Nonlocal Geometric Variational Problems: Gamow's Liquid Drop Problem and Beyond

LECTURE I

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Broad Introduction

Energy-Driven Pattern Formation

- Associate a "pattern" with an order parameter u defined over a physical domain.
- Capture and analyze observed (desired) patterns, or the dynamics to, via minimization of some often postulated "energy" defined over all possible patterns.

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- Examples include ferromagnets, ferrofluids, superconductors, elastic materials (eg. martensitic), block copolymers, social aggregation and self-organized systems (swarming, flocking) .....
- Much recent attention in the calculus of variations community.

Two Common Mathematical Themes/Structures

1. **NONCONVEXITY:** Nonconvex variational problem regularized by higher order terms

   cf. R.V. Kohn, *Energy Driven Pattern Formation*", Proc. ICM '07.

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2. **NONLOCAL:** Energetic competitions associated with short and long range interactions.

   cf. Seul & Andelman "Domain shapes and patterns: the phenomenology of modulated phases." Science '95.

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- Here we take a different, more “global” and Ansatz free approach. Invoke methods which directly address minimization of an “energy”.

From this perspective, what can mathematicians and applied mathematicians address?

- Existence and non existence of global minimizers:
  1. usually via the direct method in the calculus of variations.
  2. sometimes trivial – sometimes not (especially when the problem is posed on an unbounded domain). Key role of compactness of minimizing sequence.

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- Structural information about local and global minimizers.
- Gradient flow dynamics – choice of metric fundamentally important (cf. talks of Carrillo and Peletier).
- Simulating Minimizers and Complex Energy Landscapes: design numerical methods to address metastability and access ground states (or at least stable local minimizers).

Outline of the Lectures

Lecture 1 Overview (mostly on slides).

1. Gamow's Liquid Drop Problem
2. The problem on the torus: the nonlocal isoperimetric problem and the Ohta-Kawasaki functional
3. A recent physical motivation - diblock copolymers.
4. Analytical questions we want to address
5. Intrinsic periodicity and crystallization.

   a substantial digression to discuss the finite dimensional problem of Centroidal Voronoi Tesselation.

Lecture 2 Continuation with more analytical details (mostly on blackboard)

1. Continue with intrinsic periodicity and crystallization for NLIP.
2. Some comments about local minimizers, and the shape of minimizers for NLIP.
3. (if time permits) small volume fraction asymptotics of NLIP.
4. Return to the Liquid Drop Model – existence and nonexistence results.
5. Give details of a simple proof of Frank et al for the nonexistence when $m > 8$.

Lecture 3 A Variant of the Liquid Drop Problem (On blackboard)

1. Focus on a new shape optimization problem related to algebraic potentials ($\sim$ lectures of Carrillo).
2. Some recent existence and non existence results, joint with Burchard and Topolaglu.
3. Recent results of Frank and Lieb which build on our work.

Gamow's Liquid Drop Problem

George Gamow (1904-1968)

"A mathematician friend of mine, the late S. Banach, once told me, "The good mathematicians see analogies between theorems or theories; the very best see analogies between analogies." This ability to see analogies between models for physical theories Gamow possessed to an almost uncanny degree"

– Stanislaw Ulam

Gamow's Liquid Drop Model for the shape of atomic nuclei (1930)

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Among all $\Omega \subset \mathbb{R}^3$ with $|\Omega| = m$, minimize

$$E(\Omega) = \mathrm{Per}(\Omega) + \frac{1}{2} \int_\Omega \int_\Omega \frac{1}{|x-y|}\, dx\, dy.$$

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- the spherical shape of nuclei
- the non-existence of nuclei when the atomic number (m) is greater than some critical value.
- existence of a nucleus with minimal binding energy per unit particle.

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- The Classical Isoperimetric Problem

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- The Classical Isoperimetric Problem
- The Problem of the Equilibrium Figure $\sim$ Poincaré

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Which region of 3-space with volume m has minimal surface area?

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For the most general class (measurable sets of measure m): De Giorgi

Problem of the Equilibrium Figure – Poincaré $\sim$ 1887

Shape of a fluid body of mass m in equilibrium.

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$$\int_\Omega \int_\Omega -\frac{1}{C\,|x-y|}\,dx\,dy, \qquad |\Omega| = m$$

where $-(C|x-y|)^{-1}$, $C > 0$ is the potential resulting from the gravitational attraction between two points x and y in the fluid.

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Rigorous proof involves the Riesz Rearrangement Inequality

We Give Some Details

Marriage (or "Divorce") of the Two: Among all $\Omega \subset \mathbb{R}^3$ with $|\Omega| = m$, minimize

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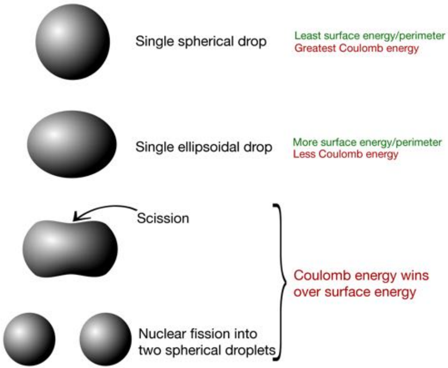
Gamow's heuristic:



Mass Scaling

Easy to see Gamow's heuristic from scaling in m: consider $\lambda\Omega$ for $\lambda > 0$

$$E(\lambda\Omega) = \lambda^2\, Per(\Omega) + \lambda^5\, \frac{1}{2}\int_\Omega\int_\Omega \frac{1}{|x-y|}\, dxdy.$$

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What is remarkable about Gamow's problem is that, from the perspective of the global minimizer, there is (most probably) always a clear winner (cf. Lecture 2).

Precise Formulation: Notion of a Set of Finite Perimeter

Functions of Bounded Variation: Let $\Sigma \subset \mathbb{R}^3$ and $u \in L^1(\Sigma)$. Define the total variation of u to be

$$\begin{aligned} \|\nabla u\|(\Sigma) &= \text{“}\int_\Omega |\nabla u|\text{”} \\ &= \sup\left\{ \int_\Sigma u \operatorname{div}\phi \, dx \;\middle|\; \phi \in C_c^1(\Sigma, \mathbb{R}^3),\ |\phi(x)| \le 1 \right\}. \end{aligned}$$

If $\|\nabla u\|(\Sigma) < \infty$, we say $u \in BV(\Sigma)$

Sets of finite perimeter and Caccioppoli sets: A set $\Omega \subset \mathbb{R}^3$ is said to be of finite perimeter iff $\chi_\Omega \in BV(\mathbb{R}^3)$. We define

$$Per(\Omega) = \|\nabla \chi_\Omega\|(\mathbb{R}^3).$$

Precise Formulation of the LD Model

For $m > 0$, consider minimizers of

$$E(z) = \int_{\mathbb{R}^3} |\nabla z| + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{z(x)\, z(y)}{|x - y|} \, dx \, dy$$

over

$$\left\{ z \in BV(\mathbb{R}^3, \{0,1\}) \,\middle|\, \int_{\mathbb{R}^3} z(x) \, dx = m \right\}.$$

Note that existence is **not** straight forward via the direct method.

Universality of the LD Model

- The spirit of energetic competitions involving competing short- and long-range interactions is ubiquitous in the contemporary calculus of variations.

- The way in which Gamow's Problem simply but directly encapsulates this competition is behind a universality, with LD model's phenomenology shared by many other systems operating at very different length scales: from femtometer nuclear scale to nanoscale in condensed matter systems, to centimeter scale for fluids and certain reaction-diffusion systems, all the way to cosmological scales.

Mathematical “Rediscovery” of the LD Model

Surprisingly, the LD problem only recently received direct attention from mathematicians, after it *resurfaced* as an asymptotic limit in the Ohta-Kawasaki functional (1986) for self-assembly of diblock copolymers (C-Peletier 2010).

This functional can be viewed as the diffuse-interface Liquid Drop problem on a finite domain.

Very Different, and Indeed RICHER, Situation on a Finite Domain

“The LD problem on the Torus”

For fixed $m \in (0,1)$,

$$\text{Minimize} \quad \int_{\mathbb{T}^3} |\nabla u| \; + \; \gamma \int_{\mathbb{T}^3} |\nabla v|^2$$

over $u \in BV(\mathbb{T}^3, \{0,1\})$, $\quad \fint_{\mathbb{T}^3} u \;=\; m \quad$ with $\quad -\Delta v = u - m$ on $\mathbb{T}^3$.

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$$\int_{\mathbb{T}^3} |\nabla v|^2 = \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} G(x,y) u(x)\, u(y)\, dx\, dy$$

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We will call this problem the nonlocal isoperimetric problem (NLIP).

The Direct Method $\implies$ Existence of a Minimizer

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- Lower semi-continuity of total variation implies

$$\int_{\mathbb{T}^3} |\nabla u| \leq \liminf \int_{\mathbb{T}^3} |\nabla u_n|.$$

- Coulombic term is continuous

$$\int_{\mathbb{T}^3} \int_{\mathbb{T}^3} G(x,y) u_n(x)\, u_n(y)\, dx\, dy \longrightarrow \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} G(x,y) u(x)\, u(y)\, dx\, dy.$$

- Thus $u \in BV(\mathbb{T}^3, \{0,1\})$ is a minimizer.

New Phenomena – modulated phases on an intrinsic scale

- Fourier (take $|\mathbb{T}^3| = 1$):

$$\|u - m\|^2_{H^{-1}(\mathbb{T}^3)} = \sum_{\mathbf{k} \neq \mathbf{0}} \frac{|\hat{u}_{\mathbf{k}}|^2}{|\mathbf{k}|^2}$$

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NLIP in terms of w where $w' = \pm 1$:

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NLIP in terms of w where $w' = \pm 1$:

$$\int_0^1 |w''| + w^2\, dx.$$

First Variation

- boundary regularity of a (local) minimizer (Topaloglu-Sternberg '11) ✓
- necessary condition for a minimizer $u = \chi_\Omega$ is

$$\boxed{H(x) + 4\gamma v(x) = \lambda \quad \text{for all } x \in \partial\Omega}$$

$H(x)$ is the mean curvature of $\partial\Omega$
$v(x) = G(x, y) * u(y)$, the potential.

- in 1D, vanishing first variation implies periodicity.
- very hard to get a handle on this condition in higher D.

Diffuse Interface Version: The Ohta Kawasaki Functional

$$\textbf{Minimize} \quad \int_{\mathbb{T}^3} \epsilon\,|\nabla u|^2 \; + \; \frac{1}{\epsilon} u^2(1-u)^2 \; + \; \gamma\,|\,\nabla v\,|^2 \;\; dx$$

$$\text{where} \quad u \in H^1(\mathbb{T}^3), \quad \fint_{\mathbb{T}^3} u \; = \; m, \quad -\triangle v = u - m \;\; \text{on } \mathbb{T}^3$$

$$\begin{aligned} \int_{\mathbb{T}^3} |\nabla v|^2 dx \;\; &= \;\; \int_{\mathbb{T}^3} \int_{\mathbb{T}^3} G(x,y) u(x)\, u(y)\, dx\, dy \\ &= \;\; \|u - m\|^2_{H^{-1}} \end{aligned}$$

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Gradient term: constant phases
Double-well: phases of 0 or 1
Nonlocal term: oscillations between phases 0 and 1 with mean m.

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All three $\Longrightarrow$ **"nearly periodic" phase separation on an intrinsic scale.**

A Few Words on H^{-1}

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$|\mathbb{T}^3| = 1$. Define the H^{-1} inner product and norm on

$$\mathcal{H} \ = \{f \in L^2(\mathbb{T}^3) \,\big|\, \int_{\mathbb{T}^3} f = 0\}.$$

Given $f, g \in \mathcal{H}$ take v, w such that

$$-\triangle v = f \quad -\triangle w = g \qquad \text{on } \mathbb{T}^3.$$

Then we define

$$\langle f, g\rangle_{\mathcal{H}} \ = \int_{\mathbb{T}^3} \nabla v \cdot \nabla w \, dx \qquad \|f\|^2_{\mathcal{H}} \ = \int_{\mathbb{T}^3} |\nabla v|^2 \, dx.$$

Dual space structure: Dual of $H^1_0(\mathbb{T}^3)$ (H^1 with average 0) with respect to the distributional L^2 pairing, i.e..

$$\|f\|^2_{\mathcal{H}} \ = \ \sup_{\phi \in H^1_0} \frac{\left(\int_{\mathbb{T}^3} f\phi \, dx\right)^2}{\|\nabla \phi\|^2_{L^2(\mathbb{T}^3)}}$$

H^{-1} Gradient Flow Dynamics

Aside: a word on gradient flows.

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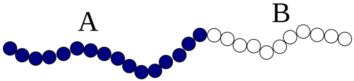
The H^{-1} gradient flow gives the modified Cahn-Hilliard equation

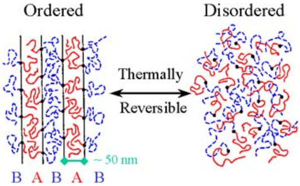
$$u_t = \triangle\left(-\epsilon^2 \triangle u - u + u^3\right) - \sigma(u - m).$$

simulation for $\sigma = 0$ simulation for $\sigma > 0$

Diversion: A Physical Application

Self Assembly of Diblock Copolymers





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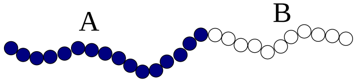
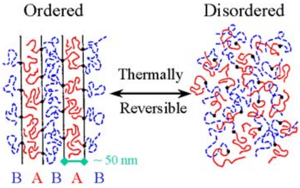
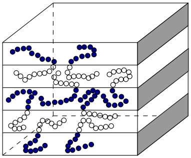
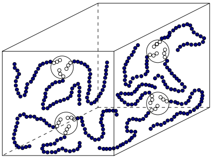








Material Parameters:

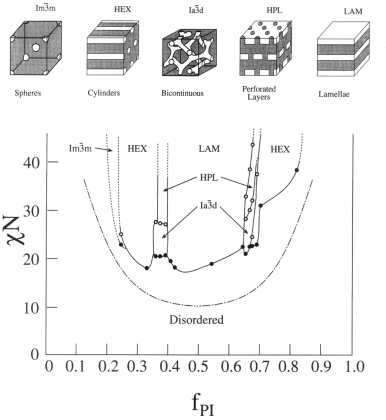
χ (Flory-Huggins interaction parameter)

N (index of polymerization)

f (molecular weight)

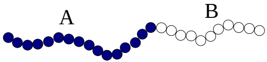
Experimental phase diagram for polystyrene-isoprene

Khandpur et al '(Macromolecules '93)



Ability for self-assembly → materials with **designer** mechanical, optical, electrical ... properties

Modelling



Include two interacting effects:

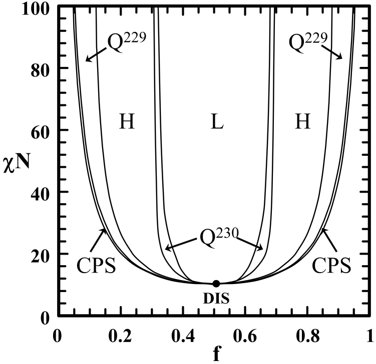
- chains like to be *randomly coiled* – behave like Brownian motion sample paths.
- part of the chain (A sub-chain) wants to separate from the other part (B sub-chain), without ever severing the covalent bond.

Hopefully captures:

- phase geometry – depending on the material parameters.

Self-Consistent Mean Field Theory

Transforms formidable task of integrating contributions to the partition function from many-chain interactions to the computation of the contribution of one polymer in a self-consistent field .



State of the art: Fredrickson group at Santa Barbara (with help from C. Garcia-Cevera)

Derivation of Ohta Kawasaki

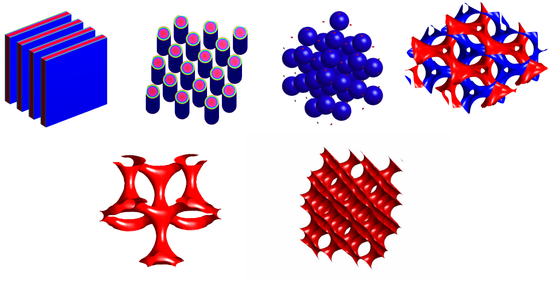
cf. Ohta-Kawasaki (*Macromolecules* '86),
C.-Ren (*J. Stat. Phys.* '03)

- Self-Consistent Mean Field Theory: The monomer density u order parameter is coupled with self-consistent external field via modified diffusion equation (Feynman-Kac). Linearize this dependence about the disordered state (Random Phase Approximation).
- validity is good close to order/disorder transition (weak segregation regime), i.e. **not** in the strong segregation regime where $\epsilon \ll 1$ (i.e. NLIP!!)

Back to Minimizers of OK and NLIP

Heuristic for Minimizers on Sufficiently Large Domain

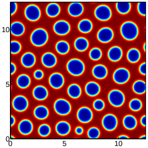
- periodic structures on an intrinsic scale ($\ll$ domain size)
- within a periodic cell, interfaces resemble a CMC surface



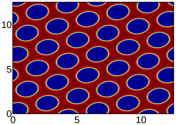
Interfaces of low energy states for different M
cf. C.-Peletier-Williams SIAP 2009

Remark: metastability is a big problem

Examples of 2D **metastable states** and their energy densities for the **same parameters**:



0.1290



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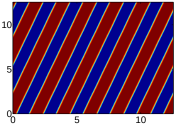

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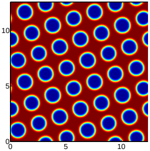
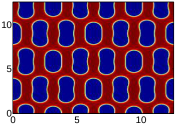


0.126258



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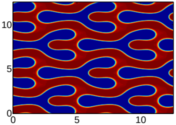

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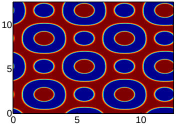

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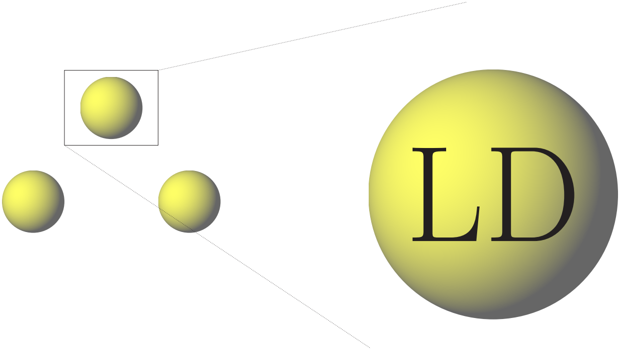
Relation with the LD Problem (Rediscovery)

Send m to 0: Asymptotic limit in which number of particles remains $O(1)$ but size tends to zero.



More details in Lecture 2

What can we hope to prove about. global minimizers of NLIP and OK?

- Intrinsic Periodicity?
- Nature of phase structure – geometry of the interface?

Intrinsic Periodicity – **1D** Done

(NLIP): follows from vanishing first variation.

(OK):

- $m = 0$ and wells ± 1: w s.t. $u = w'$:

$$\int_0^1 \epsilon^2 w_{xx}^2 \ + \ (w_x^2 - 1)^2 \ + \sigma \ w^2 \ dx,$$

cf. Müller (*Cal. Var.* '93)

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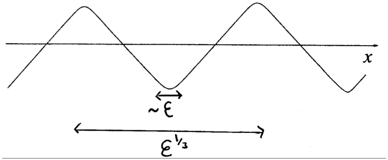

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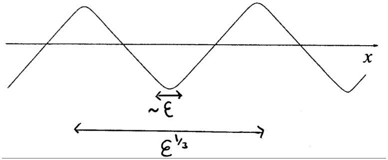

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Higher D: **VERY HARD** and only weaker statement exists.

Let's move to "simpler" finite dimensional problem to see some of the reasons why.

Substantial Digression to discuss a Finite Dimensional Nonlocal Geometric Problem

Centroidal Voronoi Tessellation (CVT)

Why introduce and discuss this now?

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- one which is directly connected to Wasserstein distances ($\sim$ talks of Carrillo and Peletier)

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- one which exhibits the difficulty of proving a crystallization result in 3D
- one which is directly connected to Wasserstein distances ($\sim$ talks of Carrillo and Peletier)
- this connection will lead us to state a rare full crystallization result by Bourne, Peletier and Theil for a novel problem which lies between (CVT) and (NLIP).

Simple Finite Dimensional Nonlocal Geometric Problem: Centroidal Voronoi Tessellation

Take N points at positions $x_i \in \Omega \subset \mathbb{R}^n$. Among all such points

$$\text{Minimize} \quad \int_{\Omega} dist^2(y, \{x_i\})\, dy$$

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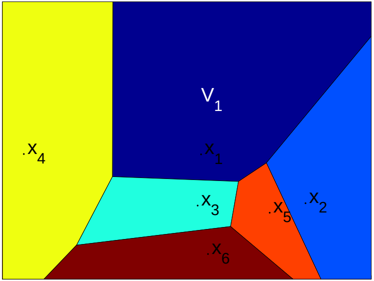
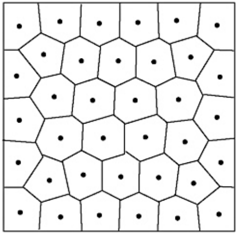
Take N points at positions $x_i \in \Omega \subset \mathbb{R}^n$. Among all such points

$$\text{Minimize} \quad \int_{\Omega} dist^2(y, \{x_i\})\, dy \;=\; \sum_{i=1}^{N} \int_{V_i} |y - x_i|^2\, dy$$

$V_i =$ Voronoi cell of x_i.



Simple characterization of a critical point and Lloyds' Method



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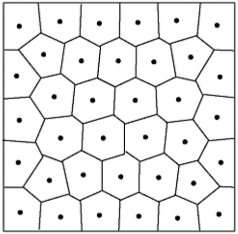


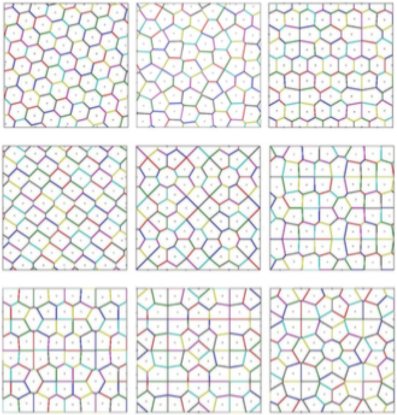
$\exists$ a simple elegant algorithm (Lloyd's Method) for generating CVTs.
Click (A. Rand)

cf. Du, Faber & Gunzburger (SIAM Rev. '99)

Complex Energy Landscape

CVTs (critical points) on the flat torus with 15 generators.

J. ZHANG, M. EMELIANENKO, AND Q. DU



Global Minimizer

- Hard to infer any geometric property of CVTs for generic (finite) n...

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So, what about $n \to +\infty$? Some questions:

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

Crystallization and Gersho's Conjecture

Gersho's Conjecture

There exists a polytope V with $|V| = 1$ which tiles the space with congruent copies such that the following holds: let X_n be a sequence of global minimizers (i.e. X_n is the minimizer over n points), then the Voronoi cells of points X_n are asymptotically congruent to a scaled V as $n \to +\infty$.

Note:

1. the polytope V can depend on the dimension d.

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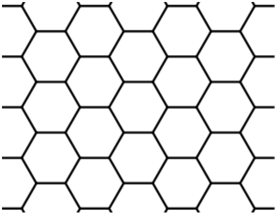
Note:

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.

2D

Known results:

1. Gersho's conjecture is fully proven in $2D$ (T'oth, Gruber, etc.): the optimal Voronoi tessellation is the triangular lattice ("honeycomb").

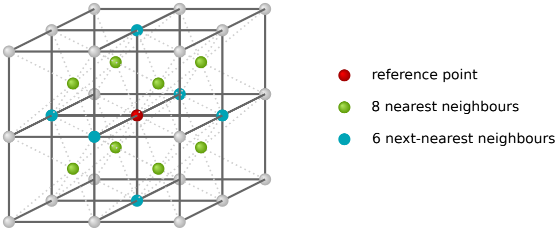


2. Open for higher dimensions.

Gersho in 3D

Conjecture

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



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

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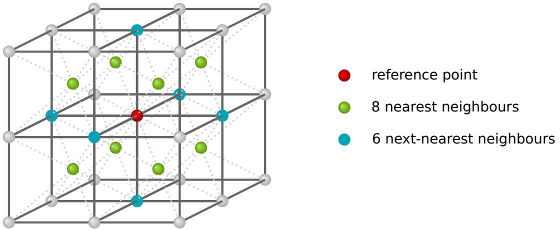

Numerical results seem to support this (Du et al. 2005).

Note that

1. Gersho's conjecture is **nonlocal** and **infinite dimensional**.
2. No a priori bounds on the geometric complexity of Voronoi cells until very recent work with Xin Yang Lu.

Connection with Optimal Transport

Let $\mu = \rho(y)dy$ and ν a Borel probability measure. Consider the set $\mathcal{M}(\mu, \nu)$ of measures π on the product space $\Omega \times \Omega$ such that

$$\pi(y, \Omega) = \mu(y) \text{ and } \pi(\Omega, \cdot) = \nu.$$

We call π a transport plan.

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Kantorovich's reformulation of optimal transportation for Euclidean cost is given as

$$W_2^2(\mu, \nu) = \inf_{\pi} \left\{ \int_{\Omega \times \Omega} |y - z|^2 d\pi(y, z) \,\middle|\, \pi \in \mathcal{M}(\mu, \nu) \right\},$$

also known as the Wasserstein-2 distance

Classical Formulation of Monge

Transport map $q : \mathrm{supp}(\mu) \to \mathrm{supp}(\nu)$

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

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

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

Connection with CVT

Fix $\mu = \rho(y)\,dy$ and for a selection of N points in Ω, $\mathbf{x} = \{x_i\}$,

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

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Thus finding CVTs via minimization of the CVT energy is equivalent to minimizing $W_2^2(\mu, \nu_{\mathbf{x}})$ (with μ having a constant density) over all possible $\mathbf{x} = \{x_i\}$.

i.e.

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

Aside – rigid shapes

Minimize the previous Wasserstein distance where the weighted measure at points is replaced with rigid shapes parametrized by centroids and rotation angles.

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Minimize the previous Wasserstein distance where the weighted measure at points is replaced with rigid shapes parametrized by centroids and rotation angles.

Thesis of Lisa Larsson (Larsson, C, Nave SISC '15, SIAP '16): quick way to simulate energy minimization.

- click
- click
- click

A Modified NLIP Problem with Wasserstein Interactions

recall OK

Bourne, Peletier and Theil CMP 2014

A Modified NLIP Problem with Wasserstein Interactions

recall OK

Bourne, Peletier and Theil CMP 2014

$\Omega \subset \mathbb{R}^2$ with $|\Omega| = 1$. Minimize over

$$\mu = \sum_{x \in Z} v_x \delta_x \qquad v_x > 0, \ \sum_{x \in Z} v_x = 1, \ \ Z \text{ any finite subset of } \Omega$$

$$\boxed{E(\mu) \ = \ \lambda \sum_{x \in Z} (v_x)^{1/2} \ + \ W_2^2(dy, \mu).}$$

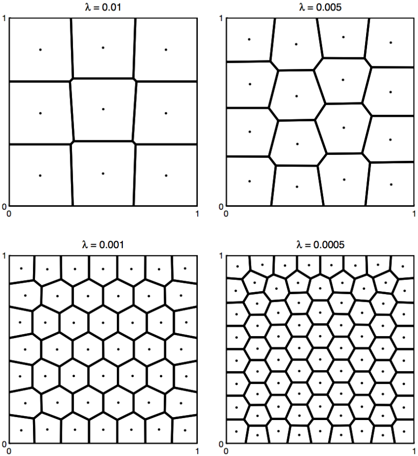
Note:

- weights are now free
- number of particles and the length scale not fixed but set by energy minimization (like in NLIP)

Heuristic/Numerics for Minimizers

Optimal number of particles $\sim \lambda^{-2/3}$.

As $\lambda \to 0$: regular hexagonal pattern (triangular lattice)



Rigorous Crystallization

For the first, Ω polygon with at most 6 sides.

Theorem:

- For any $\lambda > 0$, energy of any configuration is bounded below by the energy of an optimal hexagonal pattern (triangular lattice.
  If the energy bound can be achieved then the structure is exactly on a triangular lattice.
- Let Ω bounded and connected. Then as $\lambda \to 0$ the bound can be asymptotically attained.

Key Constant: Optimal Energy over a Polygon

$$c_n = \inf_P \left\{ \min_{y \in P} \int_P |x - y|^2 dx \,\middle|\, P \text{ a } n\text{-gon with area } 1 \right\}$$

Naturally, c_6 plays a key role in their proof.

Next Lecture: an intrinsic periodicity result for NLIP in $\mathbb{R}^n$.