

Department of Probability and Mathematical Statistics



FACULTY
OF MATHEMATICS
AND PHYSICS
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Gibbs-Delaunay Tessellations
Simulation and estimation

12 September 2018

Section 1

Point processes

Poisson point process

We're on $(\mathbb{R}^d, \mathcal{B})$, Euclidean space, λ^d Lebesgue measure.
Denote \mathcal{B}_0 the set of bounded Borel sets.

Definition. Poisson point process

Let μ be a locally finite non-atomic measure on \mathbb{R}^d . A point process Φ satisfying

- $\Phi(B) \sim \text{Pois}(\mu(B))$ 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.

is called a **Poisson point process** with the **intensity measure** μ .

If $\mu = z\lambda^d$ we call the process **homogenous** and z the **intensity**.

For $\Lambda \in \mathcal{B}_0$, denote the distribution of $\Phi \cap \Lambda$ as π_Λ^z .

For the case $z = 1$, use π_Λ .

$\Phi : (\Omega, \mathcal{A}, P) \rightarrow (\mathcal{F}_{lf}, \mathcal{F})$ where

- $\mathcal{F}_{lf} = \{\gamma \subset \mathbb{R}^d \mid \gamma \cap \Lambda \text{ is finite for all } \Lambda \in \mathcal{B}_0\}$ and
- \mathcal{F} is generated by sets of the form
 $\{\gamma \in \mathcal{F}_{lf} \mid N_\Lambda(\gamma) = n\}, n \in \mathbb{N}, \Lambda \in \mathcal{B},$ where $N_\Lambda(\gamma) = \text{Card}(\gamma \cap \Lambda).$

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We can view π_Λ as a reference measure on $(\mathcal{F}_{lf}, \mathcal{F}, \pi_\Lambda)$ and define new processes through that.

Poisson point process with intensity z :

$$\pi_\Lambda^z(d\gamma) \propto z^{N_\Lambda(\gamma)} \pi_\Lambda(d\gamma).$$

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Poisson point process with intensity z :

$$\pi_\Lambda^z(d\gamma) \propto z^{N_\Lambda(\gamma)} \pi_\Lambda(d\gamma).$$

Add a new term to obtain the finite volume Gibbs point process:

$$z^{N_\Lambda(\gamma)} e^{-H(\gamma)} \pi_\Lambda(d\gamma).$$

Take $\Lambda \in \mathcal{B}_0$.

Definition. Finite volume Gibbs point process

The **finite-volume Gibbs point process** on Λ (fGPP) is a point process Γ defined by its density with respect to π_Λ :

$$f(\gamma) = \frac{1}{C_\Lambda^z} z^{N_\Lambda(\gamma)} e^{-H(\gamma)} \quad \gamma \in \mathcal{F}_\Lambda,$$

where

- $z > 0$,
- $H : \mathcal{F}_\Lambda \mapsto \mathbb{R} \cup \{+\infty\}$ is a measurable function called the **energy function**,
- $C_\Lambda^z = \int z^{N_\Lambda} e^{-H} d\pi_\Lambda$ is the normalizing constant.

Denote P_Λ^z the distribution of the finite-volume Gibbs point process on Λ , called the **finite Gibbs measure**.

Energy function H

Requirements and an example

Typically, we require H to satisfy:

- **Non-degeneracy:**

$$H(\emptyset) < +\infty.$$

- **Hereditarity:** For any finite point configuration $\gamma \subset \mathbb{R}^d$ and $x \in \gamma$

$$H(\gamma) < +\infty \Rightarrow H(\gamma \setminus \{x\}) < +\infty.$$

- **Stability:** There exists a constant A such that for any finite point configuration γ

$$H(\gamma) \geq AN_{\mathbb{R}^d}(\gamma).$$

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Example (Strauss interaction): For $R > 0$,

$$H(\gamma) = \sum_{\{x,y\} \subset \gamma} 1_{[0,R]}(\|x - y\|)$$

For $\gamma \in \mathcal{F}_{lf}$ and $x \in \mathbb{R}^d$, define the **local energy** of x in γ by

$$h(x, \gamma) = H(\gamma \cup \{x\}) - H(\gamma).$$

Proposition (Georgii, Nguyen, Zessin). GNZ equations

For any positive measurable function $f : \mathbb{R}^d \times \mathcal{F}_{lf} \rightarrow \mathbb{R}$,

$$\int \sum_{x \in \gamma} f(x, \gamma \setminus \{x\}) P_{\Lambda}^z(d\gamma) = z \int \int_{\Lambda} f(x, \gamma) e^{-h(x, \gamma)} dx P_{\Lambda}^z(d\gamma).$$

Section 2

Triangulations

Delaunay triangulation

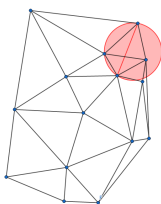
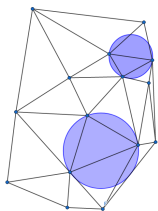
Through empty sphere property

A $d + 1$ -tuple $T = \{x_1, \dots, x_{d+1}\} \subset \gamma$ satisfies the **empty sphere property** if the open circumscribed ball $\mathcal{B}(T)$ does not contain any points from γ .

Definition. Delaunay triangulation in \mathbb{R}^d

A **Delaunay triangulation** of $\gamma \in \mathcal{F}_d$ is the set $\text{Del}(\gamma)$ defined by

$$\text{Del}(\gamma) = \{T \subset \gamma : \text{card}(T) = d + 1, T \text{ satisfies the empty sphere property} \}.$$



Additional assumption on γ (**No cospherical points**): no $d + 2$ points x_1, \dots, x_{d+2} are cospherical, i.e. there is no point $x \in \mathbb{R}^d$ such that $d(x, x_1) = \dots = d(x, x_{d+2})$.

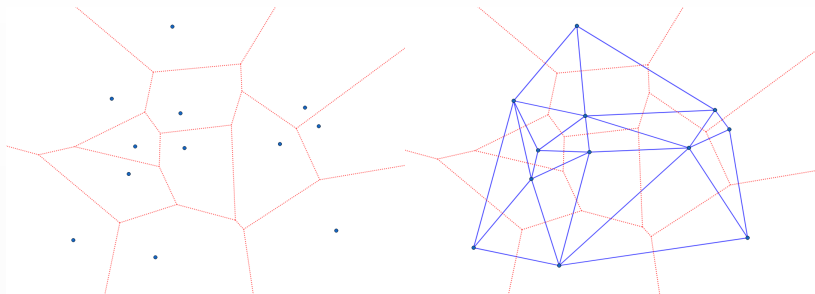
$d(x, y)$ is the Euclidean distance between points x and y .

Delaunay triangulation

Through Voronoi tessellation

For $x \in \gamma$, the **Voronoi cell** of x in γ is

$$C(x, \gamma) = \{z \in \mathbb{R}^d : \|x - z\| \leq \|y - z\| \ \forall y \in \gamma\}.$$

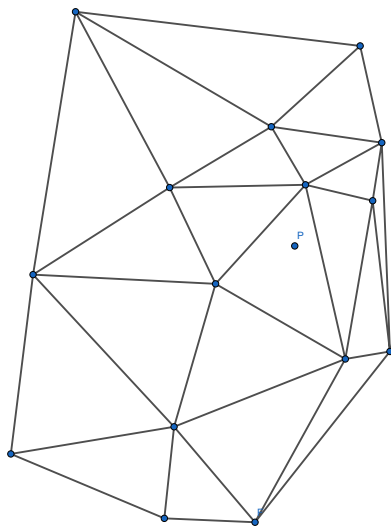


Then the Delaunay triangulation can be defined as

$$Del(\gamma) = \{\{x, y\} \subset \gamma : C(x, \gamma) \cap C(y, \gamma) \neq \emptyset\}.$$

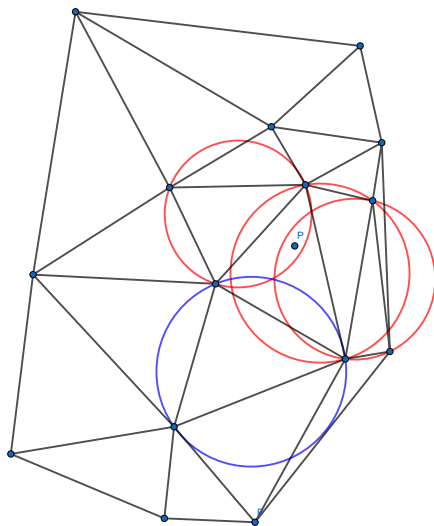
Delaunay triangulation

Building a Delaunay triangulation



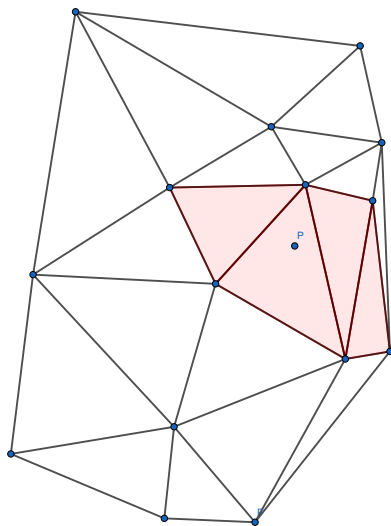
Delaunay triangulation

Building a Delaunay triangulation



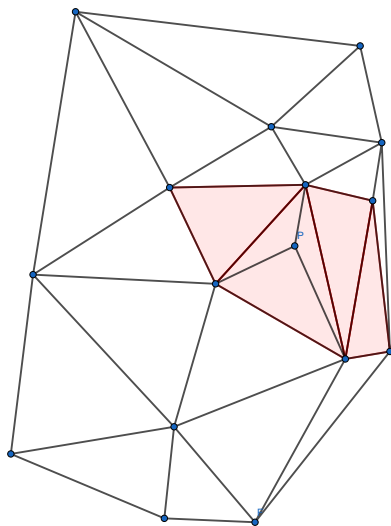
Delaunay triangulation

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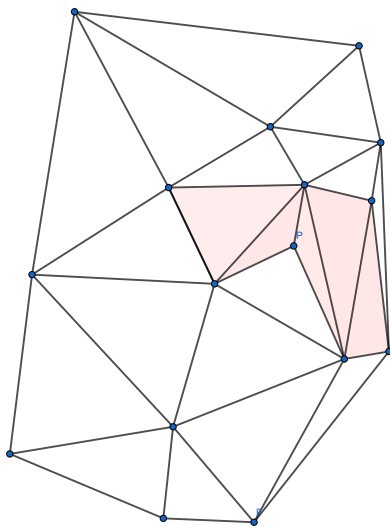
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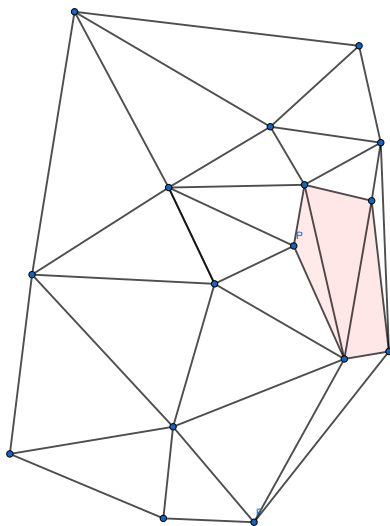
Delaunay triangulation

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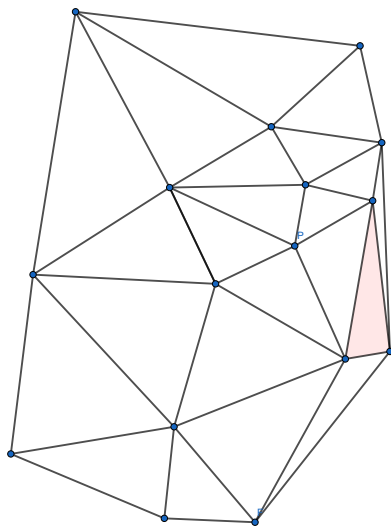
Delaunay triangulation

Building a Delaunay triangulation



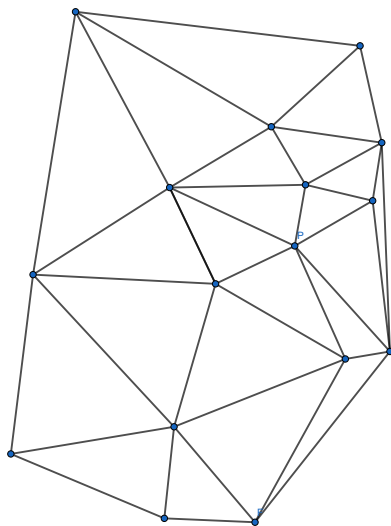
Delaunay triangulation

Building a Delaunay triangulation



Delaunay triangulation

Building a Delaunay triangulation



Delaunay triangulation in 2D

Geometric predicates, 2D

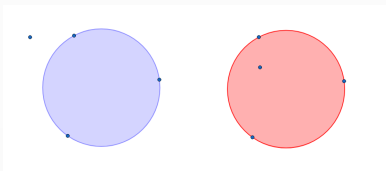
In $2D$, for p_1, \dots, p_4 , with $p_i = (x_i, y_i)$, such that

$$ORIENTATION(p_1, p_2, p_3) = \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix} > 0$$

In order for p_4 to be outside the circumsphere defined by p_1, p_2, p_3 it must hold that

$$INCIRCLE(p_1, p_2, p_3, p_4) = \begin{vmatrix} x_1 & y_1 & w_1 & 1 \\ x_2 & y_2 & w_2 & 1 \\ x_3 & y_3 & w_3 & 1 \\ x_4 & y_4 & w_4 & 1 \end{vmatrix} > 0$$

where $w_i = x_i^2 + y_i^2, i = 1, \dots, 4$



Delaunay triangulation in 3D

Geometric predicates, 3D

In 3D, for p_1, \dots, p_5 with $p_i = (x_i, y_i, z_i)$, such that

$$\text{ORIENTATION}(p_1, p_2, p_3, p_4) = \begin{vmatrix} x_1 & y_1 & z_1 & 1 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \end{vmatrix} > 0$$

in order for p_5 to be outside the circumsphere defined by p_1, \dots, p_4 it must hold that

$$\text{INCIRCLE}(p_1, p_2, p_3, p_4, p_5) = \begin{vmatrix} x_1 & y_1 & z_1 & w_1 & 1 \\ x_2 & y_2 & z_2 & w_2 & 1 \\ x_3 & y_3 & z_3 & w_3 & 1 \\ x_4 & y_4 & z_4 & w_4 & 1 \\ x_5 & y_5 & z_5 & w_5 & 1 \end{vmatrix} > 0$$

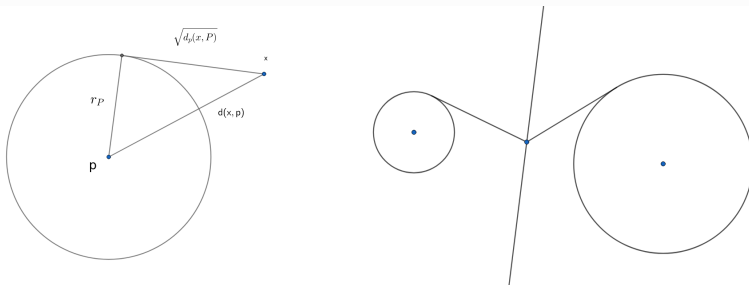
where $w_i = x_i^2 + y_i^2 + z_i^2, i = 1, \dots, 5$.

Laguerre-Delaunay triangulation

Power metric

- Generators are not points, but **spheres**.
- $\gamma = \{P_1, \dots, P_n\} = \{(p_1, r_{p_1}), \dots, (p_n, r_{p_n})\}$ can be thought of as **marked point process**.
- Metric is not Euclidean, but **power distance**.

$$d_p(x, P) = d(x, p)^2 - r_P^2$$



Laguerre-Delaunay triangulation

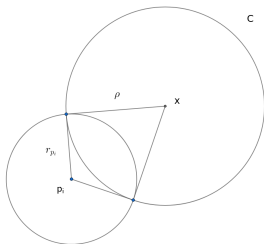
Inscribed sphere and cospherical spheres

Definition. Inscribed sphere

A sphere $C = (x, \rho)$ is **inscribed** among $d + 1$ spheres P_1, \dots, P_{d+1} if

$$\rho^2 = d_p(x, P_1) = d_p(x, P_2) = \dots = d_p(x, P_{d+1})$$

The spheres P_1, \dots, P_{d+1} are **cospherical** to the sphere C .



P_1, \dots, P_{d+1} are cospherical $\Rightarrow C$
intersects $P_i, i = 1, \dots, d + 1$ at a right
angle.

Laguerre-Delaunay triangulation

Definition

Definition. Empty sphere, empty sphere property

The inscribed sphere is called an **empty sphere** if no sphere from γ intersects C at an acute angle and if no sphere from γ is contained in C .

Spheres P_1, \dots, P_{d+1} satisfy the **empty sphere property** if their inscribed sphere is an empty sphere.

Definition. Laguerre-Delaunay triangulation in \mathbb{R}^d

A **Laguerre-Delaunay triangulation** of a locally finite set $\gamma = \{(p_1, r_{p_1}), \dots, (p_n, r_{p_n})\}$ is the set $\mathcal{LDel}(\gamma)$ defined by

$$\mathcal{LDel}(\gamma) = \{T \subset \gamma : \text{card}(T) = d + 1, T \text{ satisfies the empty sphere property} \}.$$

Laguerre-Delaunay triangulation in 3D

Geometric predicates, 3D

For P_1, \dots, P_5 , where $P_i = (x_i, y_i, z_i, r_i)$ such that

$$\text{ORIENTATION}(P_1, P_2, P_3, P_4) = \begin{vmatrix} x_1 & y_1 & z_1 & 1 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \end{vmatrix} > 0,$$

in order for the sphere P_5 to be outside the inscribed sphere defined by spheres P_1, \dots, P_4 it must hold that

$$\text{INCIRCLE}(P_1, P_2, P_3, P_4, P_5) = \begin{vmatrix} x_1 & y_1 & z_1 & w_1 & 1 \\ x_2 & y_2 & z_2 & w_2 & 1 \\ x_3 & y_3 & z_3 & w_3 & 1 \\ x_4 & y_4 & z_4 & w_4 & 1 \\ x_5 & y_5 & z_5 & w_5 & 1 \end{vmatrix} > 0$$

where $w_i = x_i^2 + y_i^2 + z_i^2 - r_i^2, i = 1, \dots, 5$



- Computational Geometry Algorithms Library
- C++ library for geometric computation.
- Has fast implementations of both 3D Delaunay and 3D Laguerre-Delaunay triangulations (called Regular triangulation).
- Offers exact arithmetic for both geometric constructions and geometric predicates.

| | Delaunay | Delaunay | Regular | Regular |
|---------------------------------|----------|---------------|----------|------------------|
| | | Fast location | | No hidden points |
| Construction from 10^2 points | 0.00054 | 0.000576 | 0.000948 | 0.000955 |
| Construction from 10^3 points | 0.00724 | 0.00748 | 0.0114 | 0.0111 |
| Construction from 10^4 points | 0.0785 | 0.0838 | 0.122 | 0.117 |
| Construction from 10^5 points | 0.827 | 0.878 | 1.25 | 1.19 |
| Construction from 10^6 points | 8.5 | 9.07 | 12.6 | 12.2 |
| Construction from 10^7 points | 87.4 | 92.5 | 129 | 125 |

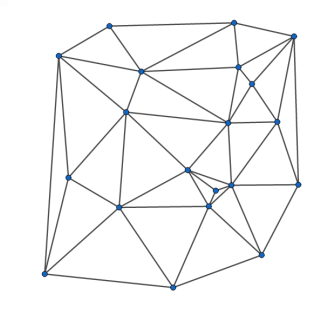
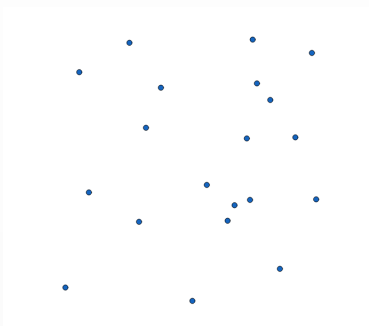
Section 3

Random triangulations

Poisson-Delaunay triangulation

Definition. Poisson-Delaunay triangulation in \mathbb{R}^d

The **Poisson-Delaunay triangulation** of the Poisson point process Φ is the set $Del(\Phi)$.



Definition. Gibbs-Laguerre-Delaunay triangulation in \mathbb{R}^d

The Gibbs-Laguerre-Delaunay triangulation of the finite marked Gibbs point process Γ is the set $\mathcal{LDel}(\Gamma)$.

Geometric aspects of the triangulation can be used to define H .
In general, the energy can have the form

$$H(\gamma) = \sum_{T \in \mathcal{LDel}(\gamma)} V_1(T) + \sum_{\{T, T'\} \subset \mathcal{LDel}(\gamma)} V_2(T, T')$$

to take interaction into account. V_1 and V_2 can be any functions from d -dimensional simplices to $\mathbb{R} \cup \{+\infty\}$.

Section 4

Simulation

Specification of the GLD model

Our model is the GLD triangulation in \mathbb{R}^3 with the energy function of the form

$$H(\gamma) = \sum_{T \in \mathcal{L}Del_{\Lambda}(\gamma)} V_1(T),$$

with V_1 defined as

$$V_1(T) = \begin{cases} \infty & \text{if } a(T) \leq \epsilon, \\ \infty & \text{if } R(T) \geq \alpha, \\ \theta Sur(T) & \text{otherwise,} \end{cases} \quad (1)$$

where

- $a(T)$ is the area of the smallest face of the tetrahedron T .
- $R(T)$ is the circumradius of T .
- $Sur(T)$ is the surface area of the tetrahedron.

Futhermore, $W = [0, W_0]$ is the weight proposal interval, where $W_0 > 0$ is the maximum weight.

Simulating a GLD triangulation

Through MCMC

- The normalizing constant C_{λ}^z is difficult to obtain.
- To sample from the distribution, we use MCMC methods.
 - Classic Birth-Death-Move Metropolis-Hastings algorithm, invented for this very purpose.

Simulating a GLD triangulation

Through MCMC

- The normalizing constant C_Λ^Z is difficult to obtain.
- To sample from the distribution, we use MCMC methods.
 - Classic Birth-Death-Move Metropolis-Hastings algorithm, invented for this very purpose.

Birth-Death-Move algorithm

Denote Λ the observation window and Δ the simulation window, $\Lambda \subset \Delta$.

$\Lambda_W := \Lambda \times [0, W]$. Choose move variance $\sigma^2 > 0$.

- 1 Start with a permissible initial configuration $\gamma_0 \subset \Delta \times W$.
- 2 Denote $n = \text{card}(\gamma_0 \cap \Lambda)$.
- 3 In each step, with probability $1/3$:
 - **Birth**: Generate a new point $x \in \Lambda_W$ uniformly. Accept with probability $\frac{zf(\gamma_0 \cup \{x\})}{(n+1)f(\gamma_0)}$,
 - **Death**: Choose $x \in \gamma_0$ uniformly. Accept with probability $\frac{nf(\gamma_0 \setminus \{x\})}{zf(\gamma_0)}$,
 - **Move**: Choose $x \in \gamma_0$ uniformly and generate $y \in \Lambda_W$ with the distribution $\mathcal{N}(x, \sigma^2 I)$. Accept with probability $\frac{f(\gamma_0 \setminus \{x\} \cup \{y\})}{f(\gamma_0)}$.
- 4 Denote the new configuration γ_1 , set $\gamma_0 \leftarrow \gamma_1$ and go to 2.

$$\pi_{\Lambda}^z \propto z^{N_{\Lambda}} \pi_{\Lambda}$$

$$P_{\Lambda}^z \propto z^{N_{\Lambda}} e^{-\theta H} \pi_{\Lambda}$$

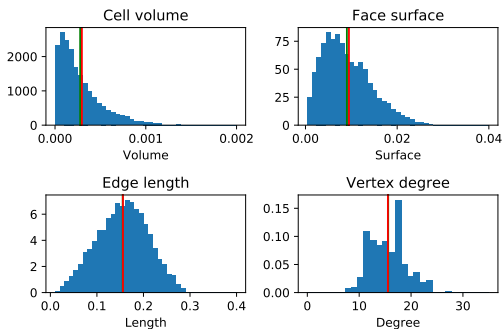
$\theta = 0 \Rightarrow$ GPP becomes PPP with intensity z .

Comparison with Poisson-Delaunay

$$\pi_{\Lambda}^z \propto z^{N_{\Lambda}} \pi_{\Lambda}$$

$$P_{\Lambda}^z \propto z^{N_{\Lambda}} e^{-\theta H} \pi_{\Lambda}$$

$\theta = 0 \Rightarrow$ GPP becomes PPP with intensity z .



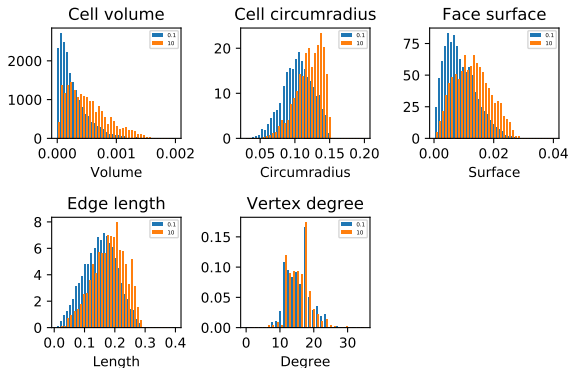
Realization of a GLD model with parameters $\theta = 0.1, z = 500, \alpha = 0.15, \epsilon = 0, W_0 = 0.001$. Red line is the expected value for Poisson-Delaunay.

Role of the parameter θ

θ positive

The model prefers configurations with lower energy.

θ multiplies the total surface area of all cells, thus with higher θ , the cells are forced to become large.



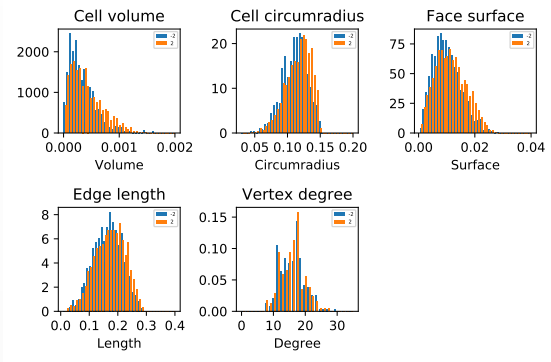
Realization of two GLD models. Blue: $\theta = 0.1$, orange: $\theta = 10$. Other parameters are $z = 500$, $\alpha = 0.15$, $\epsilon = 0$, $W_0 = 0.001$ for both models.

Role of the parameter θ

θ negative

The model prefers configurations with lower energy.

- $\theta > 0$. The sum needs to be minimized \Rightarrow fewer larger tetrahedra.
- $\theta < 0$. The sum needs to be maximized \Rightarrow many smaller tetrahedra.



Realization of two GLD models. Blue: $\theta = -2$, orange: $\theta = 2$. Other parameters are $z = 500$, $\alpha = 0.15$, $\epsilon = 0$, $W_0 = 0.001$ for both models.

Section 5

Estimation

Two-step procedure

We have 4 parameters to estimate

- Hard-core parameters.
 - The minimum face area ϵ ,
 - the maximum circumradius α .
- Smooth parameters.
 - The multiplier of $Sur(T)$, θ ,
 - the intensity of the underlying Poisson point process, z .

This is done through a **two-step procedure**

- 1 Estimate the hardcore parameters (ϵ, α) directly.
- 2 Estimate the smooth parameters (θ, z) by **Maximum Pseudo-Likelihood Estimation** (MPLE) using the estimates $(\hat{\epsilon}, \hat{\alpha})$.

Two-step procedure

1. Hardcore interaction parameters estimation

[Dereudre, Lavancier (2009)] only proves consistence for a single parameter (although experimentally both work).

Thanks to the fact that the hardcore parameter α satisfies

$$\text{if } \alpha < \alpha' \text{ then } \forall \Lambda, H_{\Lambda}^{\epsilon, \alpha, \theta}(\gamma) < \infty \Rightarrow H_{\Lambda}^{\epsilon, \alpha', \theta}(\gamma) < \infty,$$

its consistent estimator is

$$\hat{\alpha} = \inf\{\alpha > 0, H_{\Lambda}(\gamma) < \infty\},$$

which in practice is estimated as

$$\hat{\alpha} = \max\{r(T), T \in \mathcal{L}Del_{\Lambda}(\gamma)\}.$$

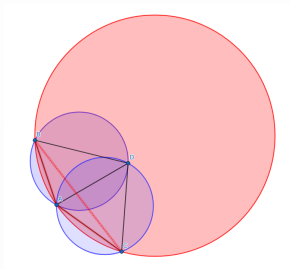
The estimate $\hat{\alpha}$ is then used in the pseudo-likelihood function in the second estimation step.

Two-step procedure

2. Maximum pseudolikelihood

MPLE depends on GNZ, which works only for **hereditary** energy functions.

$$H(\gamma) < \infty \Rightarrow H(\gamma \setminus \{x\}) < \infty \quad x \in \gamma$$

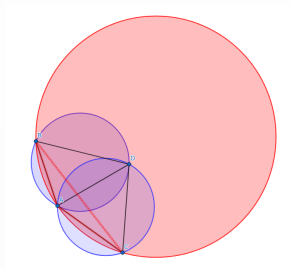


Two-step procedure

2. Maximum pseudolikelihood

MPLE depends on GNZ, which works only for **hereditary** energy functions.

$$H(\gamma) < \infty \Rightarrow H(\gamma \setminus \{x\}) < \infty \quad x \in \gamma$$



However [Dereudre, Lavancier (2009)] proved that GNZ still holds if we restrict ourselves to **removable points**.

We say a point $x \in \gamma$ is removable if $H(\gamma \setminus \{x\}) < \infty$. Denote $\mathcal{R}^\alpha(\gamma)$ the set of removable points in γ .

Two-step procedure

2. Maximum pseudolikelihood

The pseudolikelihood function is

$$PLL_{\Lambda_W}(\gamma, z, \alpha, \theta) = \int_{\Lambda_W} z \exp(-h^{\alpha, \theta}(x, \gamma)) dx + \sum_{x \in \mathcal{R}^{\alpha}(\gamma) \cap \Lambda_W} (h^{\alpha, \theta}(x, \gamma \setminus \{x\}) - \ln(z)),$$

The estimates $\hat{\theta}$ and \hat{z} are obtained through minimizing the PLL_{Λ_W} function.

$$(\hat{z}, \hat{\theta}) = \operatorname{argmin}_{z, \theta} PLL_{\Lambda_W}(\gamma, z, \hat{\alpha}, \theta).$$

Two-step procedure

2. Maximum pseudolikelihood

The pseudolikelihood function is

$$PLL_{\Lambda_W}(\gamma, z, \alpha, \theta) = \int_{\Lambda_W} z \exp(-h^{\alpha, \theta}(x, \gamma)) dx + \sum_{x \in \mathcal{R}^\alpha(\gamma) \cap \Lambda_W} (h^{\alpha, \theta}(x, \gamma \setminus \{x\}) - \ln(z)),$$

The estimates $\hat{\theta}$ and \hat{z} are obtained through minimizing the PLL_{Λ_W} function.

$$(\hat{z}, \hat{\theta}) = \operatorname{argmin}_{z, \theta} PLL_{\Lambda_W}(\gamma, z, \hat{\alpha}, \theta).$$

Differentiation yields the estimate \hat{z}

$$\hat{z} = \frac{\operatorname{card}(\mathcal{R}^{\hat{\alpha}}(\gamma) \cap \Lambda_W)}{\int_{\Lambda_W} \exp(-h^{\hat{\alpha}, \theta}(x, \gamma)) dx},$$

Two-step procedure

2. Maximum pseudolikelihood

The pseudolikelihood function is

$$PLL_{\Lambda_W}(\gamma, z, \alpha, \theta) = \int_{\Lambda_W} z \exp(-h^{\alpha, \theta}(x, \gamma)) dx + \sum_{x \in \mathcal{R}^\alpha(\gamma) \cap \Lambda_W} (h^{\alpha, \theta}(x, \gamma \setminus \{x\}) - \ln(z)),$$

The estimates $\hat{\theta}$ and \hat{z} are obtained through minimizing the PLL_{Λ_W} function.

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Differentiation yields the estimate \hat{z}

$$\hat{z} = \frac{\operatorname{card}(\mathcal{R}^{\hat{\alpha}}(\gamma) \cap \Lambda_W)}{\int_{\Lambda_W} \exp(-h^{\hat{\alpha}, \theta}(x, \gamma)) dx},$$

and the estimate $\hat{\theta}$ as the solution of

$$z \int_{\Lambda_W} (h^{\hat{\alpha}, 1}(x, \gamma) \exp(-h^{\hat{\alpha}, \theta}(x, \gamma))) dx = \sum_{x \in \mathcal{R}^{\hat{\alpha}}(\gamma) \cap \Lambda_W} h^{\hat{\alpha}, 1}(x, \gamma \setminus \{x\}).$$

Two-step procedure

2. Maximum pseudolikelihood - practical implementation

To obtain the estimate for θ , substitute the expression for \hat{z} into the equation for θ .

$$\frac{\int_{\Lambda_W} (h^{\hat{\alpha},1}(x, \gamma) \exp(-h^{\hat{\alpha},\theta}(x, \gamma))) dx}{\int_{\Lambda_W} \exp(-h^{\hat{\alpha},\theta}(x, \gamma)) dx} = \frac{\sum_{x \in \mathcal{R}^{\hat{\alpha}}(\gamma) \cap \Lambda_W} h^{\hat{\alpha},1}(x, \gamma \setminus \{x\})}{\text{card}(\mathcal{R}^{\alpha}(\gamma) \cap \Lambda_W)}. \quad (2)$$

After some algebraic manipulation, we obtain the equation

$$\int_{\Lambda_W} \exp(-\theta h^{\hat{\alpha},1}(x, \gamma)) (h^{\hat{\alpha},1}(x, \gamma) - c) dx = 0,$$

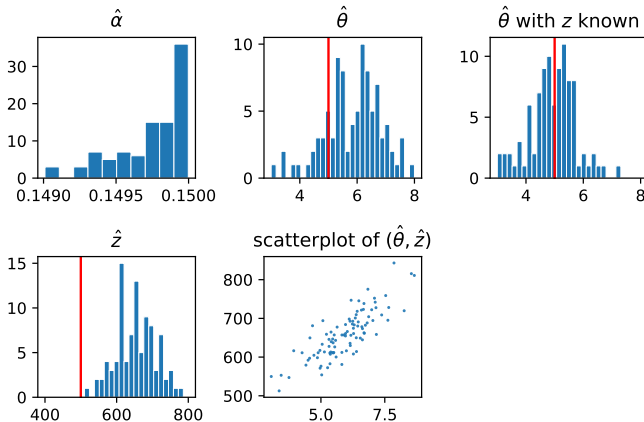
where c is the RHS of (2), which is independent of θ .

After $\hat{\theta}$ is estimated, we then obtain the estimate \hat{z} using the estimate $\hat{\theta}$ instead of θ .

All integrals are estimated by MC-integration.

Estimation results

For Gibbs-Delaunay



Estimates from 303 simulations of a Gibbs-Delaunay model with $\theta = 5$, $z = 500$, $\alpha = 0.15$, $\epsilon = 0$.

- Variational estimator

$$E\left(\sum_{x \in \Gamma} \nabla_x f(x, \Gamma \setminus \{x\})\right) = \theta E\left(\sum_{x \in \Gamma} f(x, \Gamma \setminus \{x\}) \nabla_x h(x, \Gamma \setminus \{x\})\right).$$

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- Energy with explicit interaction, e.g.

$$V_2(T, T') = \theta \left(\frac{\max(\text{Vol}(T), \text{Vol}(T'))}{\min(\text{Vol}(T), \text{Vol}(T'))} - 1 \right)$$

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- Periodic outside configuration.