Voronoi Tessellations: Optimal Quantization and Modelling Collective Behaviour

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Department of Mathematical Sciences (**G.L.** Lagrange)
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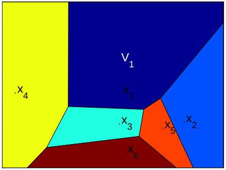
Talk consists of three parts: work of former post doc **Xin Yang Lu**, and two PhD students **Ivan Gonzalez** & **Jack Tisdell**, co-supervised with Jean-Christophe Nave.

Voronoi Tessellations

Generators $x_1, \ldots, x_N \in \Omega \subset \mathbb{R}^n$ (bounded).
Voronoi tessellation of Ω into associated Voronoi cells V_i, where

$$V_i = \{y \in \Omega : d(y, x_i) \leq d(y, x_j) \quad \text{for all } 1 \leq j \leq N\}.$$



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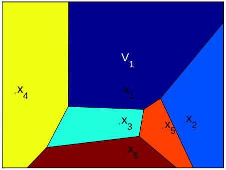

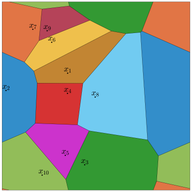

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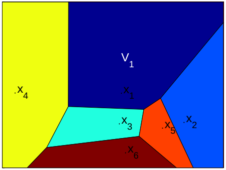
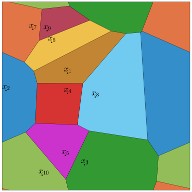
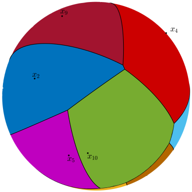
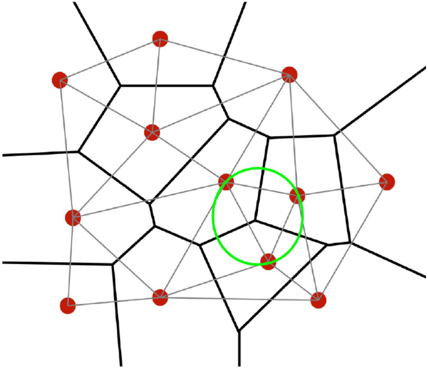




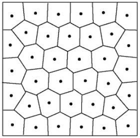


Dual Structure: Delaunay triangularization



Centroidal Voronoi Tessellation and Optimal Quantization

CVT: particular configuration of points $x_1, \ldots, x_N$ with the property that x_i is the centroid of V_i



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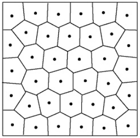

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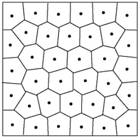

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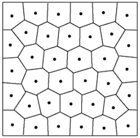

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Natural Question: Optimal Quantizer (i.e. optimal CVT) ?

SKIP: Connection with OT: Monge

Transport map $q : \mathrm{supp}(\mu) \to \mathrm{supp}(\nu)$ and *push forward* probability measure $q_{\#}\,\mu$

$$(q_{\#}\,\mu)(\mathcal{A}) \;=\; \mu\left(q^{-1}(\mathcal{A})\right) \qquad \forall \text{ Borel subsets } \;\mathcal{A}.$$

Denoting $\psi(y) = (y, q(y))$, the transport plan π can be recovered as $\pi = \mu \circ \psi^{-1}$.

$$W_2^2(\mu,\nu) = \inf_q \left\{ \int_\Omega |y - q(y)|^2 d\mu(y) \;\middle|\; \nu = q_{\#}\,\mu \right\}.$$

Brenier's Theorem proves two formulations are equivalent and $\exists$ unique transport map q which is the gradient of a convex function.

SKIP: Connection with Optimal Transport

Take $\mu = dy$ and for a selection of N points in Ω, $\mathbf{x} = \{x_i\}$,

$$\nu_{\mathbf{x}} = \sum_{i=1}^{N} m_i \delta_{x_i}, \qquad \text{where } m_i = |V_i| \qquad \left(\sum_{i=1}^{N} m_i = |\Omega| = 1 \right).$$

Unique optimal push forward is

$$q_*(y) = y - d\Big(y, \{x_i\}\Big) \nabla d\Big(y, \{x_i\}\Big).$$

$$\begin{aligned} W_2^2(\mu, \nu_{\mathbf{x}}) &= \inf_q \left\{ \int_\Omega |y - q(y)|^2 dy, \quad \mu \circ q^{-1} = \nu_{\mathbf{x}} \right\} \\ &= \int_\Omega |y - q_*(y)|^2 dy \\ &= \int_\Omega d^2\Big(y, \{x_i\}\Big) dy = \sum_{i=1}^{N} \int_{V_i} |y - x_i|^2 dy. \end{aligned}$$

SKIP: Connection with Optimal Transport

For any set set distinct points $\mathbf{x} = \{x_i\}$, let

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Optimal Quantization is **equivalent to** minimizing $W_2^2(dx, \nu_{\mathbf{x}})$ over all points $\mathbf{x} = \{x_i\}$.

That is,

$$\min_{\mathbf{x}=\{x_i\}_{i=1}^{N}} W_2^2(dx, \nu_{\mathbf{x}}).$$

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For discrete systems, the former is related to the Crystallization Conjecture: *within the confinements of a physical domain, N interacting particles arrange themselves into a periodic configuration.*

Explore these two issues in Optimal Quantization

Advantages:

- Elementary classification of critical points
- "Quasi" nonlocal behaviour: can more easily "control" (or "isolate") nonlocality.

As such, it presents a perfect paradigm to address issues 1 and 2.

Methods to generate CVTs

CVTs are important in a wide variety of applications:
Du, Faber & Gunzburger (SIAM Rev. '99)

- the simple elegant Lloyd's Method: (Click)
- Gradient descent via quasi-Newton: BFGS methods, graph Laplacian (Hateley-Wei-Chen), ...
- Stochastic (McQueen, ...)
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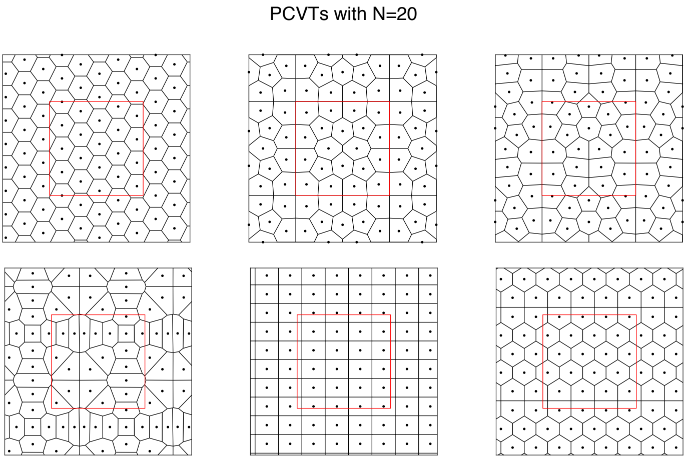
The issue: There are many many CVTs!!!
Complex energy landscape

A Few CVTs (critical points) on the square torus $N = 20$



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Joint with Xin Yang Lu (Lakehead University)
cf. C.-Lu *Comm. Math. Phys* 2020

Global minimizer

Recall our problem: Over N points $\{x_i\}_{i=1}^N$ in $\Omega \subset \mathbb{R}^n$:

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Some questions:

- Are Voronoi cells "almost congruent"?
- What should be the shape of such Voronoi cells?

Crystallization and Gersho's Conjecture

The Augmented Gersho's Conjecture in $\mathbb{R}^n$:

(a) There exists a polytope V with $|V| = 1$ which tiles the space with congruent copies such that the following holds: let $X_N = \{x_i^N\}_{i=1}^N$ be a sequence of minimizers, then the Voronoi cells of points X_N are asymptotically congruent to $N^{-1/n}V$ as $N \to +\infty$.

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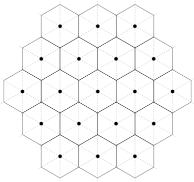
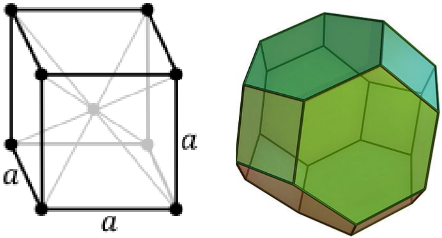
(b) In dimension $n = 2$, the optimal polytope V is a regular hexagon, corresponding to a optimal placement of points on a triangular lattice.
In dimension $n = 3$, the optimal polytope V is the truncated octahedron, corresponding to an optimal placement of points on a BCC (body centered cubic) lattice.





Left: 2D optimal placement of points on a triangular lattice with associated optimal Voronoi polytope a regular hexagon.

Right: 3D (conjectured) optimal placement of points on a BCC lattice and the associated optimal Voronoi polytope the truncated octahedron (8 regular hexagons and 6 squares).

Known results

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Note: Gersho's conjecture amounts to addressing a **nonlocal** and **non finite-dimensional** variational problem.

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This lower bound is approximately half the energy density of the BCC lattice (≈ 0.23562), the conjectured asymptotically optimal configuration.

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Precisely, it reduces the resolution of the 3D Gersho's conjecture to a (albeit huge) finite number of convex optimization problems.

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- In any Voronoi tessellation $\{V_i\}_{i=1}^N$, the average number of sides is at most 6.

- Let $\{V_i\}_{i=1}^N$ be an arbitrary Voronoi tessellation with s_i the number of sides of V_i, a_i its area, and averages

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Now we use convexity of G:

$$\begin{aligned}\sum_{i=1}^{N}\int_{V_i} |y-\bar{x}_i|^2\,dy &\geq \sum_{i=1}^{N} G(a_i, s_i)\\ &\geq NG(\bar{a}, \bar{s}) + o(N)\\ &\geq NG(\bar{a}, 6) + o(N),\end{aligned}$$

where $o(N)$ is the contribution of the boundary terms, which vanish as $N \to +\infty$.

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But: we just showed that the number of faces is bounded!

Proceeding á la Gruber in 3D

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   is convex for $m \leq N_*$.
3. verify that the optimal polytope V with m faces is space tiling.
4. we can dispense with the energetic contributions of the boundary cell.

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$$\int_V [|y-x|^2 - d^2(y,\{x,x'\})]\,dy \;\geq\; \frac{r^2|V|}{256} \;\geq\; \Gamma_1 |V|^{5/3},$$

where

$$\Gamma_1 := 0.4^{2/3}/40 \approx 0.013572, \qquad r := \max_{z' \in \partial V} |z'-x|.$$

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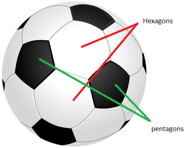

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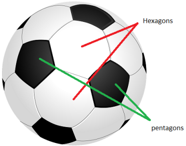

Currently these methods can be used to prove that the number of non hexagons cells must be $O(1)$ as $N \to \infty$.

Next: Address issue 2

Develop hybrid numerical algorithms to **navigate (or probe) the energy landscape** and access low energy states whose basin of attraction might be "tiny"?

Part of PhD thesis of **Ivan Gonzalez** co-supervised with Jean-Christophe Nave.

Gonzalez -C- Nave *SIAM Sci. Comp. 2021*

Take $n = 2$ and $\Omega = \mathbb{T}^2$.

How to get close to the optimal CVT?

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- On the torus with finite N, achieving this is impossible. Importance of combinatorial size effects. Trade off is subtle.
- Except for small N, basins of attraction far too small to successfully implement gradient flow with Monte Carlo initializations.

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4. Repeat Steps 1-3;
5. Stop at Step 2 when "low energy" state achieved.

The few parameters of the algorithm

- Q, the number of interactions of Steps 1 - 3. Typically for $N \sim 1000$, $Q = 8$ sufficient for good results.
- K_q, the number of interactions of MACN in Step 1 for $q = 1, \dots Q$.

How to assess a "low energy" state?

- Global measure of optimality: Compute the normalized energy and compare with *"theoretical minimum"*:

$$E(X) = \sum_{i=1}^{N} \int_{V_i} |y - x_i|^2 \, dy = \sum_{i=1}^{N} E_i \qquad E_{min} = N E_{hex}$$

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- Local measures of optimality: Optimal geometry of Voronoi cells: $H = \%$ of hexagonal cells

  $R_\epsilon = \%$ of 'almost" regular hexagonal cells.

Results for $N = 1000$

- a sample run (click) ;
- summarize experiments in a table (click) .

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- 3D simulations? (appearance of BCC structure).

Now Something Rather Different but Still Directly Linked to Voronoi Tessellations and MACN:

Modelling Collective Behaviours:

Voronoi-Topological-Perception (VTP)

Work with **Ivan Gonzalez, Jack Tisdell** and Jean-Christophe Nave.

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- Certainly are not the first to use Voronoi diagrams in collective behaviour (cf. Chaté, Ginelli, Grégoire, Lindhe, ...)
- However, we present a novel and effective synthesis of the three competing components (repulsion, alignment, and homing) - relative weights easily motivated by a few realistic and cognitively cheap assumptions on agents' perception and decisions based on their Voronoi environment.

Discrete time model for N agents in some domain where their Voronoi region represents their "personal space".

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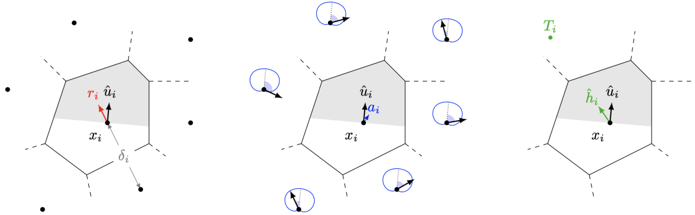
The three active ingredients:



(a) **Repulsion**. Unit repulsion vector r_i always points away from nearest neighbor or domain boundary. The distance δ_i to this nearest neighbor determines the relative weight of r_i and $\hat{h}_i$.

(b) **Alignment**. Alignment a_i is given by a weighted average of the velocities of Voronoi-neighbors. The circularly-wrapped weighting functions are indicated by the blue curves where the relative angle marked with light blue sectors is the argument.

(c) **Homing**. Unit homing vector $\hat{h}_i$ points toward target T_i, if it is nonempty and does not contain x_i. (Here the target is shown as a dot but may be any region, in general.)

Alingement averaging for a_i

$$\tilde{a}_i = \tilde{a}_i(X, U) = \frac{1}{\#\mathcal{N}_i} \sum_{j \in \mathcal{N}_i} g(\theta_{ij}) \hat{u}_j.$$

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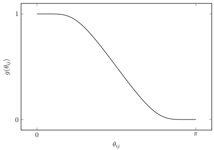

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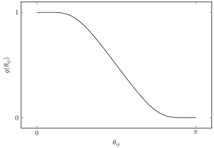

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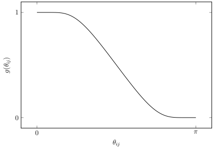

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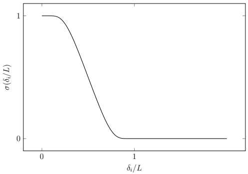

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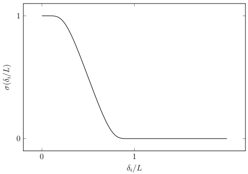
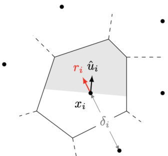


Personal-space speed scale

$$\rho_i = \tanh\left(\frac{\mathcal{A}_i}{\pi L^2/2}\right).$$



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- **Two effective dimensionless parameters:**

$$\nu \quad \text{and} \quad \mu := \frac{L}{(|\Omega| / N)^{1/2}}.$$

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- **Compute observables** along the way:

Observables

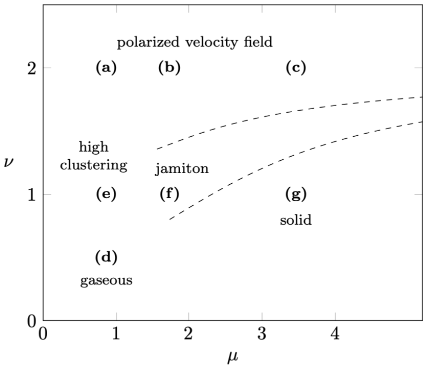
- Polarization (untargeted): $\mathcal{P}(U) = \frac{\|\sum_i u_i\|}{\sum_i \|u_i\|}$.
  Max $= 1$ when all velocities are in the same direction.
- Angular momentum (point targets)
- Energetic clustering:

$$\frac{E(X)}{E_N}, \qquad E_N \text{ energy of } N \text{ reg. hex. of area } |\Omega|/N.$$

Ratio big when there is clustering, close to 1 where there is none.

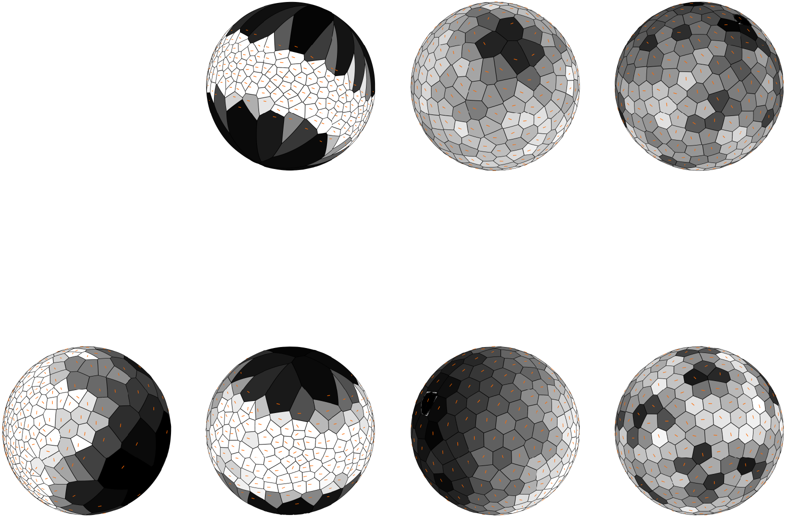
Simplest case: No targets

Phase Diagram:



https://jacktisdell.github.io/Voronoi-Topological-Perception/

Similar PD for untargeted sphere



Point Targets: single, double, triple

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- **Many further advances possible with VTP:** sources, sinks, obstacles, different agent behaviours, leadership . . .
- So far quite generic. Can model be tailored to a particular biological species or human crowds?
- **Drawback:** no asymptotic regimes to analyze
  For now just numerics.

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