n \to +\infty$.

Note:

1. the polytope V can depend on the dimension d.
2. Nothing is said about the geometry of V.
3. This conjecture is for $n \to +\infty$. Nothing is said, or expected, for finite n.

So Gersho's conjecture is a **crystallization problem**.

Crystallization problems are notoriously easy-looking, but relatively hard:

1. Seems *obviously* true in simulations...
2. It is *never* easy when it comes to proofs...

An example from Ohta-Kawasaki:

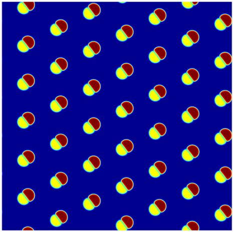

Figure: Image courtesy of Chong Wang et al.

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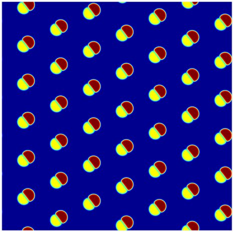

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Minimizers seems to distribute along a triangular lattice, with all double bubbles being parallel...

...But proving it will be anything but trivial.

Even "simpler" crystallization problems are highly nontrivial:

1. Heitmann and Radin (1980): interaction energy

$$V(r) := \begin{cases} +\infty & \text{if } 0 \leq r < 1, \\ -1 & \text{if } r = 1, \\ 0 & \text{if } r > 1, \end{cases}$$

2. Theil (2005): Lennard-Jones like interaction energy in 2D

Minimizers of both of these problems crystallize into a triangular lattice... These energies are highly **nonlocal** and **nonconvex**.

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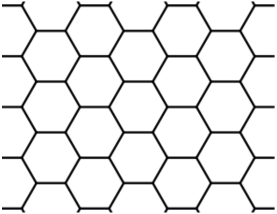
Gersho's conjecture: State of art

Known results:

1. Gersho's conjecture is fully proven in $2D$ (Fejes Tóth, Gruber, etc.): the optimal Voronoi tessellation is the triangular lattice ("honeycomb").



2. Open for higher dimensions.

Gruber's arguments for 2D:

1. optimal with k edges are regular k-gons.
2. The function $(k, A) \mapsto g(k, A)$ is convex.

$$g(k, A) := \text{energy of optimal convex } k\text{-gon with area } A.$$

3. The average number of sides in a Voronoi tessellation is 6 (by Euler's polytope formula).

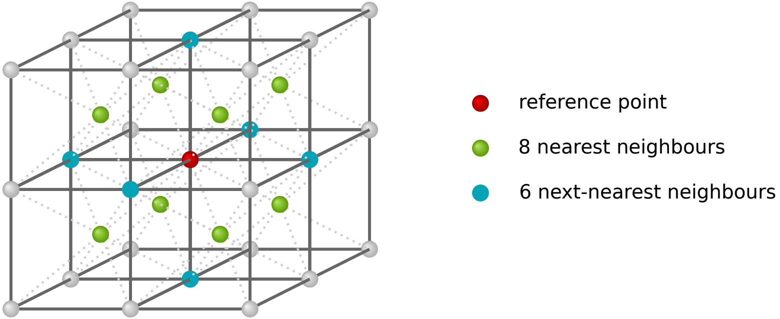
Then, for any arbitrary tessellation Y_n (with $\sharp Y_n = n$), of Q, let $\{V_k\}$ be the collection of Voronoi cells, and let α_k be the number of faces of V_k. Thus it follows

$$\begin{aligned} E(Y_n) = \sum_{k=1}^{n} \int_{V_k} |x-y|^2 \mathrm{d}x &\geq \sum_{k=1}^{n} g(\alpha_k, |V_k|) \\ &\geq ng(6, 1/n) + \text{error due to boundary effects.} \end{aligned}$$

Since the error due to boundary effects is a higher order term compared to $ng(6, 1/n)$, it follows that the optimal tessellation (as $n \to +\infty$) consists of congruent copies of a space tiling polyhedron realizing $g(6, 1/n)$.

Conjecture

The optimal lattice in 3D is the body centered cubic (BCC) lattice.



Numerical results seem to support this (Du et al. 2005).

Main difficulties in 3D:

1. No regular k-hedra.
2. Very difficult to compute the energy of a generic k-hedron.

Moreover:

1. Gersho's conjecture is **nonlocal** and **infinite dimensional**.
2. No a priori bounds on the geometric complexity of Voronoi cells.

Even deeper difficulties in 3D

Deeper causes: existence of universally optimal lattices.

- (Cohn, Viazovska et al.) $\mathbb{R}^8$ does have a universally optimal lattice ($\mathbb{E}_8$), and so does $\mathbb{R}^{24}$ (Leech lattice).
- (unproven, but likely to be true) $\mathbb{R}^2$ should have a universally optimal lattice (triangular lattice).
  This lattice is optimal for several problems:
  - sphere packing
  - optimal foam
  - crystallization of two-body interaction potentials
  - total first eigenvalues of $-\Delta$
- $\mathbb{R}^3$ is hugely unlikely to have a universally optimal lattice... BCC (Body Centered Cubic), FCC (Face Centered Cubic), HCP (Hexagonal Close Packing), and even non lattice structures (e.g. Weaire-Phelan structure) are potentially optimal configurations...

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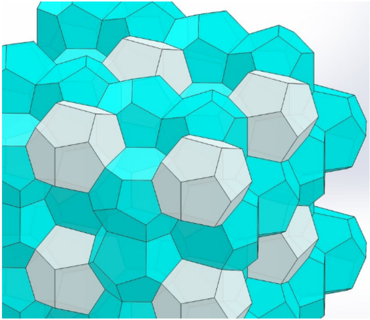

Figure: The Weaire-Phelan structure.

The Weaire-Phelan structure disproved the century old Kelvin conjecture that the "optimal foam" (i.e. packing with smallest surface area) was given by the bitruncated cubic honeycomb structure.

The Weaire-Phelan structure uses **two** polyhedra, and shows little regularity when sectioned along planes...

Figure: If you take sections of the Wearie-Phelan structure...

Geometric complexity of optimal CVTs

Main result:

Upper bound on the number of faces (Choksi and L.)

There exists a computable $N \approx 10^{20}$ such that Voronoi cells in optimal CVTs have at most N faces.

The constant N is quite large, but **finite**.

Domain $Q = [0,1]^3$, n generators. Expected averages.

1. Average diameter of each Voronoi cell $O(n^{-1/3})$.
2. Average volume of each Voronoi cell $O(n^{-1})$.
3. Average energy of each Voronoi cell $O(n^{-5/3})$.

Since the second moment is "convex", an optimal tessellation should be made of cells whose properties should not differ too much from the averages...

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Prove that all the above quantities differ from the average by a uniform multiplicative constant. But, there is far too little regularity to use anything "powerful".

Main idea (quite simple one...)

- remove a point from some cell: this **increases** the energy
- add such point elsewhere: this **decreases** the energy

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Key ingredients.

1. Crucial: reduction when adding another point.
2. Lower bound on the distance to a closest neighbor.
3. Lower/upper bound on the diameter of Voronoi cells.
4. Lower bound on the volume of Voronoi cells.
5. Boundary cells can be ignored.

Maximum geometric complexity of Voronoi cells (Choksi, L.)

For any $y \in Y_n$, its Voronoi cell V is a convex polyhedron with at most

$$N = \frac{9\pi\Gamma_4^2}{16\Gamma_1}$$

faces.

- All faces of any Voronoi cell belong to axial plane of the line segment between 2 generators, whose Voronoi cells share a boundary.
- **Can't be too far away**: if two atoms $y', y'' \in Y_n$ satisfy

$$|y' - y''| > 2\Gamma_4 n^{-1/3} \geq 2\text{maximum diameter}$$

  then their Voronoi cells do not share boundaries.
- **Upper bound on diameter**: ... so if y, y' share boundary, then the *entire* Voronoi cell of y' is in the ball

$$B(y, 3\Gamma_4 n^{-1/3})...$$

- **Lower bound on volume**: each Voronoi cell has volume at least $\Gamma_1 \Gamma_4^{-2} n^{-1}$, and diameter at most $\Gamma_4 n^{-1/3}$...

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- ... **Volume argument** $B(y, 3\Gamma_4 n^{-1/3})$ can contain only

$$N := \frac{\frac{4}{3}\pi(3\Gamma_4 n^{-1/3})^3}{\Gamma_1 \Gamma_4^{-2} n^{-1}} = \frac{9\pi\Gamma_4^2}{16\Gamma_1} \approx 10^{20}$$

entire Voronoi cells. Thus V can share boundaries with at most N other Voronoi regions.

Voronoi tessellations on the sphere

Voronoi tessellations are not exclusive to the plane:

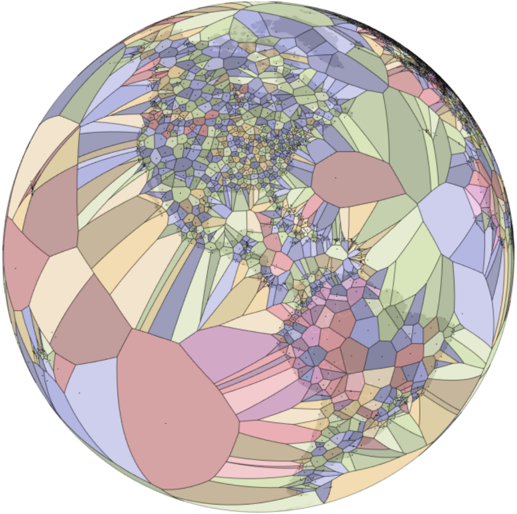

Figure: What is your closest airport?

The same question can be posed with the domain being S^2 instead of $[0,1]^3$: as the number of generators diverge, are "almost all" (i.e. all except $o(n)$ many) the Voronoi cells going to be asymptotically congruent to some fixed polytope?

Idea: the sphere S^2 is "really like" the plane $\mathbb{R}^2$, at least locally... So "almost all" the Voronoi cells going to be asymptotically congruent to a (rescaled) regular hexagon...

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Key difference: S^2 is geometrically more rigid, mainly due to the Euler polytope formula

$$\#\text{vertices} - \#\text{edges} + \#\text{faces} = 2.$$

The number of *defects* (i.e. non hexagonal cells) should be controlled, with something much tighter than $o(n)$.

Main result:

Only finitely many non hexagonal cells (Choksi, L.)

There exist computable constants M, N such that, whenever the number of generators $n > N$, the optimal configuration satisfies the following geometric properties:

- the number $k = k(n)$ of hexagonal cells is at least $n - M$;
- denote by $\{V_i\}$ the hexagonal cells, $i = 1, \cdots, k$ and let $A_n := \sum_i |V_i|$. Denote by H the regular hexagon of area A_n/k. Then

$$\lim_{n \to +\infty} \sum_i \inf_{x \in S^2} |V_i \triangle (H + x)| = 0.$$

  That is, the **total** mismatch between the Voronoi cells and regular hexagons is vanishing.

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Thank you for your attention!