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Gibbs-Delaunay Tessellations
Simulation and estimation

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Section 1

Point processes

We're on $(\mathbb{R}^d, \mathcal{B})$.

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 $B \in \mathcal{B}_0$,
- $\Phi(B_1), \dots, \Phi(B_n)$ 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 $\Theta \cap \Lambda$ 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 $N_\Lambda(\gamma) = \text{Card}(\gamma \cap \Lambda)$.

We can view π_Λ as a reference measure on $(\mathcal{F}_{lf}, \mathcal{F}, \pi_\Lambda)$.

Then we can define new point processes through defining their density w.r.t. π_Λ .

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** (fGPP) is a point process 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.

- Physical motivation
- Other examples of energy functions
- Allows working explicitly with geometrical structures such as random tessellations

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). GZN equations

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

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

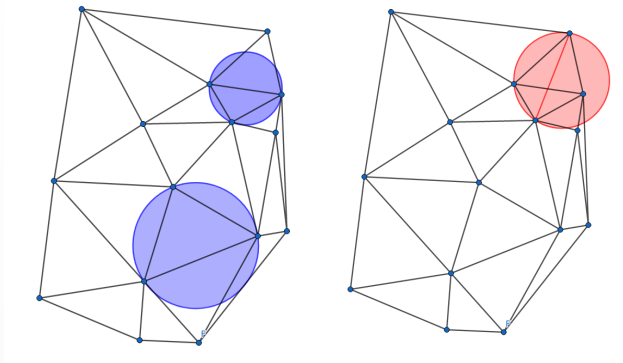
Section 2

Triangulations

Delaunay triangulation

Through empty sphere property

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



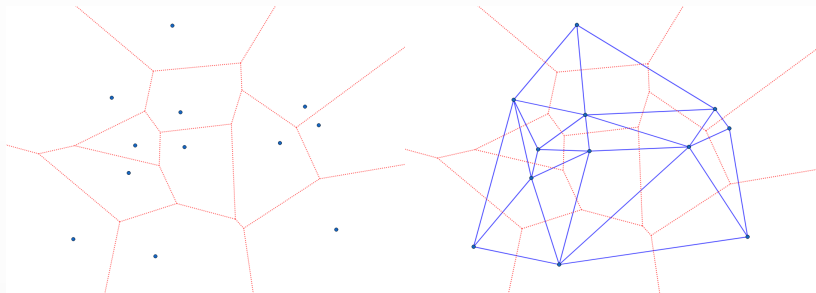
Additional assumption on γ (**No cospherical points**): no $d + 2$ points x_1, \dots, x_{d+2} are cospherical, i.e. there is no point $x \in \mathbb{R}^d$ such that $d(x, x_1) = \dots = d(x, x_2)$.

Delaunay triangulation

Through Voronoi tessellation

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

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

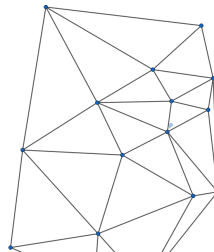
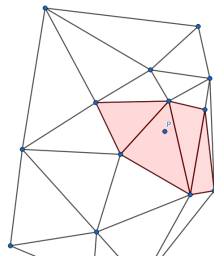
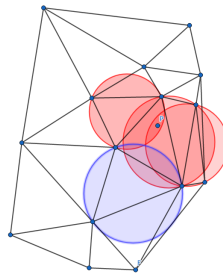
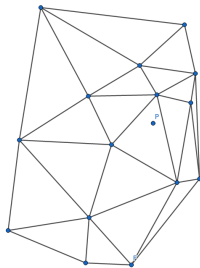


Then the Delaunay tessellation can be defined as

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

Delaunay triangulation

Building a Delaunay triangulation



Delaunay triangulation

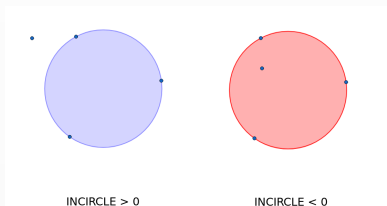
Geometric predicates, 2D

In 2D

$$\text{INCIRCLE}(P_1, P_2, P_3, P_4) = \begin{vmatrix} x_1 & y_1 & w_1 & 1 \\ x_2 & y_2 & w_2 & 1 \\ x_3 & y_3 & w_3 & 1 \\ x_4 & y_4 & w_4 & 1 \end{vmatrix}$$

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

$$\text{ORIENTATION}(P_1, P_2, P_3) = \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix} > 0$$



Delaunay triangulation

Geometric predicates, 3D

In 3D

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

where $w_i = x_i^2 + y_i^2 + z_i^2, i = 1, \dots, 5$
if the following condition is satisfied

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

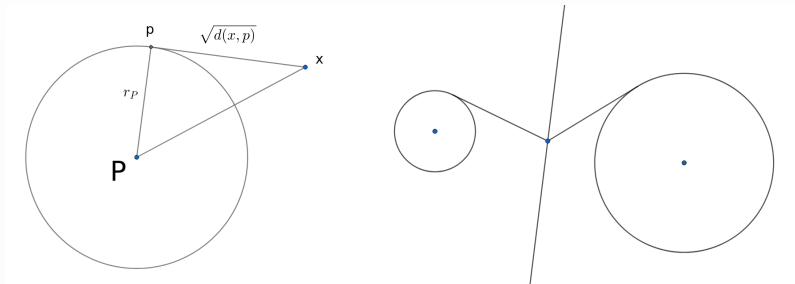
Laguerre-Delaunay triangulation

Power metric

Generators are not points, but **spheres**.

Metric is not Euclidean, but **power distance**.

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



Laguerre-Delaunay triangulation

Inscribed sphere and empty sphere property

Laguerre-Delaunay triangulation

Geometric predicates, 3D

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

where $w_i = x_i^2 + y_i^2 + z_i^2 - r_i^2, i = 1, \dots, 5$
if the following condition is satisfied

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

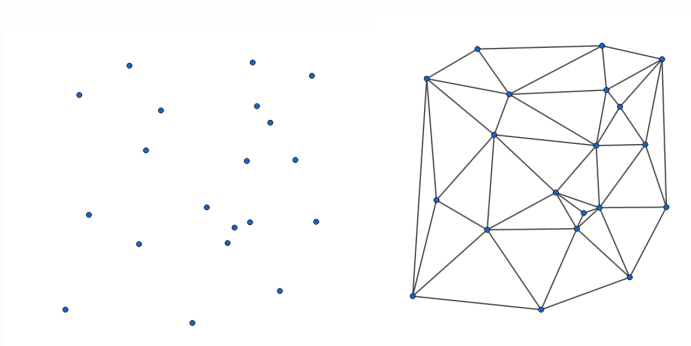
Why? Because both are **regular triangulations** - convex hulls of lifted sets of points.

Section 3

Random triangulations

Poisson-Delaunay triangulation

For Poisson point process Φ , define **Poisson-Delaunay triangulation** as $Del(\Phi)$.



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

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

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

Add example(s)?

In the model we used, the energy function is of the form

$$H(\gamma) = \sum_{T \in Del_{\lambda}(\gamma)} V_1(T),$$

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.

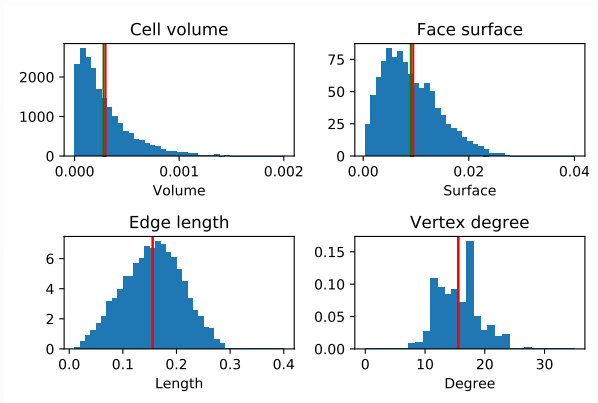
Section 4

Simulation

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

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

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

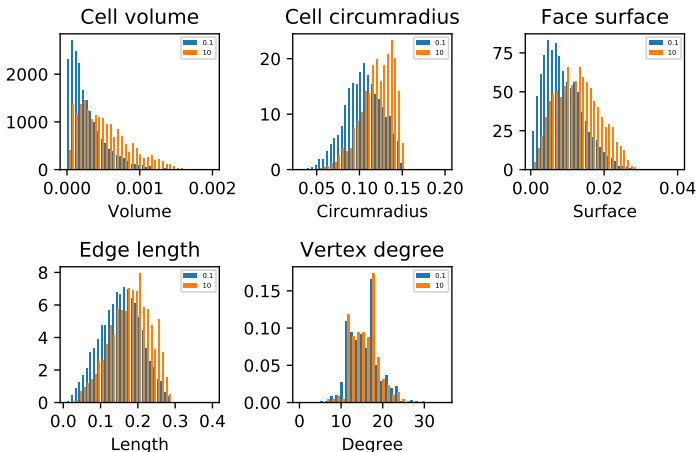


Role of the parameter θ

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.

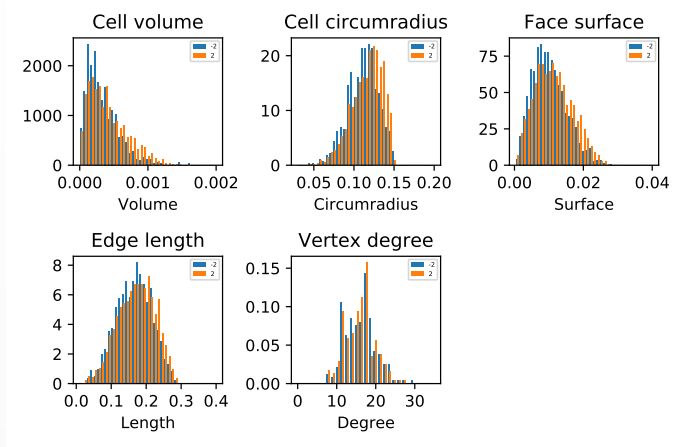


Role of the parameter θ

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.



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** (MPLE) using the estimates $(\hat{\epsilon}, \hat{\alpha})$.

Two-step procedure

1. Hardcore interaction parameters estimation

[Ref] 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

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

which in practice is estimated as

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

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.

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

However [Ref] 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

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

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

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

Yielding the estimate \hat{z}

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

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

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

Two-step procedure

2. Maximum pseudolikelihood - practical implementation

We obtain the estimate of θ by substituting the expression for \hat{z} into the equation for θ . This leads to the equation

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

After some manipulation, we obtain the equation

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

After $\hat{\theta}$ is estimated, we then obtain the estimate \hat{z} with $\hat{\theta}$ instead of θ . All integrals are estimated by MC-integration.

are not great so far.

- Variational estimate
- Energy with explicit interaction
- Periodic outside configuration
- ...