Central limit theorems for point processes with focus on Gibbsian functionals

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joint work with M. Otto & A. M. Svane

DSTS spring meeting, Aalborg, May 09, 2023

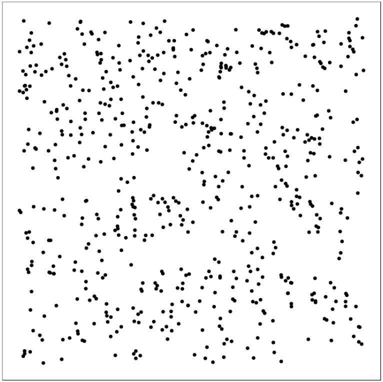
1 Motivation

2 Complete spatial randomness

3 Gibbs point processes

4 Main results

- Dataset consisting of ***634 neurons***
- ***Minicolumn Hypothesis.*** Arrangement in vertical columns



Christoffersen, Møller & Christensen. *Modelling columnarity of pyramidal cells in the human cortex*

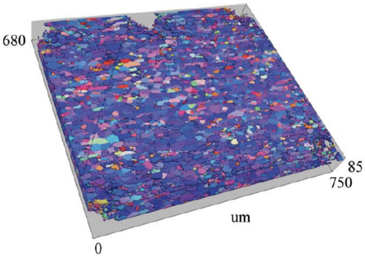
Rafati & et. al. *Detection and spatial characterization of minicolumnarity in the human cortex*

Virtual material design

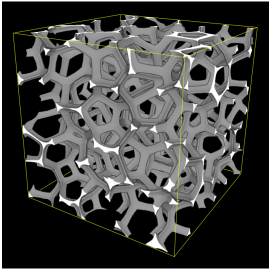
▷ Stochastic-geometry models for heterogeneous materials

⇝ Computation of material characteristics through simulations

Statistical hypothesis tests?



Extra low carbon strip steel



Aluminium alloy foam

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Null model

$\mathcal{P} = \{X_1, \ldots, X_N\}$ = Poisson point process

- $X_1, X_2, \cdots =$ iid random vectors in sampling window Q
- $N =$ Poisson random variable

Test statistics

- $H := \sum_{X_i \in Q} g(X_i, \mathcal{P})$
- $g(X_i, \mathcal{P}) :=$ Score function

Examples

- $g(X_i, \mathcal{P}) = \#\{X_j : |X_i - X_j| < r\} \rightsquigarrow$ Ripley's K-function
- $g(X_i, \mathcal{P}) =$ Area/Perimeter of Voronoi cell at X_i
- $H =$ Persistent Betti numbers $\rightsquigarrow$ Christophe & Anne Marie

Issue. Distribution of test statistic not known

$\rightsquigarrow$ Asymptotically exact tests in large windows

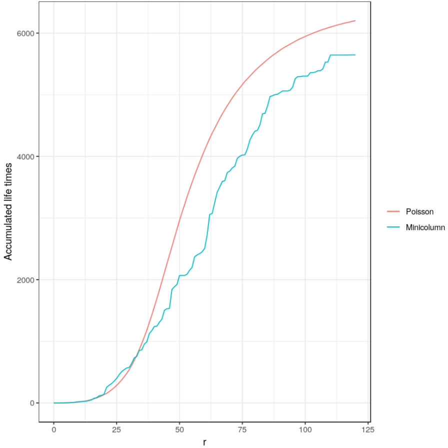
- $H_n := H(\mathcal{P}_n) := H(\mathcal{P} \cap Q_n)$

Asymptotic normality

$$\frac{H_n - \mathbb{E}[H_n]}{\sqrt{|Q_n|}} \Rightarrow \mathcal{N}(0; \sigma^2)$$

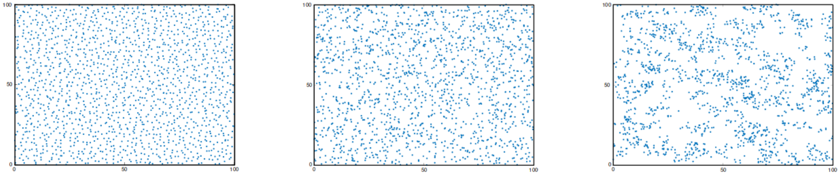
- Penrose & Yukich; (2003). $\rightsquigarrow$ Foundational general result
- Biscio, Chenavier, H. & Svane; (2020). $\rightsquigarrow$ 2D M-bounded persistent Betti numbers

Application to minicolumn dataset

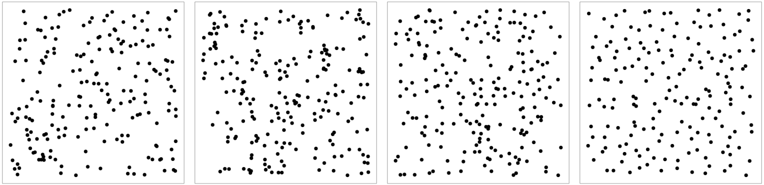


***p*-value = 0.012**

Beyond complete spatial randomness?



Y. Hiraoka, T. Shirai. *Limit theorems for persistence diagrams*



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3 **Gibbs point processes**

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Idea. Interactions via density wrt. Poisson process to reflect

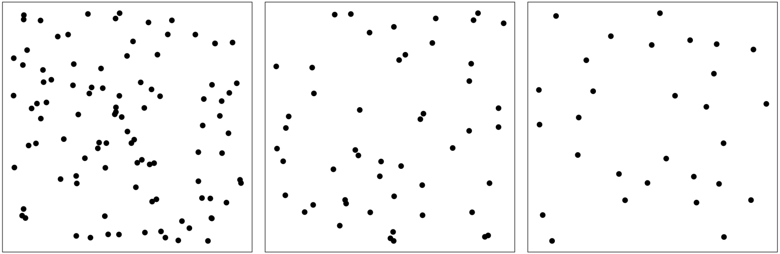
$\rightsquigarrow$ ***Gibbs point processes $\mathcal{X}_n$.***

$$\mathbb{P}(\mathcal{X}_n \in A) = \mathbb{E}[f(\mathcal{P}_n)\mathbb{1}\{\mathcal{P}_n \in A\}]$$

Strauss process.

$$f(\varphi) = \frac{1}{Z}\gamma^{s_R(\varphi)}$$

- $s_R(\varphi) = \#\{\{x, y\} \subseteq \varphi \colon |x - y| < R\} =$ number of R-close pairs



Strauss process with $\gamma = 1$ (left), $\gamma = 0.5$ (middle), $\gamma = 0$ (right) by `spatstat`

Advantages.

- Very flexible interactions
- Simulation methods available $\rightsquigarrow$ (Møller & Waagepetersen, 2004)
  - MCMC methods
  - Perfect simulation
- Parameter estimation via maximum pseudolikelihood
- Interaction quantification via ***Papangelou intensity***

$$\kappa(x, \varphi) := \frac{f(\{x\} \cup \varphi)}{f(\varphi)}$$

- Strauss process: $\kappa(x, \varphi) = \gamma^{t_R(x,\varphi)}$; $t_R(x, \varphi) := \#(\varphi \cap B_R(y))$

Disadvantages.

- Mainly repulsive point patterns
- Simulation may be slow
- No closed-form moments $\rightsquigarrow$ determinantal point processes
- Problems in modelling densely packed hard sphere systems

CLTs in growing domains $\rightsquigarrow$ ***infinite-volume Gibbs processes***

Georgii-Nguyen-Zessin (GNZ) equation

$$\mathbb{E}\Big[\sum_{X_i \in \mathcal{X}} h(X_i, \mathcal{X})\Big] = \lambda \mathbb{E}\Big[\int h(x, \mathcal{X} \cup \{x\})\kappa(x, \mathcal{X})\mathrm{d}x\Big]$$

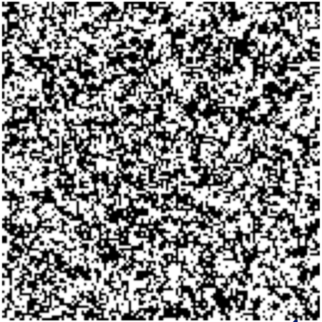
- Close relation to ***statistical physics***

Existence

- Achievable by ***tightness arguments***

Uniqueness

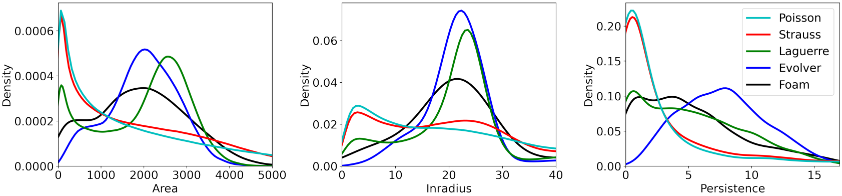
- Highly non-trivial
- Often possible for ***small intensities***
- Non-uniqueness related with ***phase transition***



Ising model

Null models. Poisson and Strauss ($\gamma = 0.01 \rightsquigarrow$ highly repulsive)

Exploratory analysis. KDE for the face areas, face-inradii and total persistences.



z-scores

H_0\Statistic	T_{Area}	T_{I}	T_{Pers}
Poisson	12.8	14.94	35.94
Strauss	11.84	14.36	32.48
Laguerre	6.92	1.85	1.33
Evolver	12.42	4.03	20.47

H., Krebs & Redenbach. *Persistent homology based goodness-of-fit tests for tessellations*

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4 **Main results**

Consider functionals of the form

- $H_n := H(\mathcal{X}_n)$

H is ***weakly stabilizing*** if

- $H((\varphi \cap A) \cup \{y\}) - H(\varphi \cap A) \to \Delta(y, \varphi, \infty) < \infty$ for $A \uparrow \mathbb{R}^d$

Theorem A. CLT for weakly stabilizing functionals

Let H be translation-invariant. Assume that H together with $\mathcal{X}_n$ satisfy conditions on moments and ***weak stabilization***. Then, for some $\sigma \geqslant 0$,

$$|Q_n|^{-1/2}(H_n - \mathbb{E}[H_n]) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \sigma^2).$$

Example. Persistent Betti numbers

Consider sums of ***stabilizing score functions:***

- $H_n = \sum_{X_i \in \mathcal{X}_n} g\big(X_i, \mathcal{X}_n\big)$
- $g(x, \varphi) = g(x, \varphi \cap B_{R(x,\varphi)}(x))$
- $\{\varphi \colon R(x, \varphi) \leqslant r\} = \{\varphi \colon R(x, \varphi \cap B_r(x)) \leqslant r\}$

Exponential stabilization

$$\limsup_{r\uparrow\infty} \sup_n \sup_{x \in Q_n} \frac{\log \mathbb{P}(R(x, \mathcal{X}_n \cup \{x\}) > r)}{r^\alpha} < 0$$

Theorem B. Quantitative normal approximation

Let g be translation covariant. Assume that g together with $\mathcal{X}_n$ satisfies conditions on moments, variance lower bound & ***exponential stabilization***. Then,

$$d_{\mathsf{K}}\Big(\frac{H_n - \mathbb{E}[H_n]}{\sqrt{\mathsf{Var}(H_n)}}, \mathcal{N}(0,1)\Big) \leqslant O\Big(\frac{(\log |Q_n|)^a}{\sqrt{|Q_n|}}\Big),$$

where $d_{\mathsf{K}}(X, Y) := \sup_{u \in \mathbb{R}} |\mathbb{P}(X \leqslant u) - \mathbb{P}(Y \leqslant u)| =$ Kolmogorov distance.

Example. Total edge length in Voronoi tessellation

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Poisson point processes

Theorem A.

(Penrose & Yukich, 2001)

- Proof based on ***Martingale CLT***

$$H_n - \mathbb{E}[H_n] = \sum_{i \leqslant k_n} \Delta_{i,n} := \sum_{i \leqslant k_n} \mathbb{E}[H_n | \mathcal{F}_{i,n}] - \mathbb{E}[H_n | \mathcal{F}_{i-1,n}],$$

- Relies on ergodic theorem

Theorem B.

(Lachièze-Rey, Schulte & Yukich, 2019)

- Proof based on ***Malliavin-Stein theory***
- No log-corrections

Gibbs point processes

Theorem A. /

Theorem B.

(Schreiber & Yukich, 2013), (Xia & Yukich, 2015)

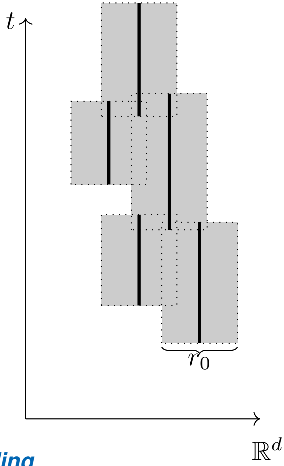
- ▷ ***Graphical construction***
- ▷ Constraint on intensity, e.g., for Strauss $|B_{(r_0+1)}(o)|\tau < 1$

(Chen, Röllin & Xia, 2022)

- ▷ ***Palm coupling***
- ▷ Require fast decay of correlations

(Cong & Xia, 2023+)

- ▷ No Gibbs assumption needed
- ▷ Restricted to Wasserstein distance



~~***Graphical construction***~~ $\rightsquigarrow$ ***Disagreement coupling***

Gibbs processes $\mathcal{X}$

- Finite interaction range $r_0 > 0$
- Papangelou intensity bounded by some $\alpha_0 > 0$
- $\alpha_0 < \alpha_c(r_0)$, the critical intensity for Poisson continuum percolation

Theorem A.

- Weak stabilization
- Growth condition. $|H(\varphi \cup \{y\}) - H(\varphi)| \leqslant \exp\big(c\varphi(B_r(y))\big)$

Theorem B.

- Exponential stabilization
- $\sup_{n\geqslant 1} \sup_{x_1,\dots,x_5 \in Q_n} \mathbb{E}\big[g(x_1, \mathcal{X}_n \cup \{x_1, \dots, x_5\})^5\big] < \infty$
- $\mathsf{Var}(H_n) \in \Omega(|Q_n|)$
- $g(x, \varphi \cup \{y\}) = 0$ if $g(x, \varphi) = 0$ $\rightsquigarrow$ hereditary condition

Summer School on TDA & Spatial Statistics Aalborg, 26/06/23–30/06/23

http://www.dstda.com

- Wojciech Chachólski (KTH)
- Anne Estrade (Université Paris Cité)
- Erika Roldán (MPI Leipzig)
- Rasmus Waagepetersen (Aalborg University)

Literature

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Normal approximation for functionals on Gibbs processes via disagreement couplings

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based on joint work with C. Hirsch & A. M. Svane

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May 09, 2023

Quantitative normal approximation

Let

$$H_n := \sum_{X_i \in \mathcal{X}_n} g(X_i, \mathcal{X}_n).$$

Theorem. Assume that g together with $\mathcal{X}$ satisfy conditions on moments, variance lower bounds and exponential stabilization. Then

$$\mathrm{d_K}\left(\frac{H_n - \mathbb{E}H_n}{\sqrt{\mathrm{Var}(H_n)}}, \mathcal{N}(0,1)\right) \leq O\left(\frac{(\log|Q_n|)^a}{\sqrt{|Q_n|}}\right),$$

where $\mathrm{d_K}(X, Y) := \sup_{u\in\mathbb{R}} |\mathbb{P}(X \leq u) - \mathbb{P}(Y \leq u)|$ Kolmogorov distance.

Proof outline

We use a technique from Chen–Röllin–Xia 2021 that combines

- Palm calculus
- Stein's method

to bound the Kolmogorov distance using a Palm coupling.

To apply this method to Gibbs functionals, we exploit

- Gibbs interpretation of the Palm measure
- Disagreement coupling.

Palm measures

- Ξ point process with intensity measure Λ
- Ξ_x Palm measure of Ξ at $x \in \mathbb{R}^d$ if

$$\mathbb{E} \int f(x, \Xi) \, \Xi(dx) = \mathbb{E} \int f(x, \Xi_x) \, \Lambda(dx), \quad f \geq 0.$$

Stein's method for normal approximation

- $h_u(w)$ smooth approximation of the indicator $1\{w \leq u\}$.
- Let $N \sim \mathcal{N}(0,1)$ and consider the Stein equation

$$f_u'(w) - wf_u(w) = h_u(w) - \mathbb{E}h_u(N), \quad u \in \mathbb{R}.$$

- Let H be such that $\mathbb{E}H = 0$ and $\mathrm{Var}(H) = 1$. Assume that

$$\mathbb{E}[Hf(H)] = \mathbb{E}\int_{-\infty}^{\infty} f'(H+t)\hat{K}(t)\,dt.$$

  for all sufficiently smooth f for some $\hat{K}(t)$.
- Put $K(t) := \mathbb{E}\hat{K}(t)$. For all $u \in \mathbb{R}$ we have

$$\begin{aligned}\mathbb{P}(H \leq u) - \mathbb{P}(N \leq u) &\approx \mathbb{E}h_u(H) - \mathbb{E}h_u(N)\\ &= \mathbb{E}\int_{-\infty}^{\infty} f_u'(H)K(t)\,dt - \mathbb{E}\int_{-\infty}^{\infty} f_u'(H+t)\hat{K}(t)\,dt.\end{aligned}$$

How to choose $\hat{K}(t)$?

- $\Xi := \sum_{X_i \in \mathcal{X}_n} g(X_i, \mathcal{X}_n)\, \delta_{X_i}$ with intensity measure Λ
- Palm versions Ξ_x, $x \in \mathbb{R}^d$, defined on the same prob. space
- Let $\lambda := \mathbb{E}|\Xi|$, $\sigma^2 := \mathrm{Var}(|\Xi|)$ and set

$$H := \frac{|\Xi| - \lambda}{\sigma^2}, \qquad H_x := \frac{|\Xi_x| - \lambda}{\sigma^2}, \qquad \Delta_x := H_x - H.$$

Then

$$\mathbb{E}[Hf(H)] = \mathbb{E} \int \frac{f(H_x) - f(H)}{\sigma^2}\, \Lambda(dx) = \mathbb{E} \iint_0^{\Delta_x} \frac{f'(H+t)}{\sigma^2}\, dt\, \Lambda(dx)$$

$$= \mathbb{E} \iint_{-\infty}^{\infty} \frac{f'(H+t)}{\sigma^2} \big(1\{\Delta_x > t > 0\} - 1\{\Delta_x < t \le 0\}\big)\, dt\, \Lambda(dx).$$

Therefore let

$$\hat{K}(t) := \frac{1}{\sigma^2} \int \big(1\{\Delta_x > t > 0\} - 1\{\Delta_x < t \le 0\}\big)\, \Lambda(dx).$$

How to couple Ξ and Ξ_x, $x \in \mathbb{R}^d$?

- Let $\mathcal{X}_x^{\Xi}$ Palm process of $\mathcal{X}$ at x wrt Ξ
- Then $\Xi_x := \sum_{X_i \in \mathcal{X}_x^{\Xi}} g(X_i, \mathcal{X}_x^{\Xi})\, \delta_{X_i}$ is a Palm version of Ξ

We use the following Gibbs interpretation of $\mathcal{X}_x^{\Xi}$:

Lemma. Let $\mathcal{X}$ be a Gibbs process with PI κ. Then the reduced process $\mathcal{X}_x^{\Xi} \setminus \{x\}$ is a Gibbs process with PI κ^x given by

$$\kappa^x(y, \omega) := \kappa(y, \omega \cup \{x\}) \frac{g(x, \omega \cup \{x, y\})}{g(x, \omega \cup \{x\})}$$

where $0/0 := 0$.

Poisson embedding of finite Gibbs processes

- total ordering $<$ on $\mathbb{R}^d$
- For $B \subset \mathbb{R}^d$ with $|B| < \infty$ define partition function

$$Z_B(\psi) := \int e^{-H(\mu,\psi)}\, \Pi_B(d\mu) \in (0, +\infty], \quad \psi \in \mathsf{N}.$$

- Define $p \colon \mathbb{R}^d \times \mathsf{N} \to [0,1]$ by

$$p(x,\psi) := \kappa(x, \psi_{(-\infty,x)}) \frac{Z_{(x,\infty)}(\psi_{(-\infty,x)} \cup \{x\})}{Z_{(x,\infty)}(\psi_{(-\infty,x)})}$$

where $\infty/\infty := 0$.

- Φ Poisson process on $\mathbb{R}^d \times \mathbb{R}_+$ with intensity measure $\lambda_d \otimes \lambda_1$

Let

$$x_1 := \min\{x \in \mathbb{X} : \exists t \geq 0 : (x,t) \in \Phi \text{ and } t \leq p(x,0)\},$$
$$x_{n+1} := \min\{x > x_n : \exists t \geq 0 : (x,t) \in \Phi,\ t \leq p(x,\{x_1,\dots,x_n\})\}.$$

Let $\tau := \sup\{n \geq 1 : x_n \in \mathbb{R}^d\}$ and define for $\tau < \infty$,

$$T(\Phi) := \{x_1,\dots,x_\tau\}.$$

Theorem. $T(\Phi)$ is Gibbs process with PI κ.

Disagreement coupling

- Iterative Poisson embedding yields

  Theorem. We find Gibbs processes $\mathcal{X}$, $\mathcal{X}_x^{\Xi} \setminus \{x\}$, $x \in \mathbb{R}^d$, such that for every Borel set $P \subset Q_n$ with $\mathrm{dist}(P, \{x\} \cup Q_n^c) > r$,

  $$\mathbb{P}(\mathcal{X} \cap P \neq (\mathcal{X}_x^{\Xi} \setminus \{x\}) \cap P) \leq c_1 e^{-c_2 r}, \quad r \geq r_0.$$

- This allows us to control

  $$\hat{K}(t) := \frac{1}{\sigma^2} \int \big(1\{\Delta_x > t > 0\} - 1\{\Delta_x < t \leq 0\}\big)\, \Lambda(dx).$$

  and, therefore, to bound

  $$d_K(H, \mathcal{N}(0,1)).$$