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Voronoï tessellations: applications in Astronomy, Biology, Physics, etc.
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Drawback: Strong independent structures coming from the Poisson process $\rightarrow$ Interactions between the cells?
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One solution:

Gibbs modifications of Poisson Voronoï tessellations.
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- Parametric estimations.

Gibbs modifications of Poisson Voronoï tessellations.
## Definitions

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2. **Definitions**
Notations

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- $\pi^z_\Lambda$: $\pi^z$ restricted on $\Lambda$. 
Gibbs measures

Let \((H_\Lambda)_{\Lambda \in \mathcal{B}(\mathbb{R}^2)}\) be a family of energies

\[
H_\Lambda : \mathcal{M}(\Lambda) \times \mathcal{M}(\Lambda^c) \longrightarrow \mathbb{R} \cup \{+\infty\}
\]

\[(\gamma_\Lambda, \gamma_{\Lambda^c}) \longmapsto H_\Lambda(\gamma_\Lambda|\gamma_{\Lambda^c})\]

We suppose that it is compatible. For every \(\Lambda \subset \Lambda'\)

\[
H_{\Lambda'}(\gamma_{\Lambda'}|\gamma_{\Lambda'^c}) = H_\Lambda(\gamma_{\Lambda}|\gamma_{\Lambda^c}) + \varphi_{\Lambda,\Lambda'}(\gamma_{\Lambda^c}).
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**Definition**

A probability measure \(P\) on \(\mathcal{M}(\mathbb{R}^2)\) is a Gibbs measure for \(z > 0\) and \((H_\Lambda)\) if for every \(\Lambda \in \mathcal{B}(\mathbb{R}^2)\) and \(P\)-almost every \(\gamma_{\Lambda^c}\)

\[
P(d\gamma_\Lambda|\gamma_{\Lambda^c}) = \frac{1}{Z_\Lambda(\gamma_{\Lambda^c})} e^{-H_\Lambda(\gamma_\Lambda|\gamma_{\Lambda^c})} \pi_\Lambda^z(d\gamma_\Lambda),
\]

where

\[
Z_\Lambda(\gamma_{\Lambda^c}) = \int e^{-H_\Lambda(\gamma'|\gamma_{\Lambda^c})} \pi_\Lambda(d\gamma'),
\]
A typical energy of a Voronoï tessellation:

\[ H_\Lambda(\gamma_\Lambda | \gamma_{\Lambda^c}) = \sum_{C \in \text{Vor}(\gamma)} V_1(C) + \sum_{C, C' \in \text{Vor}(\gamma)} V_2(C, C'). \]

- \( V_1(C) \) is given by
  \[ \begin{cases} +\infty & \text{if } h_{\text{min}}(C) \leq \epsilon \\ +\infty & \text{if } h_{\text{max}}(C) \geq \alpha \\ +\infty & \text{if } h_2(C) / \text{Vol}(C) \geq B_0 \\ \text{otherwise} & \end{cases} \]

- \( V_2(C, C') \) is given by
  \[ \theta \left( \max(\text{Vol}(C), \text{Vol}(C')) - \min(\text{Vol}(C), \text{Vol}(C')) \right)^{1/2}, \quad \theta \in \mathbb{R} \]
A typical energy of a Voronoï tessellation:

\[ H_\Lambda(\gamma_\Lambda | \gamma_\Lambda^c) = \sum_{C \in \text{Vor}(\gamma), C \cap \Lambda \neq \emptyset} V_1(C) + \sum_{C, C' \in \text{Vor}(\gamma), C \text{ and } C' \text{ are neighbors}, (C \cup C') \cap \Lambda \neq \emptyset} V_2(C, C'). \]

Our guiding example:

\[ V_1(C) = \begin{cases} +\infty & \text{if } h_{\min}(C) \leq \varepsilon \\ +\infty & \text{if } h_{\max}(C) \geq \alpha \\ +\infty & \text{if } \frac{h_{\max}^2(C)}{Vol(C)} \geq B \\ 0 & \text{otherwise} \end{cases} \]

\[ 0 < \varepsilon < \alpha, B > 1/2\sqrt{3}; \]
A typical energy of a Voronoï tessellation:

\[ H_\Lambda(\gamma_\Lambda|\gamma_{\Lambda^c}) = \sum_{\substack{C \in \text{Vor}(\gamma) \cap \Lambda \neq \emptyset}} V_1(C) + \sum_{\substack{C,C' \in \text{Vor}(\gamma) \cap \Lambda \neq \emptyset \quad C \text{ and } C' \text{ are neighbors}}} V_2(C,C'). \]

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\[ V_2(C,C') = \theta \left( \frac{\max(\text{Vol}(C), \text{Vol}(C'))}{\min(\text{Vol}(C), \text{Vol}(C'))} - 1 \right)^{\frac{1}{2}}, \quad \theta \in \mathbb{R} \]
Existence results

- **First existence results (bounded interactions):** Bertin, Billiot and Drouilhet,
  
  
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- **Existence results with hardcore interactions**
  
  \((B = +\infty)\):
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- **Existence results with hardcore interactions**

For the interaction given before:

A Gibbs measure exists but we don’t know if it is unique or not (phase transition problem!)
Simulation
### Simulations

Strong hardcore interaction
Simulations

Strong hardcore interaction $\Rightarrow$ Rigidity of the tessellation
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$\rightarrow$ Several difficulties for the simulations.
Simulations

Strong hardcore interaction ⇒ Rigidity of the tessellation → Several difficulties for the simulations.

**Birth-death-move MCMC algorithm** on \([0, 1]^2\):

1. Draw independently \(a\) and \(b\) uniformly on \([0, 1]\).
2. If \(a < 1/3\) then generate \(x\) uniformly on \([0, 1]^2\) and
   \[
   \text{if } b < \frac{f(\gamma + x)z}{(n + 1)f(\gamma)}, \text{ then } \gamma + x \mapsto \gamma \text{ otherwise "do nothing".}
   \]
3. If \(1/3 < a < 2/3\) then generate \(x\) on \(\gamma\) and
   \[
   \text{if } b < \frac{nf(\gamma - x)}{f(\gamma)z}, \text{ then } \gamma - x \mapsto \gamma \text{ otherwise "do nothing".}
   \]
4. If \(a > 2/3\) then generate \(x\) on \(\gamma\), \(y \sim \mathcal{N}(x, \sigma^2)\) and
   \[
   \text{if } b < \frac{f(\gamma - x + y)}{f(\gamma)}, \text{ then } \gamma - x + y \mapsto \gamma \text{ otherwise "do nothing".}
   \]
Examples of simulations

We fix \( z = 100, \, \varepsilon = 0, \, \alpha = 0.05 \):

\[
B = +\infty, \; \theta = 0.5 \\
B = 1, \; \theta = 0.5 \\
B = 0.625, \; \theta = 0.5 \\
B = +\infty, \; \theta = -0.5 \\
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\]
Monitoring control

$B = +\infty, \theta = 0.5$

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4 Estimation
The aim: Estimate the parameters of the interaction from one realization $\gamma$ of the Gibbs measure.
Pseudo-likelihood Estimation

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  $\rightarrow$ Empirical extremum hardcore parameters.
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- **Smooth parameters**: $z$ and $\theta$.
  $\rightarrow$ Pseudolikelihood procedure.

Why the pseudo and not the MLE? MLE is too time consuming (because of the estimation by simulations of the normalizing constant). Pseudo is proved to be asymptotically consistent and normal in most cases.

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Pseudo-likelihood Estimation

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Practical estimation procedures

Let $\Lambda_n = [-n, n]^2$ be the observation window and $\gamma$ a realization of the Gibbs measure $P$. 
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**Hardcore parameter estimators:**

- $\hat{\varepsilon} = \min\{h_{\text{min}}(C), C \in \text{Vor}(\gamma) \text{ and } C \cap \Lambda_n \neq \emptyset\}$,
- $\hat{\alpha} = \max\{h_{\text{max}}(C), C \in \text{Vor}(\gamma) \text{ and } C \cap \Lambda_n \neq \emptyset\}$,
- $\hat{B} = \max\{h_{\text{max}}^2(C)/\text{Vol}(C), C \in \text{Vor}(\gamma) \text{ and } C \cap \Lambda_n \neq \emptyset\}$. 
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- **Smooth parameter estimators**:
  
  $(\hat{z}, \hat{\theta}) = \text{argmin}_{z,\theta} PLL_{\Lambda_n}(\gamma, z, \theta, \hat{\epsilon}, \hat{\alpha}, \hat{B}),$
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with

\[
\text{PLL}_{\Lambda_n}(\gamma, z, \theta, \hat{\varepsilon}, \hat{\alpha}, \hat{B}) = \int_{\Lambda_n} z \exp(-h(x, \gamma)) \, dx + \sum_{x \in \gamma_{\Lambda_n} \cap \Lambda_n} (h(x, \gamma-x) - \ln(z)), \\
H_{\Lambda_n}(\gamma-x) < \infty
\]

where $h(x, \gamma) = H_{\Lambda_n}(\gamma + x) - H_{\Lambda_n}(\gamma)$.
Theoretical results

For the hardcore parameters:

**Theorem (Dereudre-L. (2009))**

For $P$-almost all $\gamma$

$$\lim_{n \to \infty} (\hat{\varepsilon}, \hat{\alpha}, \hat{B}) = (\varepsilon, \alpha, B).$$

For the smooth parameters:

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The true parameters: \( \varepsilon = 0, \; \alpha = 0.05, \; B = 0.625, \; z = 100 \) and \( \theta = -0.5 \).
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Conclusion

Our Gibbs Voronoi model:

- forces the shape and the maximal size of the cells
- provides some repulsive or attractive interaction between two neighbour cells.
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1. the hardcore parameters are estimated in a natural way,
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1. the hardcore parameters are estimated in a natural way,
2. the smooth parameters are estimated by pseudo-likelihood where the hardcore parameters are plugged in.

This is consistent and allows to distinguish between the repulsive and the attractive case in a non-trivial situation.


Some theoretical points
The problem of heredity

**Definition**

The family of energies \((H_\Lambda)_\Lambda\) is said **hereditary** if for every \(\Lambda\), every \(\gamma \in \mathcal{M}(\mathbb{R}^2)\) and every \(x \in \Lambda\)

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H_\Lambda(\gamma) = +\infty \Rightarrow H_\Lambda(\gamma + \delta x) = +\infty.
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It is a standard assumption in classical statistical mechanics. (Example: The classical hard ball model is hereditary.)
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The Gibbs Voronoi Tessellations are **not hereditary**.

\(\rightarrow\) When one adds a point in a too large cell, the new tessellation may be allowed.
Theorem (*Nguyen-Zessin (1979), hereditary case*)

Suppose that the energy \((H_\Lambda)\) is *hereditary*. \(P\) is Gibbs measure with intensity measure \(\nu\) if and only if, for every bounded non negative measurable function \(\psi\) from \(\mathbb{R}^2 \times \mathcal{M}(\mathbb{R}^2)\) to \(\mathbb{R}\),

\[
E_P \left( \sum_{x \in \gamma} \psi(x, \gamma - x) \right) = E_P \left( \int_{\mathbb{R}^2} \psi(x, \gamma) e^{-h(x, \gamma)} \nu(dx) \right),
\]

where \(h(x, \gamma) = H_{\Lambda_n} (\gamma + x) - H_{\Lambda_n} (\gamma)\).

Proposition (*Dereudre, L. (2009), general case*)

Let \(P\) be a Gibbs measure with intensity measure \(\nu\), then

\[
E_P \left( \sum_{x \in \gamma_{\Lambda_n}} \psi(x, \gamma - x) \right) = E_P \left( \int_{\mathbb{R}^2} \psi(x, \gamma) e^{-h(x, \gamma)} \nu(dx) \right).
\]
Validation: residuals process

We can extend the concept of residuals (see Baddeley et al., 2005) to the non-hereditary setting.

The residuals process on a set $\Delta$ is defined for any function $\psi$ by

$$R(\Delta, \psi, \hat{h}, \hat{\nu}) = \sum_{x \in \gamma \Delta, H_{\Delta}(\gamma - x) < \infty} \psi(x, \gamma - x) - \int_{\Delta} \psi(x, \gamma) e^{-\hat{h}(x, \gamma)} \hat{\nu}(dx),$$

From the equilibrium equation given before, under the true model,

- $R(\Delta, \psi, \hat{h}, \hat{\nu}) \approx 0$
- $R(\Delta, \psi, \hat{h}, \hat{\nu})$ is approximatively gaussian.

$\rightarrow$ Several diagnostic tools can then be applied when fitting a Gibbs Voronoi model.
Validation: residuals process

We can extend the concept of residuals (see Baddeley et al., 2005) to the non-hereditary setting. The residuals process on a set $\Delta$ is defined for any function $\psi$ by

$$R(\Delta, \psi, \hat{h}, \hat{\nu}) = \sum_{x \in \gamma \Delta, H_{\Delta}(\gamma - x) < \infty} \psi(x, \gamma - x) - \int_{\Delta} \psi(x, \gamma)e^{-\hat{h}(x, \gamma)} \hat{\nu}(dx),$$

From the equilibrium equation given before, under the true model,

- $R(\Delta, \psi, \hat{h}, \hat{\nu}) \approx 0$
- $R(\Delta, \psi, \hat{h}, \hat{\nu})$ is approximatively gaussian.

Several diagnostic tools can then be applied when fitting a Gibbs Voronoi model.

For further asymptotic results on the residuals process $R$:

→ See the talk of J.-F. Coeurjolly on Friday morning.