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Introduction

- Voronoï tessellations: applications in Astronomy, Biology, Physics, microstructures, etc.
- Studied as a random object: based on Poisson point Processes.
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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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- What kind of interactions?
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- Parametric estimation of the model.
- Validation of the model.
2 Definitions
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  \[ \gamma \subset \mathbb{R}^2, \text{ such that for all } \Lambda \in \mathcal{B}(\mathbb{R}^2), \text{ card}(\gamma \cap \Lambda) < \infty. \]
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- \( \pi^z_\Lambda : \pi^z \text{ restricted on } \Lambda. \)
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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Gibbs measures

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

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

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

\[ 0 < \varepsilon < \alpha, \ B > 1/2\sqrt{3}; \]
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0 < \varepsilon < \alpha, B > 1/2\sqrt{3};

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

- **First existence results (bounded interactions):**

  Bertin, Billiot and Drouilhet:

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- **Existence results with hardcore interactions:**


For a large class of interactions:

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

Simulation on $\Lambda = [0, 1]^2$ with periodic outside configuration. Let $f(\gamma) = \exp(-H_\Lambda(\gamma_\Lambda|\gamma_\Lambda^c))$ where $\Lambda = [0, 1]^2$. 
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**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
   
   if $b < \frac{f(\gamma \cup x)z}{(n + 1)f(\gamma)}$, then $\gamma \cup x \mapsto \gamma$ otherwise "do nothing".

3. If $1/3 < a < 2/3$ then generate $x$ on $\gamma$ and
   
   if $b < \frac{nf(\gamma - x)}{f(\gamma)z}$, then $\gamma - x \mapsto \gamma$ otherwise "do nothing".

4. If $a > 2/3$ then generate $x$ on $\gamma$, $y \sim N(x, \sigma^2)$ and
   
   if $b < \frac{f(\gamma - x \cup y)}{f(\gamma)}$, then $\gamma - x \cup y \mapsto \gamma$ 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

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Another Example

\[ H_{\Lambda}(\gamma_{\Lambda} | \gamma_{\Lambda^c}) = \theta \sum_{\text{C and C'} \text{ are neighbors}} \] (length of edge between C and C').

Simulation conditioned to 400 cells, \( \theta \in \{0, 50, 100, 200, 500, 1000\} \)
4 Estimation
Choose one parametric Gibbs model.

**The aim**: Estimate the parameters of the interaction from one realization $\gamma$ of the Gibbs measure.
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- **Hardcore parameters**: $\varepsilon$, $\alpha$ and $B$.
  
  $\rightarrow$ Empirical extremum hardcore parameters.
Pseudo-likelihood Estimation

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  → 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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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_{\min}(C), \ C \in \text{Vor}(\gamma) \text{ and } C \cap \Lambda_n \neq \emptyset\}, \\
  \hat{\alpha} = \max\{h_{\max}(C), \ C \in \text{Vor}(\gamma) \text{ and } C \cap \Lambda_n \neq \emptyset\}, \\
  \hat{B} = \max\{h_{\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**:

  $(\hat{z}, \hat{\theta}) = \arg\min_{\gamma, \theta} PLL_{\Lambda_n}(\gamma, z, \theta, \hat{\varepsilon}, \hat{\alpha}, \hat{B})$,
Let $\Lambda_n = [-n, n]^2$ be the observation window and $\gamma$ a realization of the Gibbs measure $P$.

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  $(\hat{z}, \hat{\theta}) = \arg\min_{z, \theta} PLL_{\Lambda_n}(\gamma, z, \theta, \hat{\varepsilon}, \hat{\alpha}, \hat{B})$,
  
  with
  
  $PLL_{\Lambda_n}() = \int_{\Lambda_n} z \exp(-h(x, \gamma)) \, dx + \sum_{x \in \gamma \setminus \Lambda_n} (h(x, \gamma - x) - \ln(z))$, 

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

The problem of non heredity

In the pseudolikelihood contrast function, in the sum term:

\[ h(x, \gamma - x) := H_{\Lambda_n}(\gamma) - H_{\Lambda_n}(\gamma - x) \]

But in presence of hardcore interaction \( H_{\Lambda_n}(\gamma - x) \) may be infinite and so \( h(x, \gamma - x) \) does not exist.

**Definition**

A Gibbs model is **hereditary** if for every \( \Lambda \), every \( \gamma \in \mathcal{M}(\mathbb{R}^2) \) and every \( x \in \gamma \), \( H_{\Lambda}(\gamma) < +\infty \Rightarrow H_{\Lambda}(\gamma - x) < +\infty \).

\[ \gamma \cup x \text{ is allowed} \Rightarrow \gamma \text{ is allowed} \]

It is a standard assumption in classical statistical mechanics.

The Gibbs Voronoi Tessellations are **not hereditary**.

\[ \rightarrow \] When one removes a point, a too large cell may appear.
Solution for non heredity

In the contrast function, the sum is restricted to the removable points, i.e. \( \{ x \in \gamma \text{ such that } H_{\Lambda_n}(\gamma - x) < \infty \} \):

\[
PLL_{\Lambda_n}() = \int_{\Lambda_n} z \exp (-h(x, \gamma)) \, dx + \sum_{x \in \gamma_{\Lambda_n}} (h(x, \gamma - x) - \ln(z)),
\]

This property only depends on the hardcore parameters. The full estimation procedure is:

1. Estimate the hardcore parameters
2. Deduce an estimation of \( \{ x \in \gamma \text{ such that } H_{\Lambda_n}(\gamma - x) < \infty \} \)
3. Minimize \( PLL_{\Lambda_n}() \) to estimate the smooth parameters.
Solution for non heredity

In the contrast function, the sum is restricted to the **removable points**, i.e. \( \{x \in \gamma \text{ such that } H_{\Lambda_n} (\gamma - x) < \infty \} \):

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The full estimation procedure is so :

1- Estimate the hardcore parameters

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3- Minimize \( PLL \) to estimate the smooth parameters.
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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For $P$-almost all $\gamma$

$$\lim_{n \to \infty} (\hat{z}, \hat{\theta}) = (z, \theta).$$

$(\hat{z}, \hat{\theta})$ are asymptotic normal if $\varepsilon, \alpha$ and $B$ are supposed to be known.
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\((\hat{z}, \hat{\theta})\) are asymptotic normal if \(\varepsilon, \alpha\) and \(B\) are supposed to be known.
The true parameters: \( \varepsilon = 0, \alpha = 0.05, B = 0.625, z = 100 \) and \( \theta = -0.5 \).
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**Typical tessellation:** Hardcore parameter estimators:

![Diagram](image)
Estimation results

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Smooth parameter estimators:

\[ \hat{\theta} \text{ when } z \text{ is known} \]
\[ \hat{\theta} \text{ when } z \text{ is estimated} \]
\[ \hat{z} \]

Scatterplot of \((\hat{\theta}, \hat{z})\):
The true parameters: \( \varepsilon = 0, \alpha = 0.05, B = 0.625, z = 100 \) and \( \theta = 0.5 \).
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Scatterplot of $(\hat{\theta}, \hat{z})$:
Validation: the residuals process
Theorem (Nguyen-Zessin (1979), hereditary case)

Suppose that the energy \((H_\Lambda)_\Lambda\) 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 \(h(x, \gamma) = H_\Lambda(\gamma \cup x) - H_\Lambda(\gamma)\).

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

Let \(P\) be a Gibbs measure with intensity measure \(\nu\), then for any \(\Lambda \in \mathcal{B}(\mathbb{R}^2)\),

\[
E_P \left( \sum_{\substack{x \in \gamma_\Lambda \\ H_\Lambda(\gamma - x) < \infty}} \psi(x, \gamma - x) \right) = E_P \left( \int_{\Lambda} \psi(x, \gamma) e^{-h(x, \gamma)} \nu(dx) \right).
\]
Validation: residuals process

The concept of residuals for point processes was introduced in Baddeley et al., 2005. It can be extended to the non-hereditary setting.

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

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

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

- $R(\Delta, \psi, \hat{h}, \hat{z}) \approx 0$
- $R(\Delta, \psi, \hat{h}, \hat{z})$ is approximatively gaussian (without hardcore).

For asymptotic results, see Coeurjolly and L. (2010).

$\rightarrow$ Several diagnostic tools can then be applied when fitting a Gibbs Voronoi model.
One example of diagnostic tool

1- Choose a model
2- Fit the data to the model
3- Compute the raw residuals \( \psi = 1 \) on sub-boxes
4- Simulate a lot of samples from the fitted model and
   - fit the model
   - compute the raw residuals on sub-boxes
5- Compare the residuals distribution from 3- with those of 4- (with a QQ-plot)
Example of misspecification

-The true model is a Gibbs Voronoi model as presented before.
-Let us fit another model which relies on the distance between the nuclei of the cells (Delaunay point of view)

The two points of view for the same sample:

Voronoi

Delaunay
Example of misspecification

- Raw Residuals for the Voronoi model
- QQplot from bootstrap

- Raw Residuals in misspecification case
- QQplot from bootstrap
**Conclusion**

- Gibbs Voronoi model can:
  - force the shape and the maximal size of the cells
  - provide some repulsive or attractive interaction between neighbour cells.

- The simulation can be achieved by a Birth-Death-Move MCMC algorithm
  -→ very time consuming if hardcore interactions.

- A two-step estimation procedure can be applied
  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 non-trivial situations.

- A validation step is available.
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-A two-step estimation procedure can be applied
  1. the hardcore parameters are estimated in a natural way,
  2. the smooth parameters are estimated by pseudo-likelihood
     where the the hardcore parameters are plugged in.

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

-A validation step is available.


