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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

- $\Phi(B) \sim Pois(\mu(B))$ 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^z_Λ.
For the case $z = 1$, use π_Λ.

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

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

Poisson point process as a reference measure

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

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

Finite volume Gibbs point process

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:

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

where

- $z > 0$,
- $H : \mathcal{F}_{lf} \mapsto \mathbb{R} \cup \{+\infty\}$ 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.

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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$$H(\gamma) \geq A N_{\mathbb{R}^d}(\gamma)$$

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

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

Local energy and GNZ equations

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 $f : \mathbb{R}^d \times \mathcal{F}_{lf} \to \mathbb{R}$,

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

Section 2

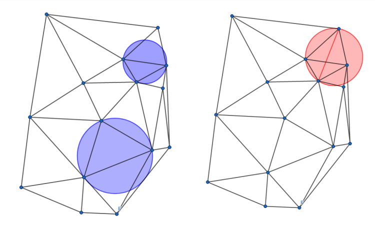
Triangulations

A $d+1$-tuplet $T = \{x_1, \dots, x_{d+1}\} \subset \gamma$ 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 $\gamma \in \mathcal{F}_{lf}$ is the set $Del(\gamma)$ defined by

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

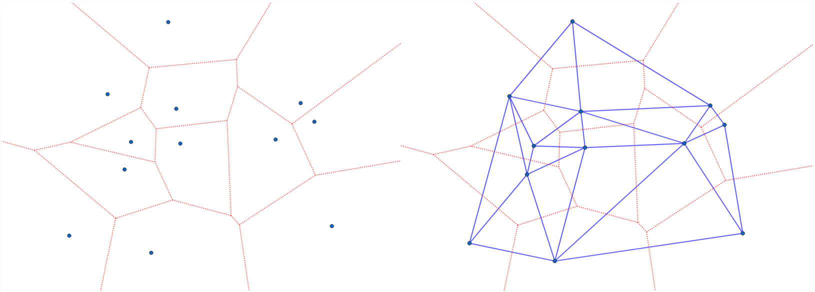


Additional assumption on γ (No cospherical points): no $d+2$ points $x_1, \dots, x_{d+2}$ are cospherical, i.e. there is no point $x \in \mathbb{R}^d$ such that $d(x, x_1) = \cdots = d(x, x_d + 2)$.

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

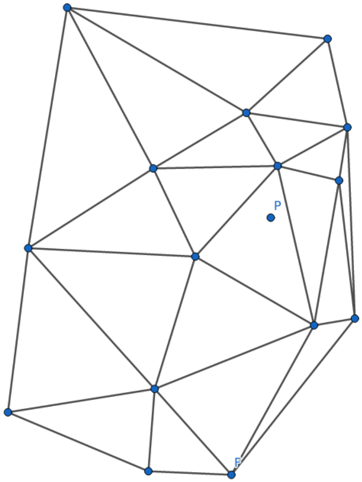
For $x \in \gamma$, the Voronoi cell of x in γ is

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



Then the Delaunay triangulation can be defined as

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



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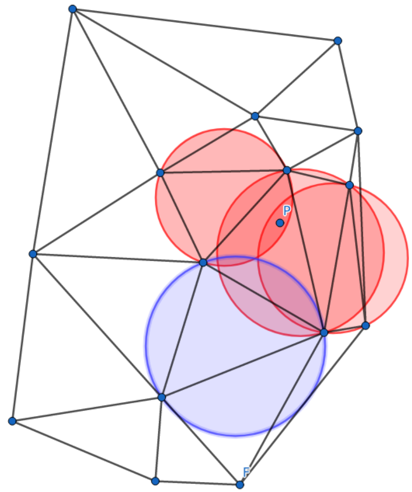
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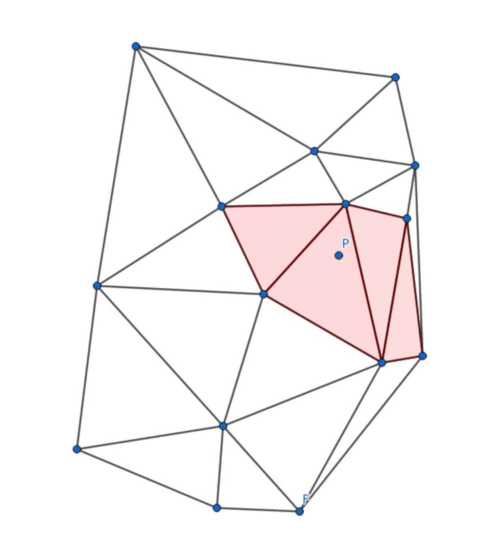

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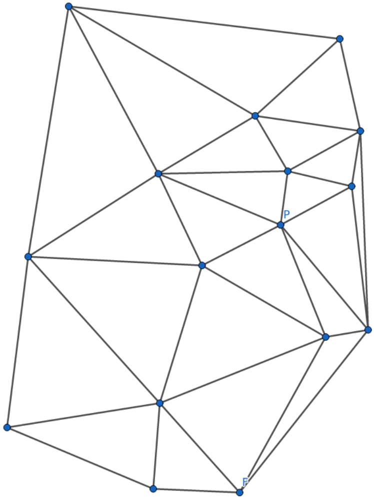
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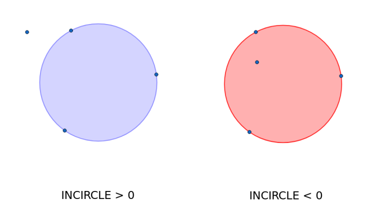
In $2D$, with $p_i = (x_i, y_i)$

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

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

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



In $3D$, with $p_i = (x_i, y_i, z_i)$

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

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

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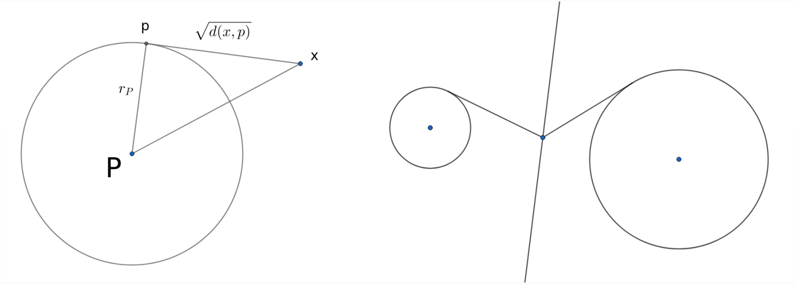
- Generators are not points, but spheres.
- $\gamma = \{P_1, \ldots, P_n\} = \{(p_1, r_{p_1}), \ldots, (p_n, r_{p_n})\}$ can be thought of as marked point process.
- Metric is not Euclidean, but power distance.

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

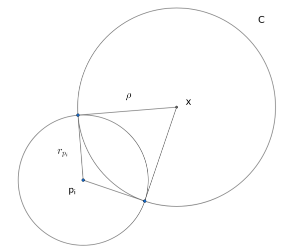


Definition. Inscribed sphere

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

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

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



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

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 $\mathcal{L}Del(\gamma)$ defined by

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

$P_i = (x_i, y_i, z_i, r_i)$

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

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

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Why? Because both are regular triangulations - convex hulls of lifted sets of points, that is

$$\gamma' = \{(P_i, w_i) : P_i \in \gamma, w_i = x_i^2 + y_i^2 + z_i^2 - r_i^2\}$$

Interlude: CGAL

- 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.

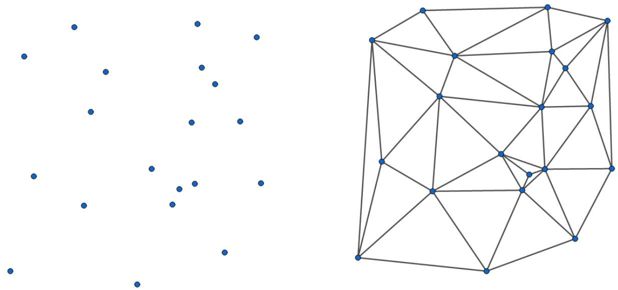
	Delaunay	**Delaunay Fast location**	**Regular**	**Regular No hidden points**
Construction from 10^2 points	0.00054	0.000576	0.000948	0.000955
Construction from 10^3 points	0.00724	0.00748	0.0114	0.0111
Construction from 10^4 points	0.0785	0.0838	0.122	0.117
Construction from 10^5 points	0.827	0.878	1.25	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

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

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



Gibbs-Laguerre-Delaunay triangulation

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

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

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

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

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

Section 4

Simulation

Specification of the GLD model

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

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

with V_1 defined as

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

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.

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- To sample from the distribution, we use MCMC methods.
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Birth-Death-Move algorithm

Denote Λ the observation window and Δ the simulation window, $\Lambda \subset \Delta$.
$\Lambda_W := \Lambda \times [0, W]$

1. Start with a permissible initial configuration $\gamma_0 \subset \Delta \times W$.
2. Denote $n = card(\gamma_0 \cap \Lambda)$.
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**: Generate a new point $y \in \Lambda_W$ uniformly and choose $x \in \gamma_0$ uniformly. 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.

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.

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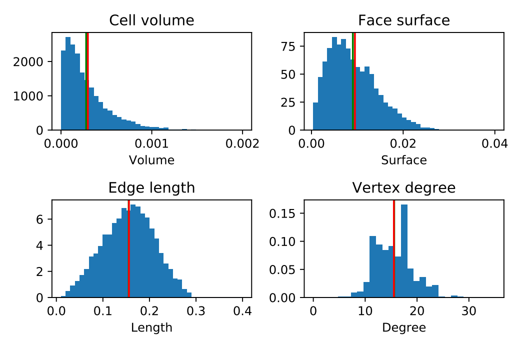
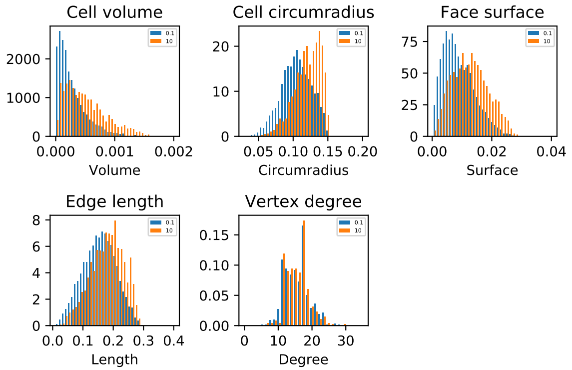


Realization of a GLD model with parameters $\theta = 0.1$, $z = 500$, $\alpha = 0.15$, $\epsilon = 0$, $W_0 = 0.001$

Role of the parameter θ

θ positive

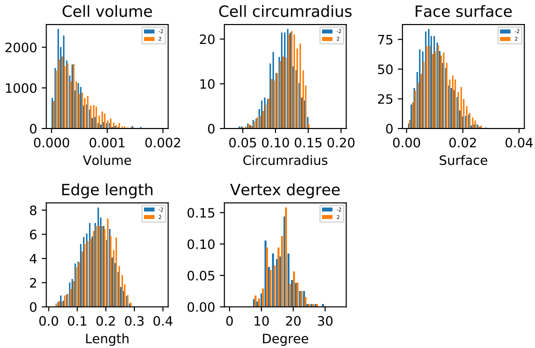
The model prefers configurations with lower energy.
θ multiplies the total surface area of all cells, thus with higher θ, the cells are forced to become large.



Realization of two GLD models. Blue: $\theta = 0.1$, orange: $\theta = 2$. Other parameters are $z = 500$, $\alpha = 0.15$, $\epsilon = 0$, $W_0 = 0.001$ for both models.

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

[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

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

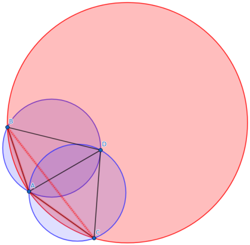
which in practice is estimated as

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

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

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

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



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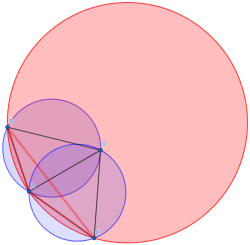

However [Dereudre, Lavancier (2009)] proved that GNZ still holds if we restrict ourselves to removable points.

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.

The pseudolikelihood function is

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

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

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

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

Differentiation yields the estimate $\hat{z}$

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

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

Differentiation yields the estimate $\hat{z}$

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

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

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

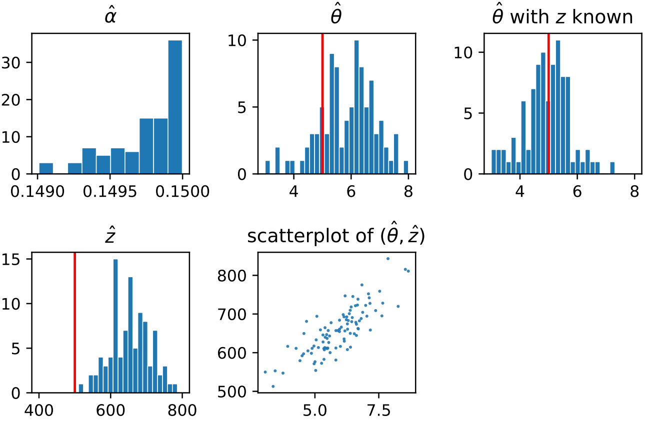
We obtain the estimate of θ by substituting the expression for $\hat{z}$ into the equation for θ. This leads to the equation

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

After some manipulation, we obtain the equation

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

where c is the RHS of (2), which is independent of θ.
After $\hat{\theta}$ is estimated, we then obtain the estimate $\hat{z}$ with $\hat{\theta}$ instead of θ.
All integrals are estimated by MC-integration.



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

- Variational estimator

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

Possible future directions

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- Energy with explicit interaction, e.g.

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

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- Periodic outside configuration.