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# A genuine test for hyperuniformity

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Hyperuniform structures, rigid point processes
and related topics

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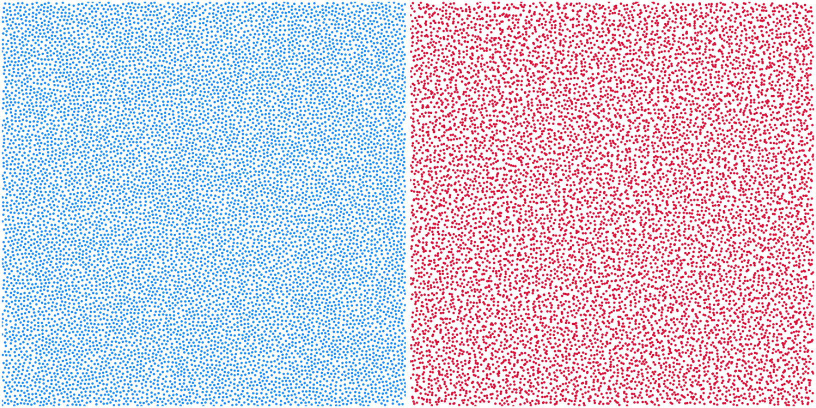
# 1. A motivating example

Realizations of two stationary point processes, both with about 10000 points. One of them has a hidden order.



# 2. The scattering intensity

## Setting

- $\eta$ is a stationary, locally square-integrable point process with positive and finite intensity $\rho$.
- $\eta$ has pair correlation function $g_2$ such that $g_2 - 1$ is (absolutely) integrable.
- $S$ is the structure factor of $\eta$.

## Theorem

*We have*

$$\rho S(k) = \lim_{r\to\infty} \lambda_d(rW)^{-1}\left(\mathbb{E}\left|\sum_{x\in\eta\cap rW} e^{-\mathrm{i}kx}\right|^2 - \mathbf{1}\{k=0\}\lambda_d(rW)\right).$$

## Definition

The empirical scattering intensity of $\eta$ is defined by

$$\mathcal{S}_r(k) := \frac{1}{\eta(W_r)}\left|\sum_{x\in\eta\cap W_r} e^{-\mathrm{i}\langle k,x\rangle} - \mathbf{1}\{k=0\}\gamma r^d\right|^2, \quad k\in\mathbb{R}^d,$$

where $W_r$ is a cube centered at 0 with side length $r>0$.

**Definition (informal version)**

The point process $\eta$ is said to be good if the empirical (local) Fourier transforms satisfy a multivariate central limit theorem.

**Theorem (informal version)**

*Assume that $\eta$ is good. Then the scattering intensities are asymptotically independent exponentially distributed random variables.*

## Definition

The standardized empirical Fourier transform of $\eta \cap W_r$ is defined by

$$T_r(k) := \frac{1}{r^{d/2}} \sum_{x \in \eta \cap W_r} e^{-\mathrm{i}\langle k,x \rangle}, \quad k \in \mathbb{R}^d.$$

## Definition

Let $\mathbb{R}^{[d]} \subset \mathbb{R}^d$ satisfy $|\mathbb{R}^{[d]} \cap \{k, -k\}| = 1$ for each $k \in \mathbb{R}^d$. Let $Z_k$, $k \in \mathbb{R}^{[d]} \setminus \{0\}$, be independent centered $\mathbb{C}$-valued normally distributed random variables. The components of $Z_k$ are assumed to be independent and to have variance $\gamma S(k)/2$.

## Definition

The point process $\eta$ is said to be good if the following holds for each $n \in$ and all distinct $k_1, \dots, k_n \in \mathbb{R}^{[d]} \setminus \{0\}$. If $H_j \colon (0, \infty) \to \mathbb{N}^d$, $j \in \{1, \dots, n\}$, satisfy $2\pi H_j(r)/r \to k_j$ as $r \to \infty$, then as $r \to \infty$,

$$\left( T_r\Big(\frac{2\pi H_1(r)}{r}\Big), \dots, T_r\Big(\frac{2\pi H_n(r)}{r}\Big) \right) \xrightarrow{d} (Z_{k_1}, \dots, Z_{k_n}).$$

## Remark

Brillinger mixing and mixing point processes are good. We believe that this is a generic property of an ergodic point process.

## Theorem

*Assume that $\eta$ is good. Let $E_k$, $k \in \mathbb{R}^{[d]} \setminus \{0\}$, be independent exponentially distributed random variables with mean $S(k)$. Let $n \in \mathbb{N}$ and $k_1, \dots, k_n \in \mathbb{R}^{[d]} \setminus \{0\}$ be pairwise distinct. Suppose that $H_j \colon (0, \infty) \to \mathbb{N}^d$, $j \in \{1, \dots, n\}$, satisfy $2\pi H_j(r)/r \to k_j$ as $r \to \infty$. Then, as $r \to \infty$,*

$$\left(\mathcal{S}_r\left(\frac{2\pi H_1(r)}{r}\right), \dots, \mathcal{S}_r\left(\frac{2\pi H_n(r)}{r}\right)\right) \xrightarrow{d} (E_{k_1}, \dots, E_{k_n}).$$

Proof: Continuous mapping theorem.

# 3. The testing problem

## Assumption

There exist $s \geq 0$ and $t \in \mathbb{R}$ such that

$$S(k) = s + t\|k\|^2 + o(\|k\|^2), \quad \text{as } k \to 0.$$

## Problem

Suppose we have a realization of $\eta$ on $W_L$ for reasonable large $L > 0$. Decide whether $s = 0$, that is whether $\eta$ is hyperuniform.

## Setting

- We observe $\eta$ on $W_L$ for some system size $L \in \mathbb{N}$.
- Take $n$ wave vectors $k_1, \dots, k_n \in \mathbb{R}^{[d]} \setminus \{0\}$ of the form $k_j = 2\pi n_j / L$ for $n_j \in \mathbb{Z}$.
- Working with the asymptotic distribution of the scattering intensities, we let $X_1, \dots, X_n$ be independent exponentially distributed random variables with $\mathbb{E}X_j = s + t\|k_j\|^2$.
- The parameter space is given by

$$\Theta := \{(s,t) \in \mathbb{R}^2 : s \geq 0, s + t\|k_1\|^2 > 0, \dots, s + t\|k_n\|^2 > 0\}.$$

  For each $(s,t) \in \Theta$ we have a probability measure $\mathbb{P}_{s,t}$.
- The null hypothesis $H_0$ is hyperuniformity and characterized by the set $\Theta_0 := \{(s,t) \in \Theta : s = 0\}$.

## Rephrased problem

Suppose given a realization $x_1, \ldots, x_n$ of $X_1, \ldots, X_n$. Does it come from a hyperuniform process? In other words: do we have $s = 0$?

## Lemma

*The* log-likelihood function *is given by*

$$\mathcal{L}(x_1, \ldots, x_n; s, t) = \sum_{j=1}^{n} \Big[ -\log(s + t\|k_j\|^2) - \frac{x_j}{s + t\|k_j\|^2} \Big].$$

# 4. Estimators

**Lemma**

*The maximizer of $\mathcal{L}(x_1, \ldots, x_n; 0, t)$ is given by*

$$\widehat{t}_0(x_1, \ldots, x_n) = \frac{1}{n} \sum_{j=1}^{n} \frac{x_j}{\|k_j\|^2}.$$

*Under the null hypothesis the estimator $\widehat{t}_0(X_1, \ldots, X_n)$ has a gamma distribution with shape parameter n and scale parameter $n/t$. In particular,*

$$\mathbb{E}_{0,t}\left[\widehat{t}_n(X_1, \ldots, X_n)\right] = t, \quad \mathbb{V}\mathrm{ar}_{0,t}\left[\widehat{t}_n(X_1, \ldots, X_n)\right] = \frac{t^2}{n},$$

*so that the estimator is unbiased and consistent.*

## Lemma (Conjecture)

*There is a unique maximizer* $(\widehat{s}(x_1, \ldots, x_n), \widehat{t}_1(x_1, \ldots, x_n)) \in \Theta$ *of* $(s, t) \mapsto \mathcal{L}(x_1, \ldots, x_n; s, t)$.

## Remark (Suggested by simulations)

- The estimators are consistent and asymptotically unbiased.
- The distribution of $\widehat{s}(X_1, \ldots, X_n)$ has an atom at 0.
- The atom size $\mathbb{P}_{s,t}(\widehat{s}(X_1, \ldots, X_n) = 0)$ converges to zero if $s > 0$ and to a constant that is independent of $t$, otherwise.
- The continuous part of the distribution of both $\widehat{s}(X_1, \ldots, X_n)$ and $\widehat{t}_1(X_1, \ldots, X_n)$ converges to a gamma distribution.

# 5. The test

## Definition

Define functions $h_0$ and $h_1$ by

$$h_0(x_1, \ldots, x_n) := \sup\{\mathcal{L}(x_1, \ldots, x_n; 0, t) : (0, t) \in \Theta\},$$
$$h_1(x_1, \ldots, x_n) := \sup\{\mathcal{L}(x_1, \ldots, x_n; s, t) : (s, t) \in \Theta\}.$$

and the (likelihood-ratio) test statistic

$$T(x_1, \ldots, x_n) := 2[h_1(x_1, \ldots, x_n) - h_0(x_1, \ldots, x_n)].$$

## Lemma

*Under $H_0$ the distribution of $T(X_1, \ldots, X_n)$ is independent of $t$. More explicitly, $\mathbb{P}_{0,t}(T(X_1, \ldots, X_n) \in \cdot)$ does not depend on $t$.*

## Remark

Running extensive simulations, we have obtained the limit distribution of $T$ under $H_0$ with high accuracy. It is a mixture of an atom at 0 and a gamma distribution.

# 6. An example

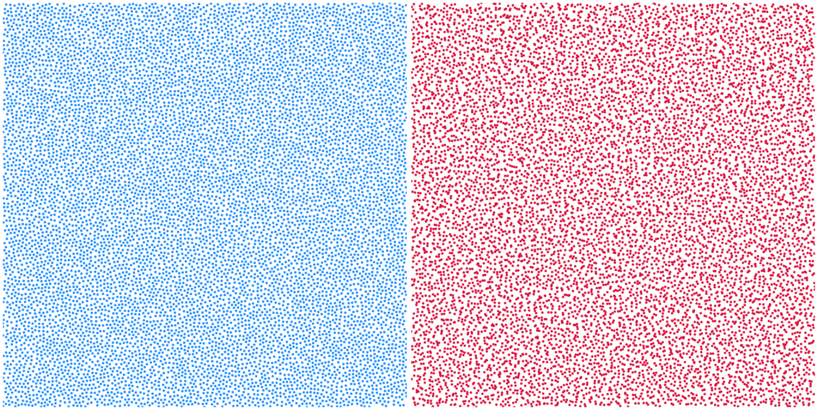
## Setting

- Consider a matching of the (stationarized) lattice $\mathbb{Z}^2$ with a Poisson process of intensity greater than 1; see Klatt, Last and Yogeshwaran '20. The matched Poisson points form a hyperuniform point process satisfying our assumption on the structure factor.
- Using independent thinning we can create versions of this process with $S(0) = s \in [0, 1)$, where $s = 0$ corresponds to the original process.

## Power of the test (applied to a single sample) for different values of $s$ and $L$:

| $s$ | $L$ | | | | | | |
|---|---|---|---|---|---|---|---|
| | 50 | 100 | 150 | 200 | 250 | 300 | 400 |
| 0.0 | 0.05 | 0.06 | 0.06 | 0.05 | 0.05 | 0.06 | 0.05 |
| 0.0001 | 0.08 | 0.20 | 0.40 | 0.64 | 0.83 | 0.93 | 1.00 |
| 0.00025 | 0.12 | 0.41 | 0.77 | 0.95 | 0.99 | 1.00 | $*$ |
| 0.0005 | 0.21 | 0.70 | 0.95 | 1.00 | $*$ | $*$ | $*$ |
| 0.00075 | 0.27 | 0.84 | 0.99 | $*$ | $*$ | $*$ | $*$ |
| 0.001 | 0.35 | 0.93 | 1.00 | $*$ | $*$ | $*$ | $*$ |
| 0.0025 | 0.68 | 1.00 | $*$ | $*$ | $*$ | $*$ | $*$ |
| 0.005 | 0.88 | $*$ | $*$ | $*$ | $*$ | $*$ | $*$ |
| 0.0075 | 0.95 | $*$ | $*$ | $*$ | $*$ | $*$ | $*$ |
| 0.01 | 0.97 | $*$ | $*$ | $*$ | $*$ | $*$ | $*$ |
| 0.025 | 1.00 | $*$ | $*$ | $*$ | $*$ | $*$ | $*$ |
| 0.05 | 1.00 | $*$ | $*$ | $*$ | $*$ | $*$ | $*$ |
| 0.075 | 1.00 | $*$ | $*$ | $*$ | $*$ | $*$ | $*$ |
| 0.1 | 1.00 | $*$ | $*$ | $*$ | $*$ | $*$ | $*$ |

# 7. Back to the motivating example



### Example

The left hand figure shows a realization of a Matérn III (packing) process close to saturation. Even though this process exhibits a high degree of local order, it is not hyperuniform. The test statistic takes a value larger than 300, i.e., it strongly exceeds the critical value of 2.39, which corresponds to a nominal significance level of 5%.

### Example

The right hand figure shows a realization of a randomly perturbed stealthy hyperuniform point pattern. This process is hyperuniform. The test statistic attains the value 0.04. Hyperuniformity is not rejected.

# 8. References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