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Gibbs-Delaunay Tessellations

Simulation and estimation

Section 1

Point processes

Poisson point process

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

- $\Phi(B) \sim Pois(\mu(B))$ for each $B \in \mathcal{B}_0$,
- $\Phi(B_1), \ldots, \Phi(B_n)$ for each $n \in \mathbb{N}$ and $B_1, \ldots, B_n \in \mathcal{B}_0$ 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} .

Poisson point process as a reference measure

- $\Phi: (\Omega, \mathcal{A}, \textit{P}) \rightarrow (\mathcal{F}_{\textit{lf}}, \mathscr{F})$ 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 $\{\gamma \in \mathcal{F}_{lf} | N_{\Lambda}(\gamma) = n\}, n \in \mathbb{N}, \Lambda \in \mathcal{B}, \text{ where } N_{\Lambda}(\gamma) = \text{Card}(\gamma \cap \Lambda).$

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

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

Finite volume Gibbs point process

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} :

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

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.

Examples and usefulness of (f)GPP

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

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). GZN equations

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

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

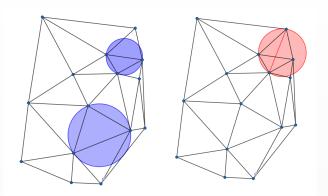
Section 2

Triangulations

Delaunay triangulation

Through empty sphere property

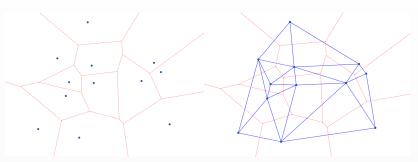
A d+1-tuplet $\{x_1,\ldots,x_{d+1}\}\subset \gamma$ has the empty sphere property if the open circumscribed ball $\mathcal{B}(T)$ does not contain any points from γ .



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

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

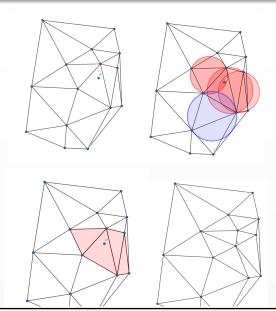
$$C(x,\gamma) = \{ z \in \mathbb{R}^d : \|x - z\| \le \|y - z\| \ \forall y \in \gamma \}.$$



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



Deulaunay triangulation

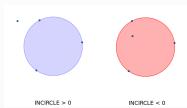
Geometric predicates, 2D

In 2D

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
$$w_i = x_i^2 + y_i^2, i = 1, ..., 4$$
 and

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



Geometric predicates, 3D

In 3*D*

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, ..., 5 if the following condition is satisfied

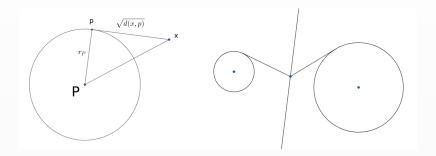
ORIENTATION(
$$P_1, P_2, P_3, P_4$$
) =
$$\begin{vmatrix} x_1 & y_1 & z_1 & 1 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \end{vmatrix} > 0$$

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, ..., 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.

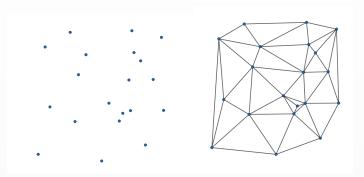
Interlude: CGAL

Section 3

Random triangulations

Poisson-Delaunay triangulation

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



Gibbs-Laguerre-Delaunay triangulation

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

$$\textit{H}(\gamma) = \sum_{\textit{T} \in \textit{Del}(\gamma)} \textit{V}_{1}(\textit{T}) + \sum_{\{\textit{T},\textit{T'}\} \subset \textit{Del}(\gamma)} \textit{V}_{2}(\textit{T},\textit{T'})$$

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)?

Specification of the GLD model

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

$$H(\gamma) = \sum_{T \in \mathit{Del}_{\Lambda}(\gamma)} V_1(T),$$

with V_1 defined as

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

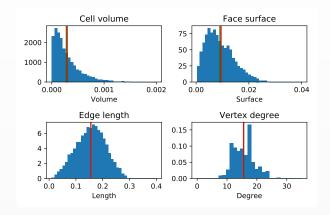
Simulation

MCMC

Comparison with Poisson-Delaunay

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

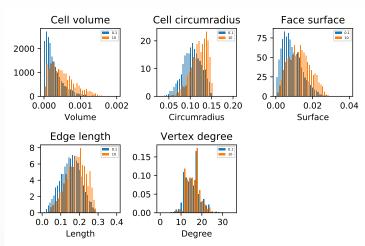
 $\theta = 0 \Rightarrow$ GPP becomes PPP with intensity z.



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.

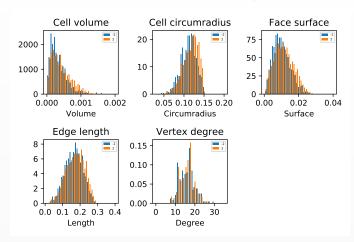


Role of the parameter θ

 θ negative

The model prefers configurations with lower energy.

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



Section 5

Estimation

Two-step procedure

Thanks to the fact that the hardcore parameter ϵ satisfies

$$\text{if }\epsilon>\epsilon' \text{ then } \forall \Lambda, \ \textit{E}^{\epsilon,\alpha,\theta}_{\Lambda}(\gamma_{\Lambda},\gamma_{\Lambda^c})<\infty \Rightarrow \textit{E}^{\epsilon',\alpha,\theta}_{\Lambda}(\gamma_{\Lambda},\gamma_{\Lambda^c})<\infty,$$

and the hardcore parameter α satisfies

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

their consistent estimators are:

$$\hat{\epsilon} = \inf\{\epsilon > 0, E_{\Lambda}(\gamma_{\Lambda}, \gamma_{\Lambda}^{c}) < \infty\},$$

$$\hat{\alpha} = \sup\{\alpha > 0, \textit{E}_{\Lambda}(\gamma_{\Lambda}, \gamma_{\Lambda}^{\textit{c}}) < \infty\}.$$

In practice, the parameters are estimated as

$$\hat{\epsilon} = \min\{a(T), T \in Del_{\Lambda}(\gamma)\},$$

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

The estimate $\hat{\beta}=(\hat{\epsilon},\hat{\alpha})$ is then used in the pseudo-likelihood function in the second estimation step.

Maximum pseudolikelihood

 $\mathbb{R}^{\beta}(\gamma)$ is the set of removable points.

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

where Λ'_n is the set of all addable points in Λ_n and $h^{\theta}(x, \gamma \setminus \{x\})$ is local energy of x in γ defined for every $x \in \mathcal{R}^{\beta}(\gamma)$ by:

$$h^{\beta,\theta}(x,\gamma\setminus\{x\})=H^{\beta,\theta}_{\Lambda}(\gamma_{\Lambda},\gamma_{\Lambda^c})-H^{\beta,\theta}_{\Lambda}(\gamma_{\Lambda}\setminus\{x\},\gamma_{\Lambda^c}).$$

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

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

Practical implementation

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

$$\int_{\Lambda_n'} \exp(-\theta h(x))(h(x)-c)dx = 0.$$

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.

Estimation results

are not great so far.

Possible future directions

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