Hyperuniformity exponent: estimation, rigidities, simulation

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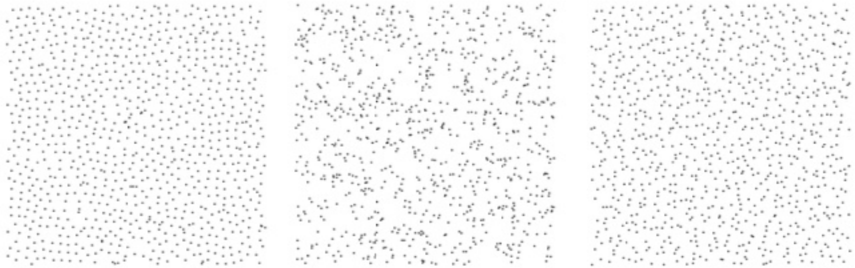
Hyperuniform processes

- A stationary hyperuniform point process $\mathbf{P} \subset \mathbb{R}^d$ is such that

$$\mathrm{Var}(\#\mathbf{P} \cap B(0,r)) = o(\underbrace{|B(0,r)|}_{\text{Poisson rate}}).$$

"Fluctuations are suppressed at large scales", "superhomogeneous"



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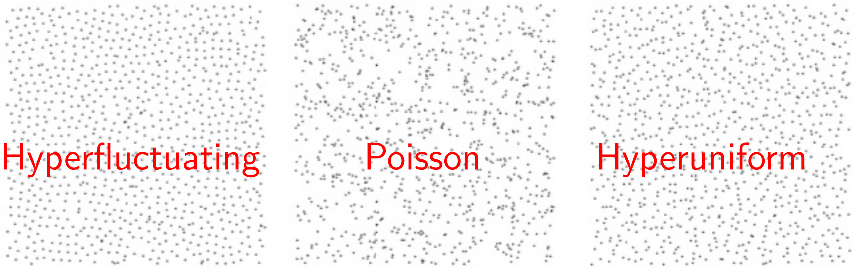
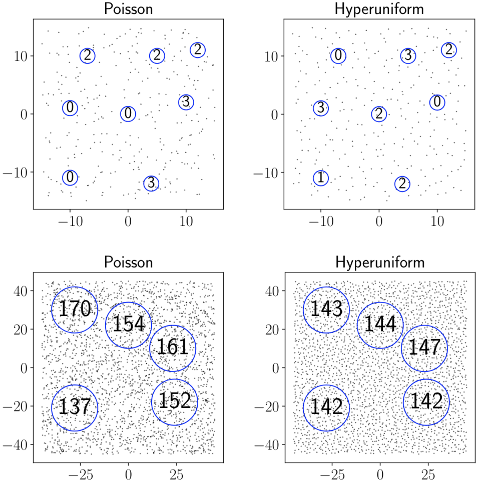


What does HU look like?

"Global order and local disorder"



Credit: Diala Hawat

History

- **Condensed matter physics**: Perturbed lattices, hard sphere models, Lloyd (k-means) algorithm, ... (Torquato, Gabrielli, Stillinger, Zhang, ...)
- **Statistical physics**: Coulomb and Riesz gases, Determinantal point processes (DPPs) (Lebowitz, Ghosh, ...)
- **Numerical integration, image processing**: "blue noise", "samples with low discrepancy"
- Eigenvalues of **random matrices** and **DPPs** (Ginibre ensembles, sine process)
- Zeros of planar random **Gaussian Analytic Function (GAF)** (Sodin, Tsirelson, ...)

Hyperuniformity exponent

For some (unit intensity) processes $\mathbf{P}$, there is $\alpha \geqslant 0$ such that, for a smooth function $f \in \mathscr{C}^\infty(\mathbb{R}^d)$:

$$\mathrm{Var}\left(\sum_{x\in\mathbf{P}} f(x/R)\right) \sim R^{d-\alpha}\int f$$

- **Numerical integration:** The larger the α, the better is the sample to estimate $\int f$!
- Poisson: $\alpha = 0$ (think of $f = 1_{B(0,1)}$ for the scaling order)
- It is indispensable to use smooth functions as for $f = 1_{B(0,1)}$, $\alpha \leqslant 1$ **[Beck '87]**.
- "Class I": $\alpha > 1$, "Class II": $\alpha = 1$, "Class III": $\alpha < 1$.

Structure factor $\mathcal{S}$

- Define $\mathcal{S}$ as the non-negative measure satisfying for f a test function

$$\mathrm{Var}\left(\sum_{x\in\mathbf{P}} f(x)\right) = \int |\hat{f}|^2 d\mathcal{S}.$$

  (exists if $\mathbf{E}(\#\mathbf{P}\cap B(0,1))^2 < \infty$)

- If $\mathcal{S}(du) \sim u^\beta du$ as $u \to 0$, then $\beta = \alpha$ under some density assumptions (e.g. **[Mastrilli, Blaszczyszyn, Lavancier '24]**).
- **Infinite Ginibre ensemble** (DPP coming from random matrices / Coulomb gas): $\alpha = 2$ as

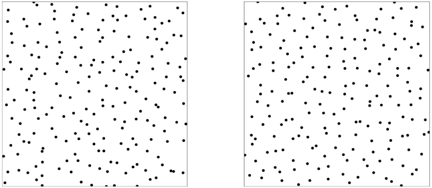
$$\mathcal{S}(du) = (1 - e^{-u^2})du$$

“Amorphous” point processes

- For a “nicely” behaved standard HU process $\mathbf{P}$, $\alpha = 2$:

$$\mathcal{S}(du) = \left(\underbrace{\mathcal{S}(0)}_{=0\ (\mathrm{HU})} + O(u^2) \right) du$$

- **GAF process**: $\alpha = 4$ only “non-lattice” known process with $\alpha > 2$



Left: DPP ($\alpha = 2$) *Right:* Zeros of the planar GAF (Gaussian Analytic Function) ($\alpha = 4$) *Ben Hough et al.*

Estimating $\mathcal{S}$ and α for amorphous processes

- **Estimate** $\mathcal{S}$: Scattering intensity / empirical structure factor: on a rectangular window $W = \prod_j [-R/2, R/2]^d$,

$$\hat{\mathcal{S}}(k) = \frac{1}{R^d} \Big| \sum_{k \in \mathbf{P} \cap W} e^{-ikx} \Big|^2.$$

- **[Gautier, Hawat, Bardenet, Lr '23]** Assume the pair correlation g exists and is integrable. As $R \to \infty$,

$$\sup_{k \in A_R} \left| \hat{\mathcal{S}}(k) - \mathbf{E}(\hat{\mathcal{S}}(k)) \right| \to 0$$

A_R : points $\neq 0$ for which one coordinate is a multiple of $2\pi/R$.

- We cannot estimate $\mathcal{S}(k)$ for $\|k\| \leqslant \pi/\sqrt{d}R$

Tapered estimators

- Let T a square integrable function. Define the tapered estimator

$$\hat{\mathcal{S}}_T(k) = \frac{1}{R^d} \left| \sum_{x \in \mathbf{P}} T(x/R) e^{-ikx} \right|^2 .$$

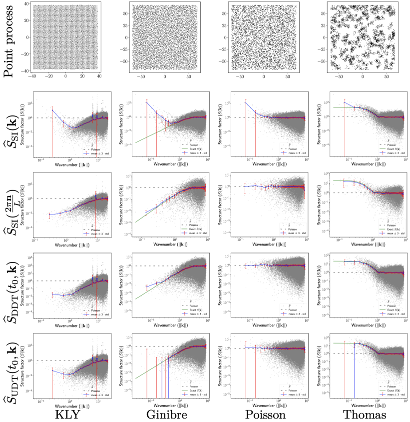
We have $\hat{\mathcal{S}}(k) = \hat{\mathcal{S}}_T(k)$ for $T = \mathbf{1}\,[0,1]^d$.

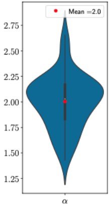
- Multi-tapered versions (inspired by **[Rajala, Olhede, Murrell '20]**)

$$\sum_j w_j \hat{\mathcal{S}}_{T_j}(k)$$

Package `structure_factor` (with D. Hawat, G. Gautier, R. Bardenet)

Functionalities for estimating $\mathcal{S}$ (several methods)





(b) Ginibre

Violin plot of estimation of α over 50 trials of 10^4 points

D. Hawat

[Mastrilli, Blaszczyszyn, Lavancier '24]

- Estimator of α based on multi-tapering :

$$\hat{\alpha} = d - \sum_j \frac{w_j}{\ln(R)} \ln\left(\sum_i T_j(f_i, R)^2\right)$$

(the f_i replace the complex exponentials)

- Converges to α in probability under continuity assumptions
- CLT under Brillinger mixing if $\alpha \leqslant d$

Lattice computations

- **[Coste '21]** : $\hat{\mathcal{S}} - \delta_0 \to \mathcal{S}$ a.s. in the sense of distributions if $\mathbf{P}$ is ergodic
- "$\alpha = \infty$" : Shifted lattice $\mathbf{P} = \mathbb{Z}^d + U, U \sim \mathscr{U}_{[0,1]^d}$: $f_R = f(\cdot/R)$

$$\begin{aligned}\sum_{k\in\mathbb{Z}^d} f_R(k+U) &= c_d \sum_{m\in\mathbb{Z}^d} e^{iRm\cdot U} \hat{f}_R(m) \text{ (Poisson formula)}\\ &= c_d R^d \sum_m e^{iRm\cdot U} \hat{f}(Rm)\\ &= c_d R^d \Big(\underbrace{\hat{f}(0)}_{deterministic} + \sum_{m\neq 0} e^{iRm\cdot U} \underbrace{\hat{f}(Rm)}_{\text{fast decay}} \Big)\end{aligned}$$

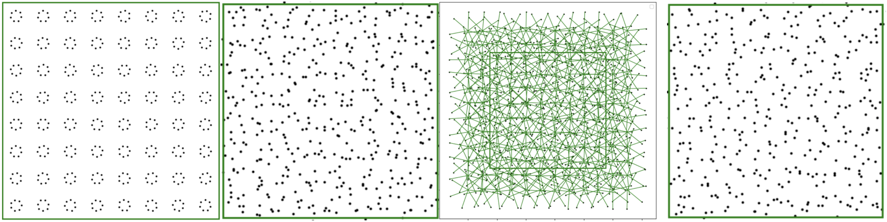
- $\alpha = 2$: Perturbed lattice $\mathbf{P} = \{k + X_k + U, k \in \mathbb{Z}^d\}, X_k$ iid centred,

$$\mathcal{S}(du) = \sum_{m\in\mathbb{Z}^d\setminus\{0\}} |\Phi_{X_0}(m)|^2 \delta_m(du) + (1 - \underbrace{|\Phi_{X_0}(u)|^2}_{\text{CF of } X_0}) du$$

$$\Phi_{X_0}(u) = 1 - \mathbf{E}(X_0^2) u^2 + o(u^2) \Rightarrow \alpha = 2$$

Lattice of clusters ($\alpha = 2p$)

- Put p equidistant points rotated by a random angle at distance r from each point of $\mathbb{Z}^2$:



$r = 0.2, p = 7$ $r = 1.3, p = 7$ Making of $r = 1.3, p = 6$

- **[Sodin & Tsirelson '04]**: $p = 3$, "toy model" for GAF ($\alpha = 4$)

Proposition (Lr '24)

If p is **prime**, $\mathcal{S}(du) \leqslant c\|u\|^{2p} du$ *as* $u \to 0$, "$\alpha \geqslant 2p$".

Any corresponding continuous (amorphous) model?

Lattice or not lattice?

- There seem to be **two main categories**: (perturbed) **lattices**, with an **atomic component** in $\mathcal{S}$, and "amorphous"/mixing/isotropic ones (Ginibre, GAF, DPPs, Coulomb gases), with a **purely continuous** $\mathcal{S}$.
- What if the perturbations $X_k, k \in \mathbb{Z}^d$ form a **dependent** stationary field? **[Dereudre, Flimmel, Huesmann, Leblé '24]**
- As it turns out, in dimension $d \geqslant 2$, a HU* process $\mathbf{P}$ (with intensity 1) can be seen as a perturbed lattice in the sense that

$$\mathbf{P} = \{k + X_k + U; k \in \mathbb{Z}^d\}$$

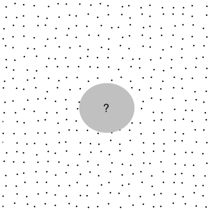
with $\{X_k\}$ stationary **dependent** and $\mathbf{E}(\|X_k\|^2) < \infty$ **[Lr,Yogeshwaran '24]**, see also **[Leblé & Huesmann '24]**, **[Butez, Dallaporta & Garcia-Zelada '24]**

- Most likely, the tail of X_0 is exponential for many models (proved for GAF in **[Nazarov, Sodin & Volberg '07]**)

Rigidity (lattices)

- A (perturbed) lattice satisfies **number rigidity**: $\mathbf{P} = \{k + X_k + U, k \in \mathbb{Z}^d\}$, X_k iid centred: for K compact

$$\#\mathbf{P} \cap K \in \sigma(\mathbf{P} \cap K^c)$$



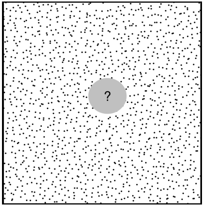
- If $X_k = 0$ (unperturbed lattice), we have **maximal rigidity**:

$$\mathbf{P} \cap K \in \sigma(\mathbf{P} \cap K^c)$$

- Do other types of processes satisfy rigidity?

Rigidity [Ghosh & Peres '17]

- Ginibre process and GAF satisfy number rigidity:



Knowledge of $\mathbf{P} \cap B(0,1)^c \Rightarrow \#\mathbf{P} \cap B(0,1) = 52$

- GAF satisfies 1-rigidity:

$$\left(\#\mathbf{P} \cap B(0,1), \sum_{x \in \mathbf{P} \cap B(0,1)} x\right) \in \sigma(\mathbf{P} \cap B(0,1)^c)$$

Definition (k-rigidity)

$\mathbf{P}$ is k-rigid iff $\displaystyle\sum_{x \in \mathbf{P} \cap B(0,1)} x^{\mathsf{m}} \in \sigma(\mathbf{P} \cap B(0,1)^c), \mathsf{m} \in \mathbb{Z}^d, |\mathsf{m}| \leqslant k$

Rigidity and HU exponent

- Ginibre, perturbed lattices in $d = 1, 2$: 0-rigid, $\alpha = 2$
- GAF ($d = 2$): 1-rigid, $\alpha = 4$.

Theorem (Lr '24)

Decompose $\mathcal{S}(du) = s(u)du + \mathcal{S}_s$ where $\mathcal{S}_s$ is singular (atomic, Cantor, ...). $\mathbf{P}$ is k-rigid if the spectral density s has a " zero of order k". If $\mathbf{P}$ is isotropic or separable, or "simple":

- *Converse is true (for "linear rigidity")*
- *Zero of order k means*

$$\int \frac{\|u\|^{2k}}{s(u)} du = \infty.$$

$\Rightarrow$ The p-flower lattice of clusters is $(p-1)$-rigid for p prime.

Simulation

- **Blue noise** comes from image processing, blue noise sampling seems to "prevent some aliasing phenomena": *Heck et al.*(2013) and *Yan et al.*(2015)

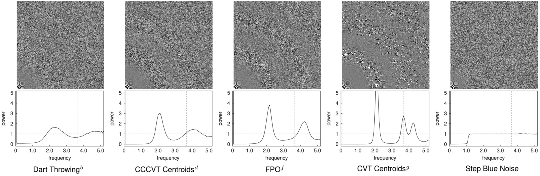


Fig. 1. A bird's eye view of the standard zone plate reveals structured aliasing for blue noise patterns that have peaks in their power spectrum. High-frequency image content is not replaced by white noise (as is the goal of stochastic sampling) but by pseudo-patterns that are conceptually similar to the moiré patterns of regular sampling. Step blue noise patterns, as defined in Section 3.1, consistently prevent such artifacts by cleanly mapping all high frequencies to white noise. (The superscripts refer to the citations in Table 1.)

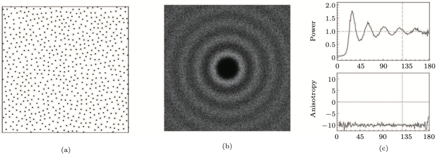
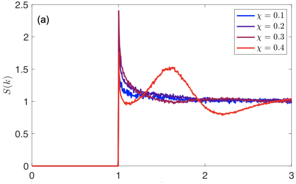


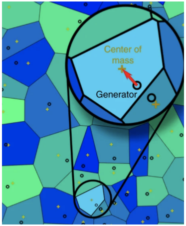
Fig. 1. Example of Poisson-disk sampling and its spectral analysis. (a) A sampled point set. (b) Power spectrum from this point set. (c) Radial means and normal anisotropy.

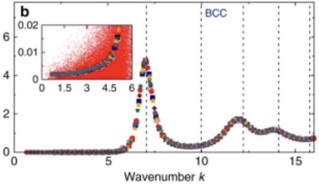
Simulations from physicists (team of Torquato)

[Morse et al. '23]: Minimization of an energy which ground states are HU



[Klatt et al. '19]: Lloyd/KMeans algorithm





Stealthy processes

The structure factor of $\mathbb{Z}^d + U$ is

$$\sum_{k \in \mathbb{Z}^d \setminus \{0\}} \delta_k.$$

In particular it has a gap around zero ($\alpha = \infty$).

Definition

A SPP $\mathbf{P}$ is **stealthy** if $\mathcal{S}(B) = 0$ for some neighbourhood (of 0).

- **What can be the structure factor of a stealthy process? Can it have a non zero continuous part? Be mixing?**
  Related to difficult problem in harmonic analysis and *quasi-crystals*

Simulation of mixing processes

- It is easy to simulate a perturbed lattice, but it has atoms, or “Braggs peaks”, and is not mixing.
- DPP simulation: not more than several thousands points
- GAF simulation: ?

A HU process without Braggs peaks and $n\ln(n)$ complexity (with A. Shapira and L. Thomassey)

- Lattice perturbed by stationary field:

$$\{k + X(k) + U; k \in \mathbb{Z}^d\}$$

  for $X : \mathbb{R}^d \to \mathbb{R}^d$ a stationary field.

- Lattice perturbed by field X with **stationary increments**

$$\mathbb{Z}^d \star X = \{k + X(k) : k \in \mathbb{Z}^d\},$$

  X requires a convention of the type $X(0) = 0 \Rightarrow$ not stationary.

Theorem (TLS '24 +)

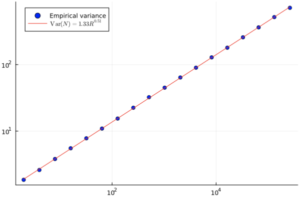
For $\mathbf{P}$ a stationary point process with Palm measure $\mathbf{P}^0$, X a field with stationary increments, $\mathbf{P}^0 \star X$ is the Palm measure of a stationary point process.

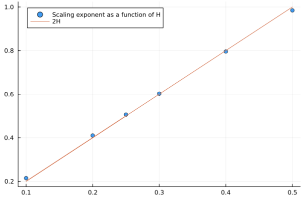
Perturbation with fractional Gaussian fields

Theorem

Let X a fractional Brownian motion on $\mathbb{R}$ with Hurst index $H < 1/2$. Let $\mathbf{P}^0 = \mathbb{Z}^d \star X$. Then $\mathbf{P}^0$ is the Palm measure of a point process $\mathbf{P}$ which structure factor $\mathcal{S}$ is purely continuous and satisfies as $u \to 0$,

$$\mathcal{S}(du) \sim u^{1-2H}.$$





left : log-log plot of the variance on $[-R, R]$. *right*: exponent in function of H

Coulomb repulsion (with D. Hawat, R. Bardenet)

- Move Poisson point x_i according to the repulsive Coulomb force $C_d(x) = \frac{x}{\|x\|^d}$

$$x_i \to x_i^\varepsilon := x_i + \varepsilon \sum_{j \neq i} C_d(x_j - x_i)$$

Theorem (HBL + M)

For any f of class $\mathcal{C}^2$ with compact support, $I_\varepsilon = \sum f(x_i^\varepsilon)$:

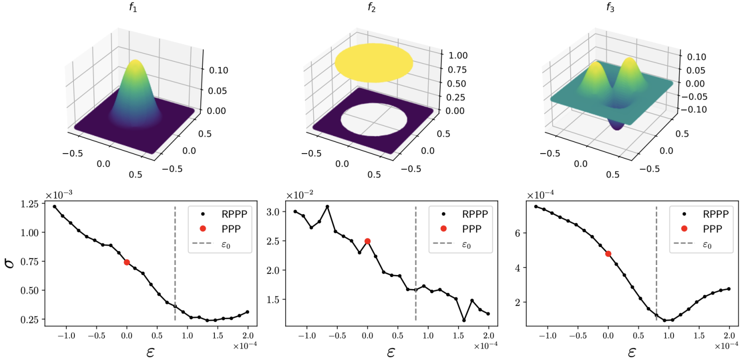
$$Var(I_\varepsilon) = Var(I_0)\,(1 - 2\varepsilon\kappa_d) + O(\varepsilon^{1+1/d})$$

Explanation: C_d (is the only kernel that) satisfies in the weak sense

$$\Delta C_d = -\kappa_d \delta_0$$

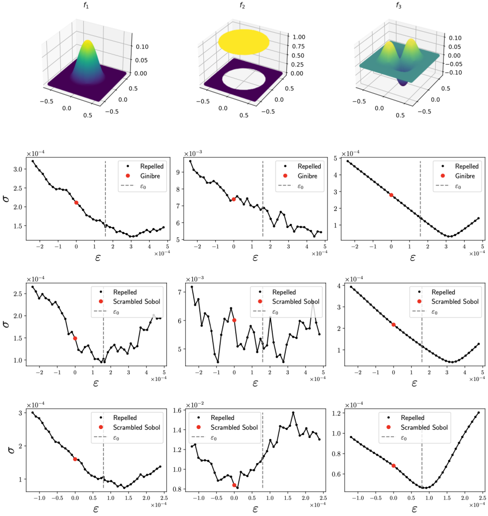
Test with MCRPP Python package

$\mathrm{Var}\left(I_\varepsilon\right) = \mathrm{Var}\left(I_0\right)\left(1 - 2\varepsilon\kappa_d\right) + O(\varepsilon^{1+1/d})$. Hence choose $\varepsilon_0 = (2\kappa_d)^{-1}$.



Variance as ε increases for resp. f_1, f_2, f_3

Test with other initial data



Variance evolution for other initial processes: Ginibre, Scrambled Sobol 2D, scrambled Sobol 3D

Workshop around Hyperuniformity in Paris on December 11-13:
https://hyperuniformity.sciencesconf.org/

Thank you for your attention!

The table

		Atomic part	Continuous part	α/Rigidity	Complexity
Stealthy	Purely lattice	✓	✗	∞	N
	Crystalline	✓	✗	∞	
	???	?	✓	∞	
	Independently perturbed lattice (locally dependent)	✓	✓	2p	N
Amorphous	GAF	✗	✓	4	?
	DPPs (Ginibre)			2	N^2?
	Coulomb			$\leqslant 2$?	?
	Riesz				
	1D $X \star \mathbb{Z}^d$	✗	✓	$1-2H$	$N\ln(N)$
Not HU	Poisson etc...			0	N