Hyperuniformity and non-hyperuniformity of quasicrystals

Tobias Hartnick (KIT)

Hyperuniform structures, rigid point processes and related topics
Lille, 21.02.2023

Joint work with Michael Björklund (Chalmers),
see [BjH22] `arXiv:2210.02151`

Table of Contents

1 Diffraction and hyperuniformity

2 Quasicrystalline point processes

3 Hyperuniformity of cut-and-project processes

4 Upper bounds

5 Lower bounds

Observing hyperuniformity

Suppose that Λ is a point process in $\mathbb{R}^2$ which models a thin film of random material. We want to understand whether Λ is hyperuniform:

$$\lim_{R\to\infty} \frac{\mathrm{Var}\left(|\Lambda \cap B_R|\right)}{R^2} \stackrel{?}{=} 0.$$

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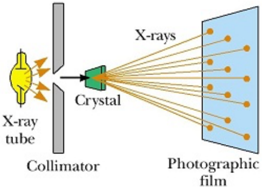
Problem

The number variance of Λ is hard to observe directly experimentally. What can be measured is the (Fraunhofer) diffraction.



Moments vs. diffraction

We consider a locally square integrable point process

$$\Lambda : (\Omega, \mathbb{P}) \to \mathrm{LF}(\mathbb{R}^2),$$

where

- $\mathrm{LF}(\mathbb{R}^2)$ denotes the space of locally finite subsets of $\mathbb{R}^2$;
- $(\Omega, \mathbb{P})$ is an auxiliary probability space;
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- the composition of Λ with any linear statistic is measurable.

It turns out that (under some idealizations) the diffraction depends only on the first two moment measures

$$M^1_\Lambda(A) := \mathbb{E}[|\Lambda \cap A|] \quad \text{and} \quad M^2_\Lambda(B) := \mathbb{E}[|(\Lambda \times \Lambda) \cap B|].$$

These are σ-finite measures on $\mathbb{R}^2$ and $(\mathbb{R}^2)^2$ respectively.

Reduced moments

Standing assumptions

All point processes in this talk are locally square integrable and stationary.

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- $M^1_\Lambda = i(\Lambda) \cdot \mathrm{Vol}_d$. (intensity)

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- $M^1_\Lambda = i(\Lambda) \cdot \mathrm{Vol}_d$. (intensity)
- There exists a positive definite measure η_Λ on $\mathbb{R}^d$ such that

$$M^2_\Lambda(A \times B) = \eta_\Lambda(\chi_A * \chi_{-B}) \quad (A, B \subset \mathbb{R}^d \text{ Borel}).$$

(reduced second moment measure = autocorrelation measure)

A mathematical model of Fraunhofer diffraction

Definition

The diffraction measure of $\Lambda : (\Omega, \mathbb{P}) \to \mathrm{LF}(\mathbb{R}^d)$ is the Fourier transform of the reduced second moment measure, i.e.

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If $\Lambda : \Omega \to \mathrm{LF}(\mathbb{R}^d)$ is Poisson, then

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In general, there is always a Bragg peak of strength $i(\Lambda)^2$ at 0. We set

$$\mathrm{diff}^0_\Lambda := \mathrm{diff}_\Lambda - i(\Lambda)^2 \cdot \delta_0.$$

Structure factor

In many unordered systems the diffraction is absolutely continuous apart from the central Bragg peak, i.e.

$$\mathrm{diff}_\Lambda^0 = f_\Lambda \cdot \mathrm{Vol}_d \quad \text{for some } f_\Lambda \in L^1(\mathbb{R}^d).$$

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Example (Poisson summation)

If $\Lambda : \mathbb{R}^d/\mathbb{Z}^d \hookrightarrow \mathrm{LF}(\mathbb{R}^d)$ is a perfect crystal, then $\mathrm{diff}_\Lambda = \sum_{x \in \mathbb{Z}^d} \delta_x$ is pure point with uniformly discrete support and all peaks at uniform strength (crystallographic diffraction $\rightsquigarrow$ no structure factor!).

Spectral hyperuniformity

Denote by $B_r \subset \mathbb{R}^d$ the Euclidean ball of radius r.

Theorem

For any square-integrable stationary point process $\Lambda : (\Omega, \mathbb{P}) \to \mathrm{LF}(\mathbb{R}^d)$,

$$\underbrace{\lim_{R\to\infty} \frac{\mathrm{Var}(|\Lambda \cap B_R|)}{R^d} = 0}_{\text{geometric hyperuniformity}} \iff \underbrace{\lim_{\varepsilon\to 0} \frac{\mathrm{diff}^0_\Lambda(B_\varepsilon)}{\varepsilon^d} = 0.}_{\text{spectral hyperuniformity}}$$

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geometric hyperuniformity *spectral hyperuniformity*

We can also state this as

$$\mathrm{Var}(|\Lambda \cap B_R|) = o(\mathrm{Var}(|\Lambda_{\mathrm{Pois}} \cap B_R|) \iff \mathrm{diff}^0_\Lambda(B_\varepsilon) = o(\mathrm{diff}^0_{\Lambda_{\mathrm{Pois}}}(B_\varepsilon)).$$

Thus hyperuniformity means that the central peak in the diffraction is substantially sharper than expected from a random material. This does not require the existence of a structure factor [BjH22].

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What is a quasicrystalline point process?

Definition

We say that $\Lambda : (\Omega, \mathbb{P}) \to \mathrm{LF}(\mathbb{R}^d)$ is quasicrystalline if it is

- hard core, i.e. there exists $r > 0$ such that for almost all Λ_ω and all $x, y \in \Lambda_\omega$ with $x \neq y$ we have $d(x, y) > r$;
- jammed, i.e. there exists $R > 0$ such that for almost all Λ_ω we have

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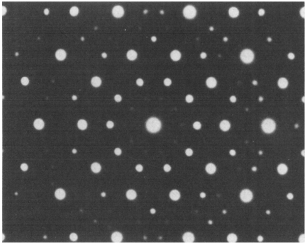
- pure point diffractive, i.e. $\mathrm{diff}_\Lambda = \sum c(x)\delta_x$ is a weighted sum of point measures;
- ergodic, i.e. its distribution is an ergodic measure.

Quasicrystallographic diffraction in real life

This picture was produced in 1983 by Dan Schechtman during a diffraction experiment at an aluminum-manganese alloy. It lost him his sabbatical position and visa in the US and later won him the Nobel Prize in Chemistry.



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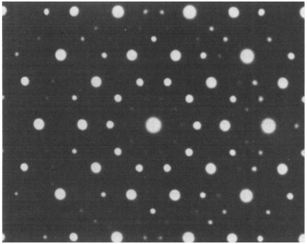

Main features

- Pure point diffractive (hence quasicrystalline).
- Sharp Bragg peaks (hence hyperuniform).
- Peaks of varying strength and exotic symmetry (hence *not* crystalline).

A one-dimensional process

Let $\Gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mathbb{Z}^2 < \mathbb{R} \times \mathbb{R}$ be a lattice (i.e. $ad - bc \neq 0$).

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If we equip Ω_Γ with the unique invariant probability measure, then the hitting times form an ergodic jammed hard core process

$$\Lambda : \Omega_\Gamma \to \mathrm{LF}(G), \quad \Lambda_\omega = \{t \in \mathbb{R} \mid \phi_t(\omega) \in \mathcal{T}_W\}.$$

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Once instance of the above process is given by

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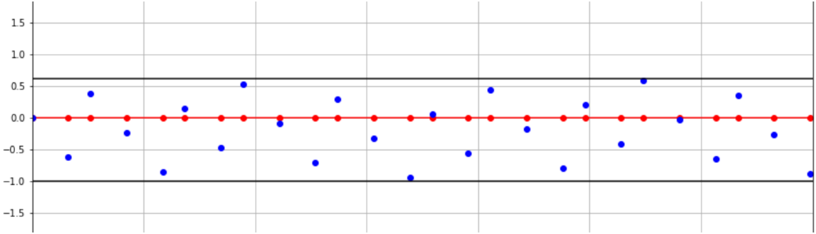
Pictorially this means:

1. Take the lattice Γ and CUT out the strip with width W.
2. PROJECT the resulting points onto $\mathbb{R}$.



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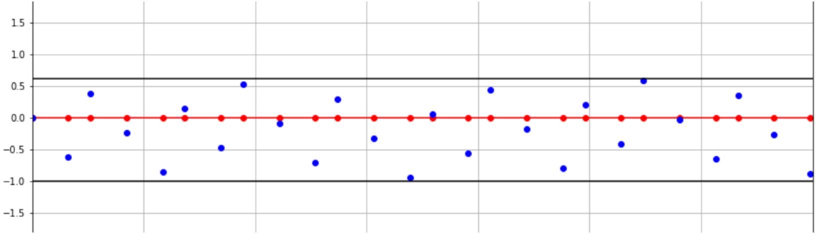

Randomness is introduced by translating the lattice randomly. We call this process a 1(+1)-dimensional cut-and-project (CUP) process.

Generalizations

The previous example admits many generalizations:

- $d_1(+d_2)$-dimensional CUP processes:
  Pick an (irreducible) lattice $\Gamma < \mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$ and a window $W \subset \mathbb{R}^{d_2}$ (e.g. a Euclidean ball or a polytope) to obtain a process in $\mathbb{R}^{d_1}$ by the same construction.

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- General transverse point processes: Any dynamical system of any locally compact second countable group over a standard Borel space admits a transversal $\mathcal{T}$ such that the corresponding hitting times form an ergodic jammed hard core process.
- The moments of such processes can be described in terms of the Palm measures. By using systems with special properties (e.g. mixing) we can get processes with further properties.

CUP processes are quasicrystallographic

Meyer's diffraction formula [Exotic Poisson summation]

If Λ is a cut-and-project process in $\mathbb{R}^{d_1}$ with lattice $\Gamma < \mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$ and window $W \subset \mathbb{R}^{d_2}$, then

$$\mathrm{diff}_\Lambda = \frac{1}{\mathrm{covol}(\Gamma)^2} \cdot \sum_{(\xi_1, \xi_2) \in \Gamma^\perp} |\widehat{\chi}_W(\xi_2)|^2 \cdot \delta_{\xi_1},$$

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The set of peaks is actually dense in $\mathbb{R}^{d_1}$, but one sees a uniform discrete set of large peaks and some background noise of small peaks.

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Our main result

Theorem A [Rough version, see [BjH22] for details]

Let Λ be a $d_1(+d_2)$-dimensional CUP process in with lattice $\Gamma < \mathbb{R}^{d_1+d_2}$ and window W, which is a Euclidean ball of some radius R_0.

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By randomizing the underlying lattice we can thus produce a jammed hard core process which is invariant under $\mathrm{GL}_{d_1}(\mathbb{R}) \ltimes \mathbb{R}^{d_1}$ (in particular, isotropic) and hyperuniform.

A toy version of Theorem A

Even in 1(+1) dimension the space of CUP processes depends on 5 parameters. We look at a 2-parameter family of examples:

Theorem T

Let $\Lambda_{a,b}$ be the CUP process in 1(+1) dimension constructed from

$$\Gamma_a = \left\{ \frac{1}{2a} \begin{pmatrix} m - na \\ m + na \end{pmatrix} \mid m, n \in \mathbb{Z} \right\} \quad \text{and} \quad W_b := [-b, b].$$

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2. For almost all $a \in \mathbb{R}$, $\Lambda_{a,b}$ is hyperuniform for all $b \in \mathbb{R}$. (Generic hyperuniformity)
3. If $a = \sum 10^{-n!}$, then $\Lambda_{a,b}$ is not hyperuniform for almost all $b \in (0/2a)$. (Non-hyperuniformity in the Liouville case)

Diffraction in our toy example

For our process $\Lambda_{a,b}$ the covolume is $\frac{1}{2a}$ and the dual lattice is

$$\Gamma_a^\perp = \left\{ \begin{pmatrix} am - n \\ am + n \end{pmatrix} \mid m, n \in \mathbb{Z} \right\},$$

hence Meyer's diffraction formula reads

$$\mathrm{diff}_{\Lambda_{a,b}}(B_\varepsilon) = 4a^2 \cdot \sum_{(m,n)\in\mathbb{Z}^2} \chi_{[-\varepsilon,\varepsilon]}(am-n) \left|\widehat{\chi}_{[-b,b]}(am+n)\right|^2$$

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where

$$\Delta_a(\varepsilon) = \{ am + n \mid m, n \in \mathbb{Z}, |am - n| \le \varepsilon \}.$$

Our task

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$$\frac{1}{\varepsilon} \sum_{\delta \in \Delta_a(\varepsilon)\setminus\{0\}} \delta^{-2} \to 0.$$
2. To show non-hyperuniformity we will actually show the strongest possible anti-hyperuniformity along a subsequence: We will construct a sequence (ε_n) of radii with $\varepsilon_n \searrow 0$ such that for all $\alpha \in (0,1)$,
$$\frac{1}{\varepsilon_n^\alpha} \sum_{\delta \in \Delta_a(\varepsilon_n)\setminus\{0\}} \frac{\sin^2(4\pi b\delta)}{\delta^2} \to \infty.$$

Table of Contents

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The arithmetic case: $a = \sqrt{2}$

$$\frac{1}{\varepsilon} \sum_{\delta \in \Delta_a(\varepsilon) \setminus \{0\}} \delta^{-2} \xrightarrow{?} 0, \quad \Delta_a(\varepsilon) = \{am + n \mid m, n \in \mathbb{Z}, |am - n| \leq \varepsilon\}$$

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$$|\delta_1 - \delta_2| \leq (2\varepsilon)^{-1}.$$
4. Since the kth pos./neg. element has abs. value $\geq k(2\varepsilon^{-1})$ we get
$$\sum_{\delta \in \Delta_a(\varepsilon)\setminus\{0\}} \delta^{-2} \leq 2\sum_{k=1}^{\infty} (k(2\varepsilon^{-1}))^{-2} = O(\varepsilon^2) = o(\varepsilon).$$

What actually happened here?

Repellence implies hyperuniformity

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We claim that almost all real numbers are 0.98-repellent, i.e. almost as repellent as $\sqrt{2}$. This is a consequence of Khintchine's theorem.

Khintchine's theorem

Theorem (Khintchine 0-1 law)

The set of all $a \in \mathbb{R}$ such that $|am - n| < m^{\alpha}$ for infinitely many $m, n \in \mathbb{Z}$ is either conull or null, depending on whether m^{α} is summable or not.

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Generic repellence

- Since $\alpha = -1.01$ is in the summable regime, we see that for almost all $a \in \mathbb{R}$ and all $m, n \in \mathbb{Z}$ with $m \gg_a 1$ we get $|am - n| \geq m^{-1.01}$.

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- Assume that $a \in \mathbb{R}$ has this property and assume that $|am - n| \leq \varepsilon$. If m is sufficiently large and ε sufficiently small, then

$$\varepsilon \geq |am - n| \geq m^{-1.01} \quad \Longrightarrow \quad m \geq \varepsilon^{-0.99}$$

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$$\begin{aligned} \varepsilon \geq |am - n| \geq m^{-1.01} \quad &\Longrightarrow \quad m \geq \varepsilon^{-0.99} \\ \Longrightarrow \quad |am + n| \geq |2am - (am - n)| &\geq 2a\varepsilon^{-0.99} - \varepsilon \geq \varepsilon^{-0.98}. \end{aligned}$$

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The counterexample

We are going to show that for

$$a := \sum 10^{-n!} = 0.110001000000000000000001\ldots$$

and all $\alpha \in (0,1)$ we have

$$\sup_{\varepsilon} \frac{\mathrm{diff}^0_\Lambda(B_\varepsilon)}{\varepsilon^\alpha} = \mathrm{const} \cdot \varepsilon^{-\alpha} \sum_{\delta \in \Delta_a(\varepsilon)\setminus\{0\}} \frac{\sin^2(4\pi b\delta)}{\delta^2} = \infty$$

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After 10 pages of hard (but in a sense elementary) analysis we get

$$\frac{\mathrm{diff}^0_{\Lambda}(B_\varepsilon)}{\varepsilon^\alpha} \geq \mathrm{const}\cdot\varepsilon^{-\alpha}\cdot \sum_{\{m \in \mathbb{Z}^2\setminus\{0\} \mid \mathrm{dist}(ma, \mathbb{Z}) \leq \varepsilon/2\}} \frac{\sin^2(4\pi mab)}{m^2} + O_{a,b}(\varepsilon^{1-\alpha}).$$

Choosing radii

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$a := \sum 10^{-n!} = 0.110001000000000000000001\ldots$ has very good rational approximants (like 0.110001), i.e. we can find a sequence (m_k) such that

$$\mathrm{dist}(m_k a, \mathbb{Z}) \leq m_k^{-k} \quad \text{and} \quad m_k \nearrow \infty.$$

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Almost done ...

Summary

If $a = \sum 10^{-n!}$, then there exist integers $m_k \nearrow \infty$ and real numbers $\varepsilon_k \searrow 0$ such that for all $\alpha \in (0,1)$,

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We may thus conclude that, even for $\alpha \ll 1$,

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i.e. strong quantitative anti-hyperuniformity along a subsequence, provided $(\sin^2(4\pi m_k ab))_{k\in\mathbb{N}}$ stays uniformly bounded away from 0.

The endgame: equidistribution

How can we ensure that $(\sin^2(4\pi m_k ab))_{k\in\mathbb{N}}$ stays uniformly bounded away from 0?

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Lemma (Equidistribution)

For any monotone sequence (m_k) there exists a subsequence (m_{k_j}) such that for almost all $b \in (0/2a)$ we have $2abm_{k_j} \to \frac{1}{4} \mod 1$.

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Corollary

If we choose the lattice parameter a to be a Liouville number and choose the window parameter $b \in (0/2a)$ sufficiently generically, then Λ is strongly anti-hyperuniform along a subsequence of radii.

Positive ANV?

In our counterexample, the limit

$$\mathrm{ANV}(\Lambda) := \lim_{R\to\infty} \frac{\mathrm{Var}(|\Lambda \cap B_R|)}{R^d}$$

and its spectral counterpart do not exist - we get wildly oscillating behaviour. But one can also construct similar point processes with a positive limit.

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How to construct processes with positive ANV

- Start from the simplest mixing transformation $\times 2 : \mathbb{R}/\mathbb{Z} \to \mathbb{R}/\mathbb{Z}$ and take its invertible extension $\mathbb{Z} \curvearrowright \mathbb{R}/\mathbb{Z} \times \mathbb{Q}_2$.
- Induce this system to an $\mathbb{R}$-system $\mathbb{R} \times \Omega$ and take any reasonable transversal.
- The corresponding transverse point process is a large random subset of a random translate of $\mathbb{Z}$ and has positive ANV.

Our main result

Theorem A [Rough version, see Björlund-H. '22 for details]

Let Λ be a $d_1(+d_2)$-dimensional CUP process in with lattice $\Gamma < \mathbb{R}^{d_1+d_2}$ and window W, which is a Euclidean ball of some radius R_0.

1. If Γ is an arithmetic lattice (as in Penrose, Fibonacci, ... and all other classical examples), then Λ is hyperuniform. (Hyperuniformity from arithmeticity)
2. For almost all lattices Γ, the process Λ is hyperuniform. (Generic hyperuniformity)
3. For some choices of Γ and R_0, the process Λ is not hyperuniform. (Non-hyperuniformity in the Liouville case)

By randomizing the underlying lattice we can thus produce a jammed hard core process which is invariant under $\mathrm{GL}_{d_1}(\mathbb{R}) \ltimes \mathbb{R}^{d_1}$ (in particular, isotropic) and hyperuniform.