

Department of Probability and Mathematical Statistics



FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University

Daniel Jahn

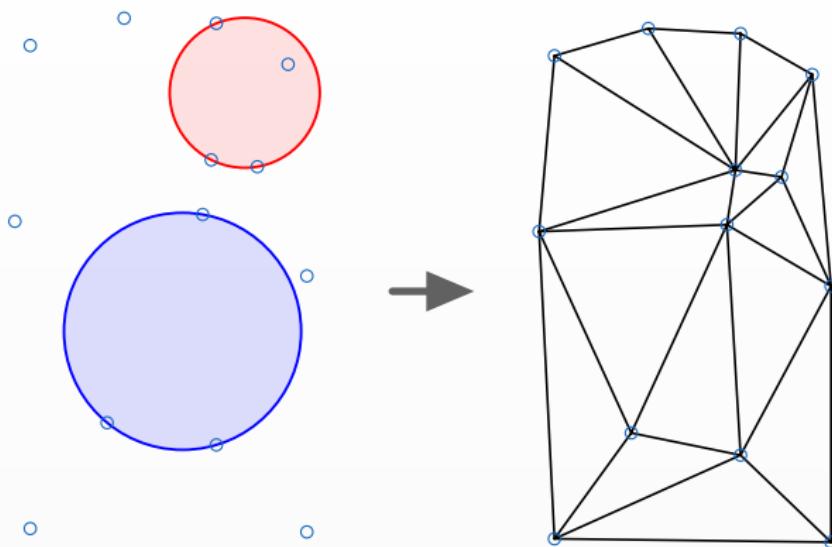
Existence of Gibbs-Laguerre-Delaunay Models

Workshop Devet Skal

27 February 2019

Delaunay tetrahedrization

Let γ be a locally finite subset \mathbb{R}^3 .



$$\mathcal{D}_4(\gamma) = \{\eta \subset \gamma : \text{card}(\eta) = 4, \eta \text{ satisfies the empty ball property } \}$$

Point processes

\mathcal{B} Borel σ -algebra on \mathbb{R}^3 , \mathcal{B}_0 bounded Borel sets, $|\cdot|$ is the Lebesgue measure.

Point process: $\Phi : (\Omega, \mathcal{A}, \mathbb{P}) \rightarrow (\mathbf{N}_{lf}, \mathcal{N}_{lf})$ where

- \mathbf{N}_{lf} is the set of all locally finite simple counting measures on \mathbb{R}^3 .
- \mathcal{N}_{lf} is generated by sets of the form

$$\{\nu \in \mathbf{N}_{lf} \mid \nu(\Lambda) = n\}, n \in \mathbf{N}_{lf}, \Lambda \in \mathcal{B}.$$

Point processes

\mathcal{B} Borel σ -algebra on \mathbb{R}^3 , \mathcal{B}_0 bounded Borel sets, $|\cdot|$ is the Lebesgue measure.

Point process: $\Phi : (\Omega, \mathcal{A}, \mathbb{P}) \rightarrow (\mathbf{N}_{lf}, \mathcal{N}_{lf})$ where

- \mathbf{N}_{lf} is the set of all locally finite simple counting measures on \mathbb{R}^3 .
- \mathcal{N}_{lf} is generated by sets of the form

$$\{\nu \in \mathbf{N}_{lf} \mid \nu(\Lambda) = n\}, n \in \mathbf{N}_{lf}, \Lambda \in \mathcal{B}.$$

Poisson point process with intensity $z > 0$ is a point process Φ such that

- $\Phi(B) \sim Pois(z|B|)$ for each $B \in \mathcal{B}_0$,
- $\Phi(B_1), \dots, \Phi(B_n)$ are independent for each $n \in \mathbb{N}$ and $B_1, \dots, B_n \in \mathcal{B}_0$ pairwise disjoint.

Point processes

\mathcal{B} Borel σ -algebra on \mathbb{R}^3 , \mathcal{B}_0 bounded Borel sets, $|\cdot|$ is the Lebesgue measure.

Point process: $\Phi : (\Omega, \mathcal{A}, \mathbb{P}) \rightarrow (\mathbf{N}_{lf}, \mathcal{N}_{lf})$ where

- \mathbf{N}_{lf} is the set of all locally finite simple counting measures on \mathbb{R}^3 .
- \mathcal{N}_{lf} is generated by sets of the form

$$\{\nu \in \mathbf{N}_{lf} \mid \nu(\Lambda) = n\}, n \in \mathbf{N}_{lf}, \Lambda \in \mathcal{B}.$$

Poisson point process with intensity $z > 0$ is a point process Φ such that

- $\Phi(B) \sim Pois(z|B|)$ for each $B \in \mathcal{B}_0$,
- $\Phi(B_1), \dots, \Phi(B_n)$ are independent for each $n \in \mathbb{N}$ and $B_1, \dots, B_n \in \mathcal{B}_0$ pairwise disjoint.

For $\Lambda \in \mathcal{B}_0$ and Poisson point process Φ with intensity $z > 0$, denote the distribution of $\Phi_\Lambda := \Phi \cap \Lambda$ as Π_Λ^z .

We obtain the probability space $(\mathbf{N}_{lf}, \mathcal{N}_{lf}, \Pi_\Lambda^z)$.

Gibbs point process

Denote

$$\mathbf{N}_\Lambda = \{\nu \in \mathbf{N}_{lf} : \nu(\mathbb{R}^3 \setminus \Lambda) = 0\}.$$

A translation-invariant probability measure P on $(\mathbf{N}_{lf}, \mathcal{N}_{lf})$ is a **Gibbs measure** with activity $z > 0$ if it satisfies the **Dobrushin-Lanford-Ruelle equation**:

$$\int f dP = \int \frac{1}{Z_\Lambda^z(\gamma)} \int_{\mathbf{N}_\Lambda} f(\zeta \cup \gamma_{\Lambda^c}) e^{-H_\Lambda(\zeta \cup \gamma_{\Lambda^c})} \Pi_\Lambda^z(d\zeta) P(d\gamma)$$

for every $\Lambda \in \mathcal{B}_0$ and every measurable $f : \mathbf{N}_{lf} \rightarrow [0, \infty)$.

$Z_\Lambda^z(\gamma) = \int e^{H_\Lambda(\zeta \cup \gamma_{\Lambda^c})} \Pi_\Lambda^z(d\zeta)$ is the **partition function**

H_Λ is the **energy function**

$$H_\Lambda(\gamma) = \sum_{\eta \in \mathcal{E}_\Lambda(\gamma)} \varphi(\eta, \gamma),$$

such that $Z_\Lambda^z(\gamma) < \infty$.

A point process whose distribution is a Gibbs measure is called a **Gibbs point process**.

D. Dereudre and F. Lavancier. Practical simulation and estimation for Gibbs Delaunay-Voronoi tessellations with geometric hardcore interaction (2011)

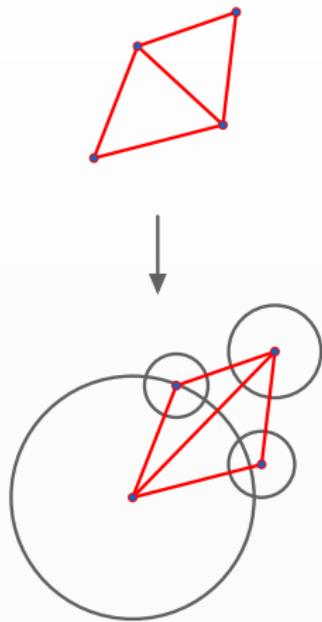
Considered Delaunay triangulation in \mathbb{R}^2 using the potential

$$\varphi(\eta) = \begin{cases} \infty & \text{if } I(T) \leq \epsilon, \\ \infty & \text{if } \chi(T) \geq \alpha, \\ \theta \text{Per}(T) & \text{otherwise,} \end{cases}$$

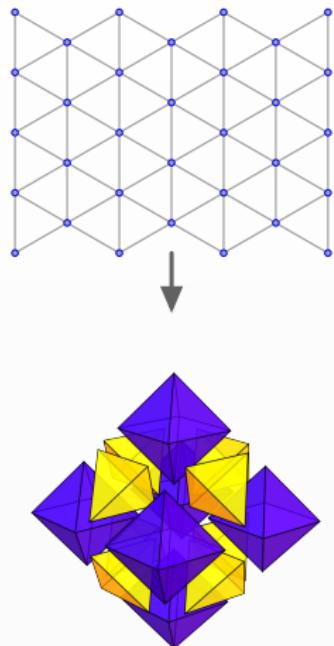
where

- $I(T)$ is the length of the shortest edge of the triangle T .
- $\chi(T)$ is the circumradius of T .
- $\text{Per}(T)$ is the perimeter of the triangle T .
- $\theta \in \mathbb{R}$, $\epsilon \geq 0$, $\alpha > 0$ such that $2\epsilon < \alpha < 1/2$.

Delaunay → Laguerre



2D → 3D

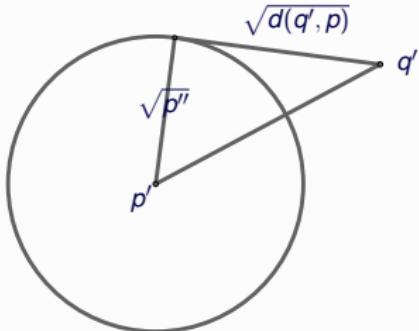


Laguerre-Delaunay

Power distance

- Generating points are now both locations and **weights**. Can be geometrically interpreted as **spheres**.
- $\gamma = \{p_1, \dots, p_n\} = \{(p'_1, p''_1), \dots, (p'_n, p''_n)\}$ can be thought of as **marked point process**.
- $\gamma \subset \mathbb{R}^3 \times S$, where $S = [0, W]$, $W > 0$.
- Distance is not Euclidean, but the **power distance**

$$d(q', p) = \|q' - p'\|^2 - p''.$$



Laguerre-Delaunay

Characteristic point, regularity

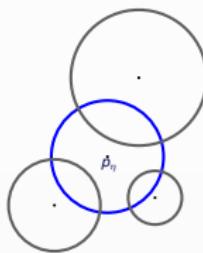
- Instead of circumscribed ball, we have the **characteristic point** $p_\eta = (p'_\eta, p''_\eta)$.

$$d(p'_\eta, p_i) = p''_\eta, \quad \text{for each } i = 1, \dots, 4.$$

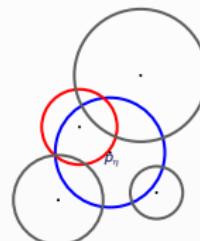
- Instead of the empty sphere property, we have **regularity**

η is **regular** if there is no other point $q \in \gamma$ such that $d(p'_\eta, q) < p''_\eta$.

$$\mathcal{LD}_4(\gamma) = \{\eta \subset \gamma : \text{card}(\eta) = 4, \eta \text{ is regular}\}$$



Points of η (gray) and their characteristic point p_η (blue).



A point (red) breaking the regularity of η .

Practical results

Implementation

The partition function Z_Λ^z is unknown → Birth-Death-Move Metropolis-Hastings algorithm.

Each step has to reconstruct a new tetrahedrization.



- Final solution: implement the MCMC algorithm and rely on Computer Graphics Algorithms Library for handling the tetrahedrization.

Current version at <https://github.com/DahnJ/Gibbs-Laguerre-Delaunay.git>

- Simulations done in C++, numerical analysis in Python and Mathematica.

Theoretical results

Goal: To prove the existence of the Gibbs-Laguerre-Delaunay models we simulated.

Results: Proved the existence of the following two classes of models.

A hyperedge potential ϕ is **unary** for the hypergraph structure \mathcal{E} if there exists a measurable function $\hat{\varphi} : \mathbf{N}_f \rightarrow \mathbb{R} \cup \{+\infty\}$ such that

$$\varphi(\eta, \gamma) = \hat{\varphi}(\eta) \text{ for } \eta \in \mathcal{E}(\gamma).$$

Bounded interaction: For $\eta \in \mathcal{LD}_4(\gamma)$ define the potential φ_S as a unary potential such that

$$\varphi_S(\eta, \gamma) \leq K_0 + K_1 \chi(\eta)^\beta$$

for some $K_0, K_1 \geq 0, \beta > 0$

Hard-core interaction: For $\eta \in \mathcal{LD}_4(\gamma)$ define the potential φ_{HC} as a unary potential such that

$$\sup_{\eta: d_0 \leq \chi(\eta) \leq d_1} \varphi_{HC}(\eta, \gamma) < \infty \text{ and } \varphi_{HC}(\eta, \gamma) = \infty \text{ if } \chi(\eta) > \alpha$$

for some $0 \leq d_0 < d_1 \leq \alpha$.

Based on *Dereudre, Drouilhet, Georgii: Existence of gibbsian point processes with geometry-dependent interactions (2012)*.

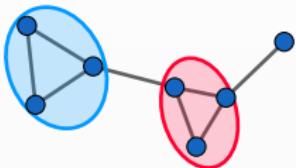
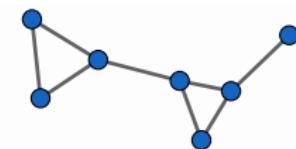
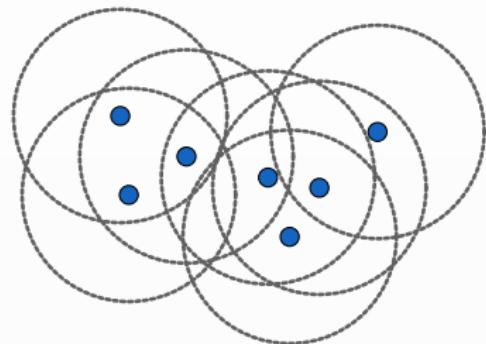
Definition. Hypergraph structure

A *hypergraph structure* is a measurable subset \mathcal{E} of $(\mathbf{N}_f \times \mathbf{N}_{lf}, \mathcal{N}_f \otimes \mathcal{N}_{lf})$ such that $\eta \subset \gamma$ for all $(\eta, \gamma) \in \mathcal{E}$. We call η a *hyperedge* of γ and write $\eta \in \mathcal{E}(\gamma)$, where $\mathcal{E}(\gamma) = \{\eta : (\eta, \gamma) \in \mathcal{E}\}$. For a given $\gamma \in \mathbf{N}_{lf}$, the pair $(\gamma, \mathcal{E}(\gamma))$ is called a *hypergraph*.

A *hyperedge potential* is a measurable function $\varphi : \mathcal{E} \rightarrow \mathbb{R} \cup \{+\infty\}$. We define $\varphi = 0$ on \mathcal{E}^c .

Many-body interaction

$$\text{LC}_r = \{(\eta, \gamma) : \eta \subset \gamma, \text{diam}(\eta) \leq r, \gamma \in \mathbb{N}_{lf}\}$$



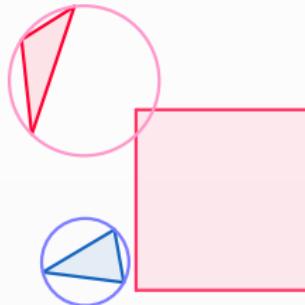
Set \mathcal{E}_Λ

Let $\Lambda \in \mathcal{B}_0$. Define the set

$$\mathcal{E}_\Lambda(\gamma) := \{\eta \in \mathcal{E}(\gamma) : \varphi(\eta, \zeta \cup \gamma_{\Lambda^c}) \neq \varphi(\eta, \gamma) \text{ for some } \zeta \in \mathbf{N}_\Lambda\}.$$

For $\eta \in \mathcal{E}(\gamma)$ such that $\varphi(\eta, \gamma) \neq 0$ we have the following implication:

$$\eta \notin \mathcal{E}(\zeta \cup \gamma_{\Lambda^c}) \text{ for some } \zeta \in \mathbf{N}_\Lambda \Rightarrow \eta \in \mathcal{E}_\Lambda(\gamma).$$



Finite horizon, range confinement, range condition.

Pseudo-periodic configurations

$M \in \mathbb{R}^{3 \times 3}$... an invertible 3×3 matrix, column vectors (M_1, M_2, M_3) .
For each $k \in \mathbb{Z}^3$ define the cell

$$C(k) = \{Mx \in \mathbb{R}^3 : x - k \in [-1/2, 1/2)^3\}.$$

Let $\Gamma \in \mathcal{N}_C$ be non-empty. Then we define the *pseudo-periodic* configurations $\bar{\Gamma}$ as

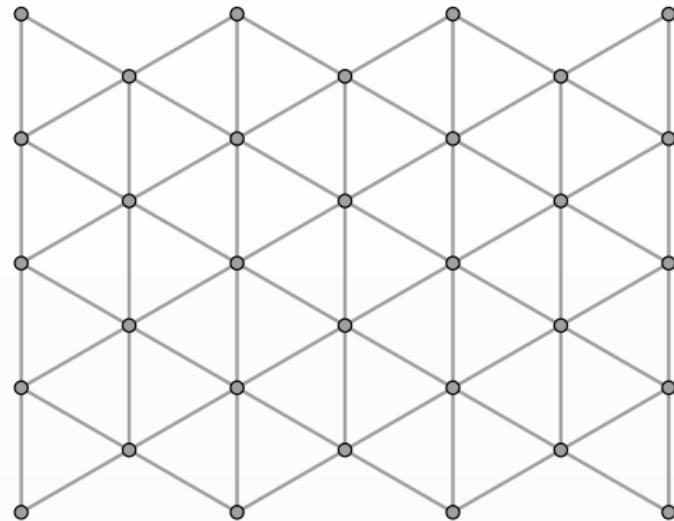
$$\bar{\Gamma} = \{\gamma \in \mathbf{N}_{lf} : \vartheta_{Mk}(\gamma_{C(k)}) \in \Gamma \text{ for all } k \in \mathbb{Z}^3\},$$

Fix some $A \subset C \times S$ and define

$$\Gamma^b = \{\zeta \in \mathbf{N}_C : \zeta = \{p\}, p \in B(0, b)\},$$

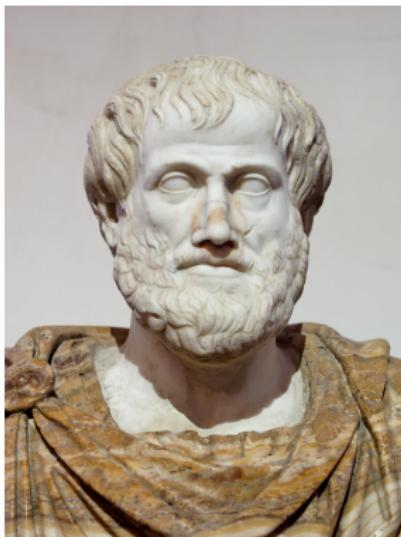
Let M be such that $|M_i| = a > 0$ for $i = 1, 2, 3$ and $\angle(M_i, M_j) = \pi/3$ for $i \neq j$.

In 2D: Equilateral triangles



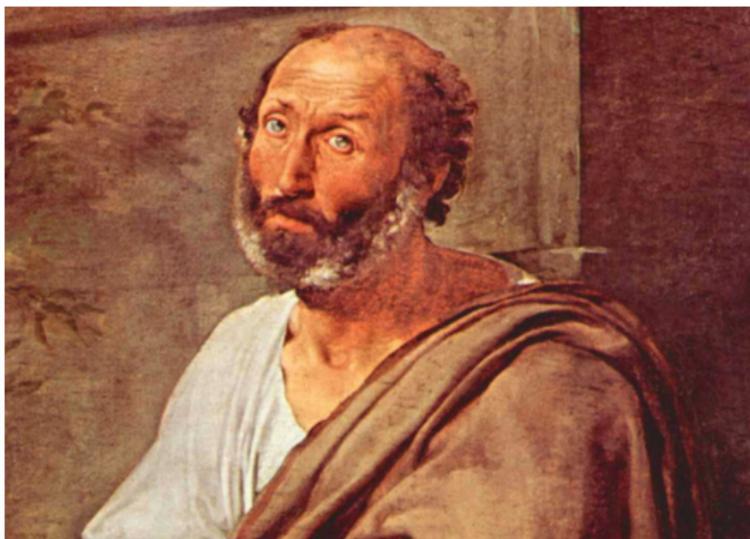
In 3D: Regular tetrahedra?

In 3D: Regular tetrahedra?



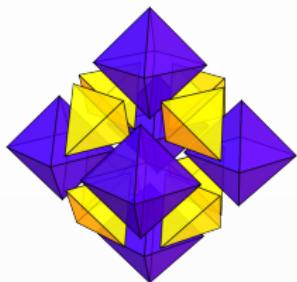
Aristotle

In 3D: Regular tetrahedra

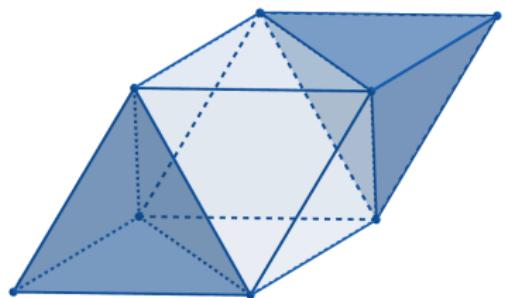


Tetrahedrons do not tessellate.

In 3D: Tetrahedral-octahedral honeycomb



Tetrahedral-octahedral honeycomb in an exploded view.



A single cell of a tetrahedral-octahedral honeycomb.





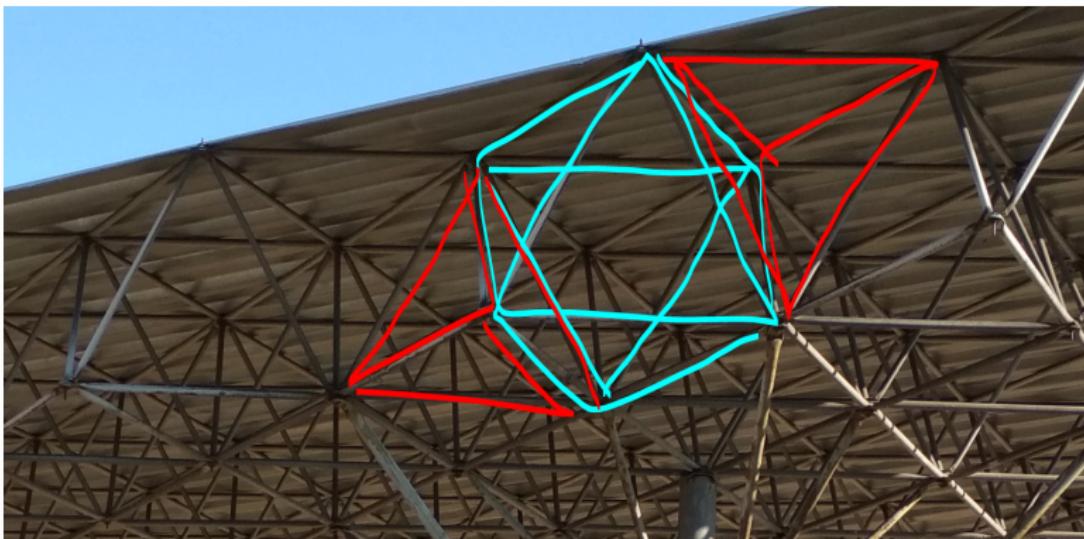


FIGURE 14

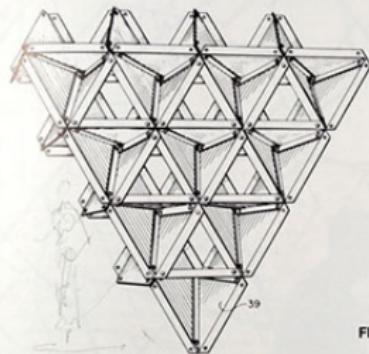


FIGURE 15

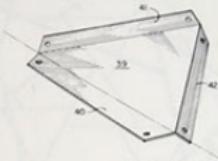
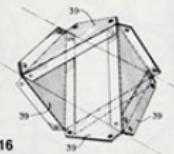
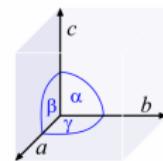
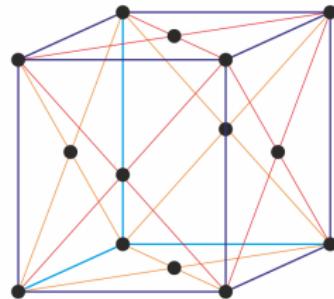


FIGURE 16



CRYSTAL LATTICE
face-centered cubic



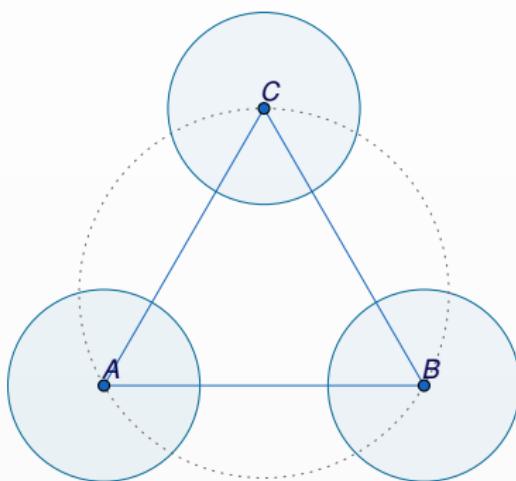
$$a = b = c$$

$$\alpha = \beta = \gamma = 90^\circ$$

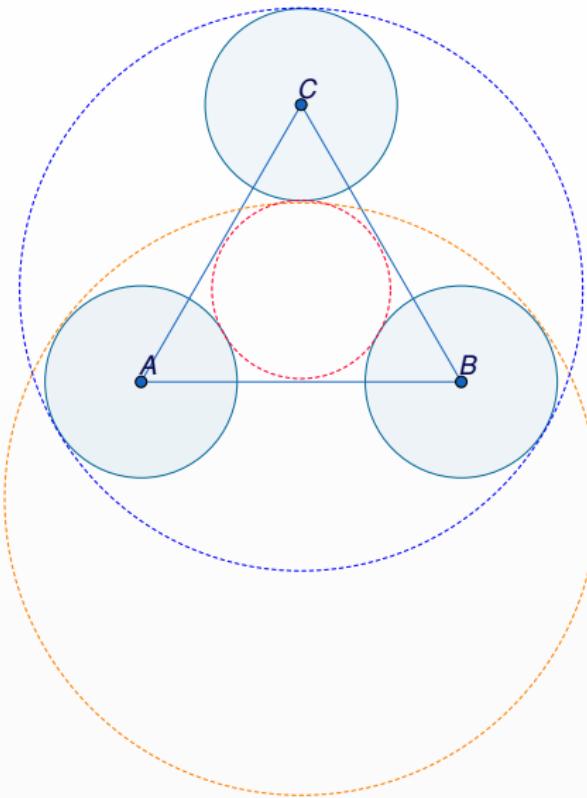
Bounding the diameter

$$\varphi_S(\eta, \gamma) \leq K_0 + K_1 \chi(\eta)^\beta$$

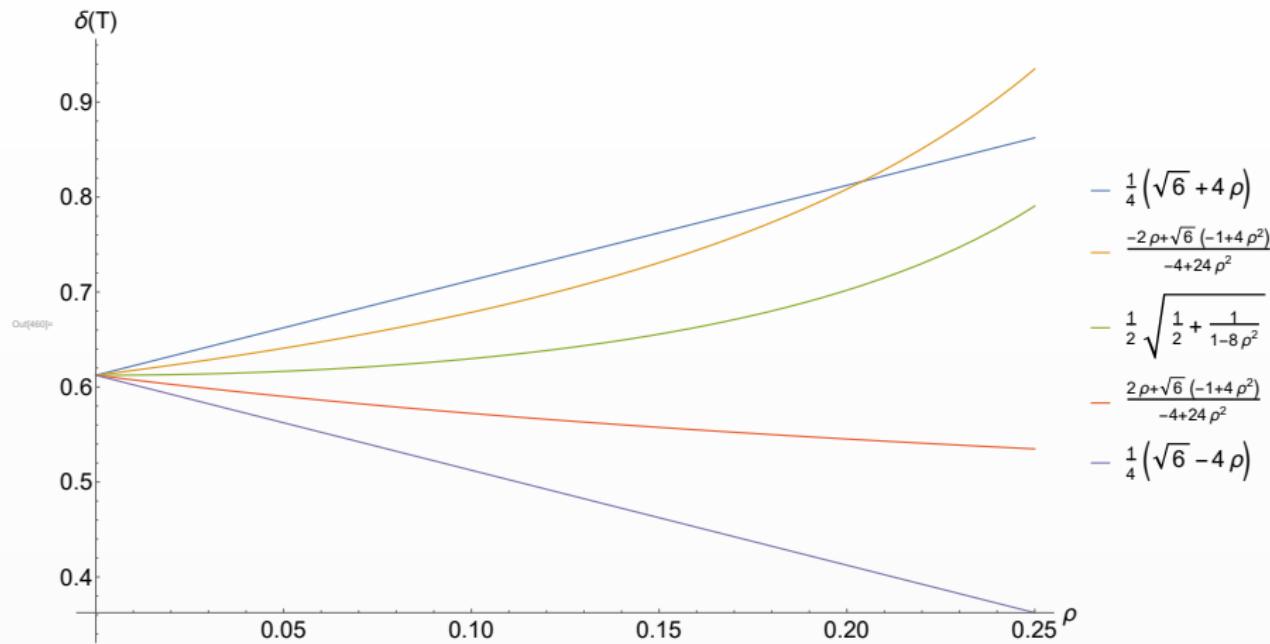
Need to bound the potential on the pseudo-periodic configurations $\tilde{\Gamma}$.



Problem of Apollonius



Apollonius spheres



$\delta(T)$ - circumdiameter of the tetrahedron

ρ - radius of the sphere in which the points can move

- ① D. Dereudre and F. Lavancier. Practical simulation and estimation for Gibbs Delaunay-Voronoi tessellations with geometric hardcore interaction. *Computational Statistics and Data Analysis*, 55(1):498-519, 2011.
- ② D. Dereudre, R. Drouilhet, and H.O. Georgii. Existence of gibbsian point processes with geometry-dependent interactions. *Probability Theory and Related Fields*, 153(3):643-670, 2012
- ③ Fropuff. The vertex configuration of a tetrahedral-octahedral honeycomb., 2006. URL
<https://en.wikipedia.org/wiki/File:TetraOctaHoneycomb-VertexConfig.svg>