On estimating the structure factor of a point process, with applications to hyperuniformity

Diala Hawat,

Guillaume Gautier, Rémi Bardenet, and Raphaël Lachièze-Rey

Université de Lille, CNRS, Centrale Lille ; UMR 9189 – CRIStAL, F-59000 Lille, France.
Université de Paris, Map5, Paris, France.

Contents

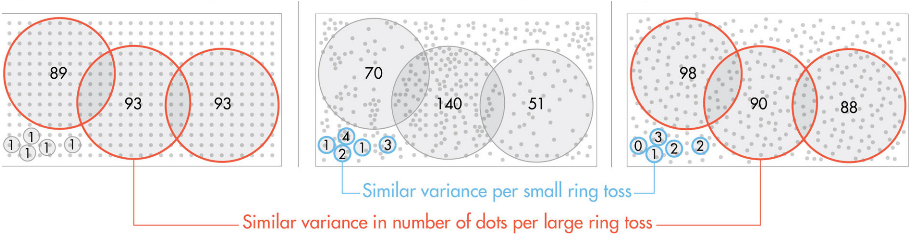
Definitions and Motivations

Hyperuniform or Superhomogeneous

Let $\mathcal{X}$ be a stationary point process of $\mathbb{R}^d$ of intensity ρ, $\mathcal{X}$ is hyperuniform iff

- Variance:

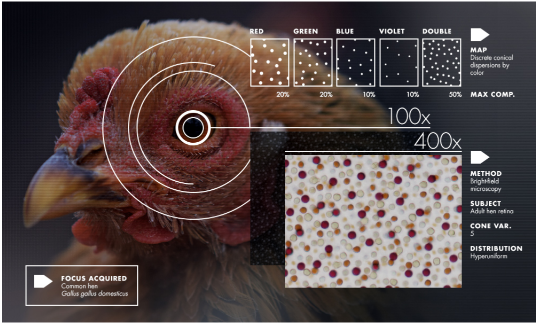
$$\lim_{R\to\infty} \frac{\mathrm{Var}\left(\mathrm{Card}(\mathcal{X}\cap B(0,R))\right)}{|B(0,R)|} = 0.$$



S. Torquato, *Hyperuniform States of Matter, 2018.*

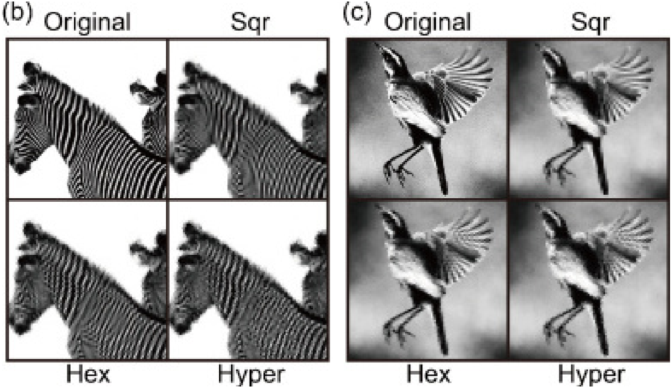
S. Coste, *Order, Fluctuations, Rigidities*, 2021.

Bird's-Eye



Y. Jiao, T. Lau, H. Hatzikirou, M Meyer-Hermann, J. C. Corbo, and S. Torquato, *Avian photoreceptor patterns represent a disordered hyperuniform solution to a multiscale packing problem,* 2014.

Image reconstruction

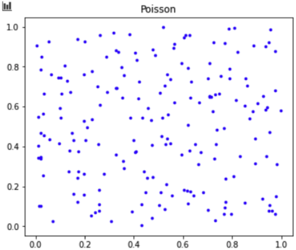


Ming-Jie Sun, Xin-Yu Zhao, and Li-Jing Li, *Imaging using hyperuniform sampling with a single-pixel camera,* 2018.

- **Monte Carlo integration:**

$$\int f(x)\mu(\mathrm{d}x) \approx \sum_{i=1}^{N} w_i f\left(\mathbf{x}_i\right)$$

- **Rate of convergence with a Poisson point process:** $O(1/\sqrt{N})$

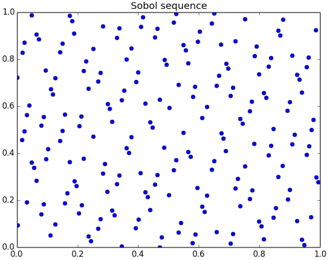


Numerical integration

- **Monte Carlo integration:**

$$\int f(x)\mu(\mathrm{d}x) \approx \sum_{i=1}^{N} w_i f(\mathbf{x}_i)$$

- **Rate of convergence with Sobol sequence:** $O(\log(N)^d/N)$



Structure Factor

Let $\mathcal{X} \subset \mathbb{R}^d$ be a stationary point process of intensity ρ

- Structure factor

$$S(\mathbf{k}) = 1 + \rho \mathcal{F}(g-1)(\mathbf{k})$$

- Pair correlation function

$$\mathbb{E}\left[\sum_{\mathbf{x},\mathbf{y}\in\mathcal{X}}^{\neq} f(\mathbf{x},\mathbf{y})\right] = \int_{\mathbb{R}^d\times\mathbb{R}^d} f(\mathbf{x}+\mathbf{y},\mathbf{y})\rho^2 g(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}$$

S. Coste, *Order, Fluctuations, Rigidities*, 2021.

S. Torquato, *Hyperuniform States of Matter, 2018.*

Structure Factor

$$\mathcal{X} \text{ is hyperuniform} \iff \lim_{R\to\infty} \frac{\mathrm{Var}(\mathrm{Card}(\mathcal{X}\cap B(0,R)))}{|B(0,R)|} = 0$$

- Structure factor

$$S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k})$$

- Pair correlation function

$$\mathbb{E}\left[\sum_{\mathbf{x},\mathbf{y}\in\mathcal{X}}^{\neq} f(\mathbf{x},\mathbf{y})\right] = \int_{\mathbb{R}^d\times\mathbb{R}^d} f(\mathbf{x}+\mathbf{y},\mathbf{y})\rho^2 g(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}$$

- $\mathcal{X}$ is hyperuniform iff

$$S(\mathbf{0}) = 0$$

S. Coste, *Order, Fluctuations, Rigidities*, 2021.

S. Torquato, *Hyperuniform States of Matter, 2018.*

Hyperuniformity class

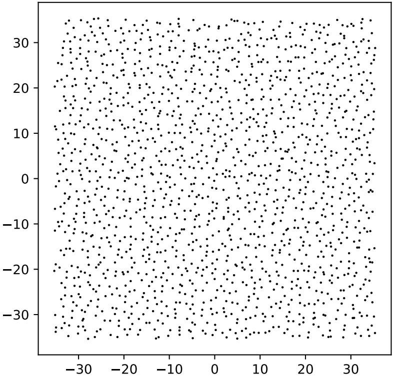
$$\mathcal{X} \text{ is hyperuniform} \iff \lim_{\mathbf{k}\to\mathbf{0}} \underbrace{1 + \rho\mathcal{F}(g-1)(\mathbf{k})}_{S(\mathbf{k})} = 0$$

- $\mathcal{X}$ is hyperuniform with $|S(\mathbf{k})| \sim c\|\mathbf{k}\|_2^\alpha$ in the neighborhood of 0 then,

α	$\mathrm{Var}\left[\mathrm{Card}(\mathcal{X} \cap B(0,R))\right]$	class
> 1	$O(R^{d-1})$	I
1	$O(R^{d-1}\log(R))$	II
$]0,1[$	$O(R^{d-\alpha})$	III

S. Cost, *Order, Fluctuations, Rigidities*, 2021.

Ginibre ensemble



Ginibre ensemble

- Intenity: $\rho_{\text{Ginibre}} = 1/\pi$
- Pair correlation function: $g_{\text{Ginibre}}(r) = 1 - \exp(-r^2)$
- Structure factor: $S_{\text{Ginibre}}(k) = 1 - \exp(-k^2/4)$
- Power decay: $\alpha_{\text{Ginibre}} = 2$
- Hyperuniform class: I

Structure factor estimators

Idea

$$S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k})$$

- **Given**: $\mathcal{X}_N = \{\mathbf{x}_i\}_1^N$ a realization of a **stationary** point process $\mathcal{X}$ of intensity ρ in $W = [-L/2, L/2]^d$
- **Need**: Use $\mathcal{X}_N$ to approximate $S(\mathbf{k}) = 1 + \rho \int_{\mathbb{R}^d}(g(\mathbf{r}) - 1)e^{-i\langle \mathbf{k},\mathbf{r}\rangle} \,\mathrm{d}\mathbf{r}$

Idea

$$S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k})$$

- **Given**: $\mathcal{X}_N = \{\mathbf{x}_i\}_1^N$ a realization of a **stationary** point process $\mathcal{X}$ of intensity ρ in $W = [-L/2, L/2]^d$
- **Need**: Use $\mathcal{X}_N$ to approximate $S(\mathbf{k}) = 1 + \rho \int_{\mathbb{R}^d} (g(\mathbf{r}) - 1) e^{-i\langle \mathbf{k}, \mathbf{r}\rangle} \, \mathrm{d}\mathbf{r}$
- **Idea**:
  1. Use $\alpha_t(\mathbf{r}, W) = \int_{\mathbb{R}^d} t(\mathbf{r}+\mathbf{y}, W) t(\mathbf{y}, W) \mathrm{d}\mathbf{y}$ s.t. $\lim_{L\to\infty} \alpha_t(\mathbf{r}, W) = 1$ and $\|t\|_2 = 1$:

$$\begin{aligned} S(\mathbf{k}) &= 1 + \rho \int_{\mathbb{R}^d} \lim_{L\to\infty} (g(\mathbf{r}) - 1)\alpha_t(\mathbf{r}, W) e^{-i\langle \mathbf{k}, \mathbf{r}\rangle} \, \mathrm{d}\mathbf{r} \\ &= \lim_{L\to\infty} \mathbb{E}[\widehat{S}(t, \mathbf{k})] - \underbrace{\rho\mathcal{F}(\alpha_t)(\mathbf{k}, W)}_{\epsilon_t(\mathbf{k}, \mathbf{L})} \end{aligned}$$

  2. Reduce bias: Consider the zeros of $\epsilon_t(\mathbf{k}, \mathbf{L})$ as the set of allowed wavevectors of $\widehat{S}$, or remove the bias term.

Scattering intenisty

- **Taper:** $t_0(\mathbf{x}, W) = \frac{1}{\sqrt{|W|}} \mathbb{1}_W(\mathbf{x})$
- $S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\Big[\underbrace{\frac{1}{\rho|W|} \Big| \sum_{\mathbf{x}\in\mathcal{X}\cap W} e^{-i\langle \mathbf{k},\mathbf{x}\rangle} \Big|^2}_{\widehat{S}_{\mathrm{SI}}(\mathbf{k})} \Big] - \rho \underbrace{\Big(\prod_{j=1}^{d} \frac{\sin(k_j L/2)}{k_j \sqrt{L}/2} \Big)^2}_{\epsilon_0(\mathbf{k},\mathbf{L})}$
- $\epsilon_0(\mathbf{k}, \mathbf{L}) = \begin{cases} 0 & \text{if } \mathbf{k} \in \mathbb{A}_{\mathbf{L}} \\ \rho L^d & \text{as } \|\mathbf{k}\|_2 \to 0 \\ 2^{2d} \prod_{j=1}^{d} \frac{1}{L k_j^2} & \text{as } \|\mathbf{k}\|_2 \to \infty \end{cases}$
- **Allowed wavevectors:**
  $\mathbb{A}_{\mathbf{L}} = \{(k_1, \cdots, k_d) \in (\mathbb{R}^d)^*, \exists j \in \{1, \cdots, d\}, n \in \mathbb{Z}^* \text{ s.t. } k_j = \frac{2\pi n}{L}\}$

Scattering intensity estimator

- **1** Estimator:

$$\widehat{S}_{\mathrm{SI}}(\mathbf{k}) = \frac{1}{\rho|W|} \left| \sum_{\mathbf{x}\in\mathcal{X}\cap W} e^{-i\langle \mathbf{k},\mathbf{x}\rangle} \right|^2$$

  2 Allowed wavevectors:
  $\mathbb{A}_{\mathbf{L}} = \left\{(k_1, \cdots, k_d) \in (\mathbb{R}^d)^*, \exists j \in \{1, \cdots, d\}, n \in \mathbb{Z}^* \text{ s.t. } k_j = \frac{2\pi n}{L}\right\}.$

- **Formulation in the literature**:

  1 Estimator:

$$\widehat{S}_{\mathrm{SI,s}}(\mathbf{k}) \triangleq \frac{1}{N} \left| \sum_{j=1}^{N} e^{-i\langle \mathbf{k},\mathbf{x}_j\rangle} \right|^2$$

  2 Allowed wavevectors:
  $\mathbb{A}_{\mathbf{L}}^{res} = \left\{\left(\frac{2\pi n_1}{L}, \cdots, \frac{2\pi n_d}{L}\right) \text{ with, } \mathbf{n} = (n_1, \cdots, n_d) \in \mathbb{Z}^d \setminus \{\mathbf{0}\}\right\}.$

Preprint: D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey *On estimating the structure factor of a point process, with applications to hyperuniformity, 2022.*

Tapered estimator

General case

- Tapered estimator:

$$S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\underbrace{\Big[\frac{1}{\rho}\Big| \sum_{j=1}^{N} t(\mathbf{x}_j, W) e^{-i\langle \mathbf{k}, \mathbf{x}_j\rangle} \Big|^2 \Big]}_{\widehat{S}_{\mathrm{T}}(t,\mathbf{k})} - \underbrace{\rho\,|\mathcal{F}(t)(\mathbf{k}, W)|^2}_{\epsilon_t(\mathbf{k},\mathbf{L})}.$$

- Debiased tapered estimator:
  1. Directly debiased:
  $$\widehat{S}_{\mathrm{DDT}}(t,\mathbf{k}) \triangleq \frac{1}{\rho}\left| \sum_{j=1}^{N} t(\mathbf{x}_j, W) e^{-i\langle \mathbf{k}, \mathbf{x}_j\rangle} - \rho\mathcal{F}(t)(\mathbf{k}, W)\right|^2$$
  2. Undirectly debiased:
  $$\widehat{S}_{\mathrm{UDT}}(t,\mathbf{k}) \triangleq \frac{1}{\rho}\left| \sum_{j=1}^{N} t(\mathbf{x}_j, W) e^{-i\langle \mathbf{k}, \mathbf{x}_j\rangle} \right|^2 - \rho\,|\mathcal{F}(t)(\mathbf{k}, W)|^2$$

Preprint: T. Rajala and S. C. Olhede and D. John Murrell *Spectral estimation for spatial point patterns, 2020.*

Multitapered estimator

$$\widehat{S}_{\mathrm{T}}(t,\mathbf{k}) = \frac{1}{\rho}\Big|\sum_{j=1}^{N} t(\mathbf{x}_j, W)e^{-i\langle \mathbf{k},\mathbf{x}_j\rangle}\Big|^2$$

More generally,

- Family of orthogonal tapers: $(t_q)_{q=1}^{P}$
- Multitapered estimator:

$$\widehat{S}_{\mathrm{MT}}((t_q)_{q=1}^{P},\mathbf{k}) = \frac{1}{P}\sum_{q=1}^{P}\widehat{S}_{\mathrm{T}}(t_q,\mathbf{k}).$$

Preprint: T. Rajala and S. C. Olhede and D. John Murrell, *Spectral estimation for spatial point patterns, 2020.*

Estimators assuming stationarity and isotropy

- Structure factor: $S(\mathbf{k}) = 1 + \rho \mathcal{F}(g-1)(\mathbf{k})$
- Isotropic case:

$$S(k) = 1 + \rho \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty (g(r)-1) r^{d/2} J_{d/2-1}(kr)\, dr.$$

Estimators assuming stationarity and isotropy

- Isotropic case:

$$S(k) = 1 + \rho \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty (g(r) - 1) r^{d/2} J_{d/2-1}(kr) \, dr.$$

- Ball window : $W = B(0, R)$
- Radial Taper: $t_0(\mathbf{x}, W) = \frac{1}{\sqrt{|W|}} \mathbb{1}_W(\mathbf{x})$

Estimators assuming stationarity and isotropy

- Isotropic case:

$$S(k) = 1 + \rho \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty (g(r) - 1) r^{d/2} J_{d/2-1}(kr) \, dr.$$

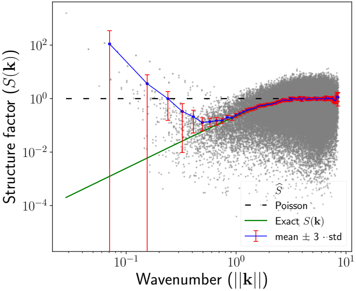
- Ball window : $W = B(0, R)$
- Radial Taper: $t_0(\mathbf{x}, W) = \frac{1}{\sqrt{|W|}} \mathbb{1}_W(\mathbf{x})$
- Bartlett's isotropic estimator

$$\widehat{S}_{\mathrm{BI}}(k) = 1 + \frac{(2\pi)^{\frac{d}{2}}}{\rho |W| \omega_{d-1}} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \frac{J_{d/2-1}(k \|\mathbf{x}_i - \mathbf{x}_j\|_2)}{(k \|\mathbf{x}_i - \mathbf{x}_j\|_2)^{d/2-1}}$$

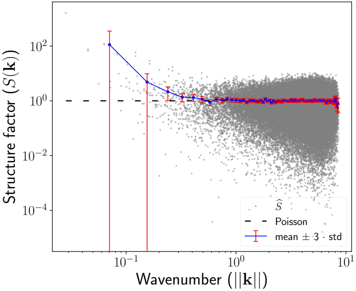
- Allowed wavenumbers: $\mathbb{A}_R = \left\{ \frac{x}{R} \in \mathbb{R}, \text{ s.t. } J_{d/2}(x) = 0 \right\}$

Scattering intensity

$$\widehat{S}_{\mathrm{SI}}(\mathbf{k}) = \frac{1}{\rho|W|} \left| \sum_{\mathbf{x} \in \mathcal{X} \cap W} e^{-i\langle \mathbf{k}, \mathbf{x} \rangle} \right|^2$$



Ginibre



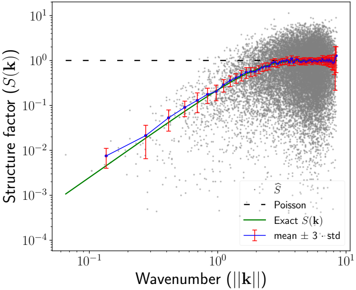
Poisson

Figure: On arbitrary wavevectors $\mathbf{k}$

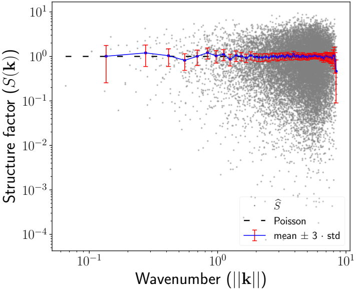
https://github.com/For-a-few-DPPs-more/structure-factor

Scattering intensity

$$\widehat{S}_{\mathrm{SI}}(\mathbf{k}) = \frac{1}{\rho|W|} \left|\sum_{\mathbf{x}\in\mathcal{X}\cap W} e^{-i\langle \mathbf{k},\mathbf{x}\rangle}\right|^2$$



Ginibre



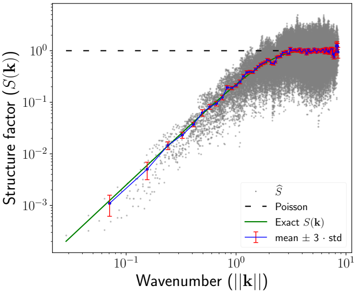
Poisson

Figure: On allowed wavevectors **k**

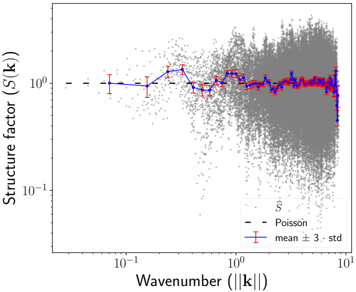
https://github.com/For-a-few-DPPs-more/structure-factor

Multitapered estimator

$$\widehat{S}_{\mathrm{DDT}}(t, \mathbf{k}) \triangleq \frac{1}{\rho} \left| \sum_{j=1}^{N} t(\mathbf{x}_j, W) e^{-i\langle \mathbf{k}, \mathbf{x}_j \rangle} - \rho \mathcal{F}(t)(\mathbf{k}, W) \right|^2$$



Ginibre

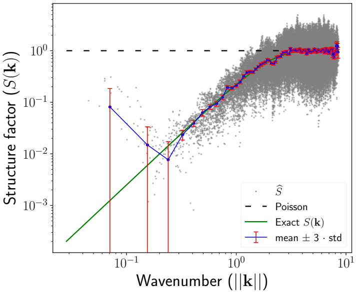


Poisson

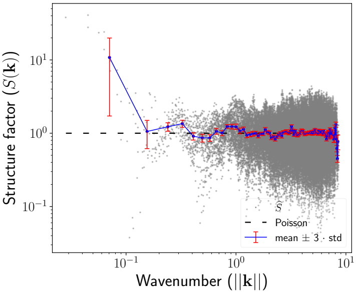
https://github.com/For-a-few-DPPs-more/structure-factor

Multitapered estimator

$$\widehat{S}_{\mathrm{UDT}}(t, \mathbf{k}) \triangleq \frac{1}{\rho} \left| \sum_{j=1}^{N} t(\mathbf{x}_j, W) e^{-i\langle \mathbf{k}, \mathbf{x}_j \rangle} \right|^2 - \rho \left| \mathcal{F}(t)(\mathbf{k}, W) \right|^2$$



Ginibre

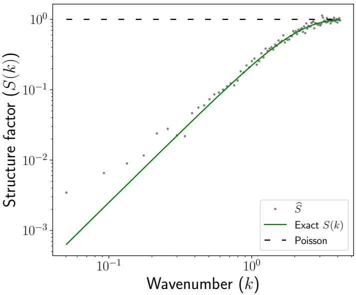


Poisson

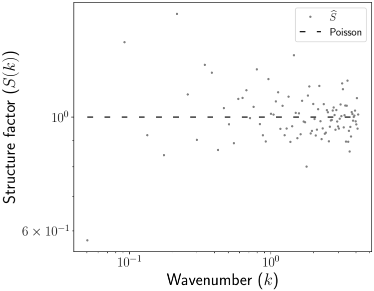
https://github.com/For-a-few-DPPs-more/structure-factor

Bartlett's isotropic estimator

$$\widehat{S}_{\mathrm{BI}}(k) \triangleq 1 + \frac{(2\pi)^{\frac{d}{2}}}{\rho|W|\omega_{d-1}} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} \frac{J_{d/2-1}(k\|\mathbf{x}_i - \mathbf{x}_j\|_2)}{(k\|\mathbf{x}_i - \mathbf{x}_j\|_2)^{d/2-1}}$$



Ginibre



Poisson

Figure: On allowed wavenumbers k

https://github.com/For-a-few-DPPs-more/structure-factor

Integrated mean square error

Sample integrated variance and MSE across 50 samples

Estimators	$\widehat{\mathrm{iVar}}$	$\mathrm{CI}[\widehat{\mathrm{iMSE}}]$	$\widehat{\mathrm{iVar}}$	$\mathrm{CI}[\widehat{\mathrm{iMSE}}]$
$\widehat{S}_{\mathrm{SI}}(2\pi\mathbf{n}/L)$	0.32	0.32 ± 0.02	1.31	1.34 ± 0.06
$\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$	0.08	$\mathbf{0.08} \pm 0.007$	0.37	$\mathbf{0.38} \pm 0.02$
$\widehat{S}_{\mathrm{BI}}(\frac{x}{R})$	3.9×10^{-3}	$\mathbf{4.0 \times 10^{-3}} \pm 3 \times 10^{-4}$	0.057	$\mathbf{0.058} \pm 9 \times 10^{-3}$
	Ginibre		Poisson	

Hyperuniformity diagnostics

Effective hyperuniformity

$$\mathcal{X} \text{ is effectively hyperuniform } \iff H = \frac{\widehat{S}(0)}{\widehat{S}(k_{peak})} \leq 10^{-3},$$

- $\widehat{S}(0)$ is a linear extrapolation of the estimated structure factor $\widehat{S}$ in $k = 0$.
- k_{peak} is the location of the first dominant peak value of $\widehat{S}$.

S. Torquato, *Hyperuniform States of Matter, 2018.*

- Need: Check if $S(\mathbf{0}) = 0$
- Problem: We don't have an unbiased estimator of $S(\mathbf{0})$
- Idea: Use biased estimators to construct an unbiased estimator

Coupled sum estimator

Need: Check if $S(\mathbf{0}) = 0$

- $(Y_m)_m$ a sequence of approximations of a r.v. Y

$$Z_m = \sum_{j=1}^{m \wedge M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}, \quad m \geq 1$$

- M is an $\mathbb{N}$-r.v. such that $\mathbb{P}(M \geq j) > 0$ for all j, and $Y_0 = 0$

C. Rhee and P.W. Glynn, *Unbiased estimation with square root convergence for SDE models, 2015*

Coupled sum estimator

Need: Check if $S(\mathbf{0}) = 0$

- $(Y_m)_m$ a sequence of approximations of a r.v. Y

$$Z_m = \sum_{j=1}^{m \wedge M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}, \quad m \geq 1$$

- M is an $\mathbb{N}$-r.v. such that $\mathbb{P}(M \geq j) > 0$ for all j, and $Y_0 = 0$
- $\mathbb{E}[Z_m] = \mathbb{E}[Y_m]$ and $Z_m \xrightarrow[m\to\infty]{\text{a.s.}} Z := \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$.
- $Y_m \xrightarrow[m\to\infty]{L^2} Y$ + some hypotheses $\Longrightarrow \mathbb{E}[Z] = \mathbb{E}[Y]$

C. Rhee and P.W. Glynn, *Unbiased estimation with square root convergence for SDE models, 2015*

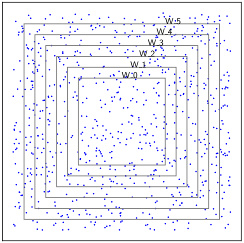
Coupled sum estimator

Need: Check if $S(\mathbf{0}) = 0$

- $(Y_m)_m$ a sequence of approximations of a r.v. Y

$$Z_m = \sum_{j=1}^{m \wedge M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}, \quad m \geq 1$$

- M is an $\mathbb{N}$-r.v. such that $\mathbb{P}(M \geq j) > 0$ for all j, and $Y_0 = 0$
- Consider an increasing sequence of sets $(\mathcal{X} \cap W_m)_{m \geq 1}$, with $W_\infty = \mathbb{R}^d$



Coupled sum estimator

Need: Check if $S(\mathbf{0}) = 0$

- $(Y_m)_m$ a sequence of approximations of a r.v. Y

$$Z_m = \sum_{j=1}^{m \wedge M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}, \quad m \geq 1$$

- M is an $\mathbb{N}$-r.v. such that $\mathbb{P}(M \geq j) > 0$ for all j, and $Y_0 = 0$
- Consider an increasing sequence of sets $(\mathcal{X} \cap W_m)_{m \geq 1}$, with $W_\infty = \mathbb{R}^d$
- Take $Y_m = 1 \wedge \widehat{S}_m(\mathbf{k}_m^{\min})$ and $\mathbf{k}_m^{\min} \xrightarrow[m \to \infty]{} \mathbf{0}$

Multiscale hyperuniformity test

Need: Check if $S(\mathbf{0}) = 0$

- Take $Y_m = 1 \wedge \widehat{S}_m(\mathbf{k}_m^{\min})$, $\mathbf{k}_m^{\min} \xrightarrow[m\to\infty]{} \mathbf{0}$, $\{W_m\}_m \uparrow$, and $W_\infty = \mathbb{R}^d$
- $Z = \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$
- M is an $\mathbb{N}$-r.v. such that $\mathbb{P}(M \geq j) > 0$ for all j, and $Y_0 = 0$

Proposition

Assume that $M \in L^p$ for some $p \geq 1$. Then $Z \in L^p$ and $Z_m \to Z$ in L^p. Moreover,

1. *If $\mathcal{X}$ is hyperuniform, then $\mathbb{E}[Z] = 0$.*
2. *If $\mathcal{X}$ is not hyperuniform and $\sup_m \mathbb{E}[\widehat{S}_m^2(\mathbf{k}_m^{\min})] < \infty$, then $\mathbb{E}[Z] \neq 0$.*

Preprint: D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey *On estimating the structure factor of a point process, with applications to hyperuniformity, 2022.*

Multiscale hyperuniformity test

Need: Check if $S(\mathbf{0}) = 0 \iff \mathbb{E}[Z] = 0$, with $Z = \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$

Test:

- M a Poisson r.v. of parameter λ
- i.i.d. pairs $(\mathcal{X}_a, M_a)_{a=1}^{A}$ of realizations of $(\mathcal{X}, M)$
- Asymptotic confidence interval $CI[\mathbb{E}[Z]]$ of level ζ

$$CI[\mathbb{E}[Z]] = \left[\bar{Z}_A - z\bar{\sigma}_A A^{-1/2}, \bar{Z}_A + z\bar{\sigma}_A A^{-1/2}\right]$$

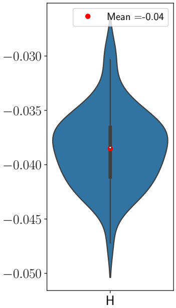
with $\mathbb{P}(-z < \mathcal{N}(0,1) < z) = \zeta$

- Assessing whether 0 lies in $CI[\mathbb{E}[Z]]$

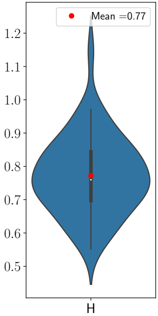
Preprint: D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey *On estimating the structure factor of a point process, with applications to hyperuniformity, 2022.*

Effective hyperuniformity

$$\mathcal{X} \text{ is effectively hyperuniform} \iff H = \widehat{S}(0)/\widehat{S}(k_{peak}) \leq 10^{-3}$$



Ginibre



Poisson

H for 50 samples from Ginibre and Poisson using Bartlett's isotropic estimator

https://github.com/For-a-few-DPPs-more/structure-factor

Multiscale hyperuniformity test

$$\mathcal{X} \text{ is hyperuniform} \iff \mathbb{E}[Z] = \mathbb{E}[\sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}] = 0$$

Table: Multiscale hyperuniformity test with 99% confidence level

	$\bar{Z}_{50}$	$CI[\mathbb{E}[Z]]$	$\bar{Z}_{50}$	$CI[\mathbb{E}[Z]]$
Ginibre	0.015	$[-0.021, 0.051]$	0.007	$[-0.003, 0.011]$
Poisson	0.832	$[0.444, 1.220]$	0.781	$[0.560, 1.001]$
$\widehat{S}$	$\widehat{S}_{\mathrm{SI}}$		$\widehat{S}_{\mathrm{BI}}$	

Multiscale hyperuniformity test

$$\mathcal{X} \text{ is hyperuniform} \iff \mathbb{E}[Z] = \mathbb{E}[\sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}] = 0$$

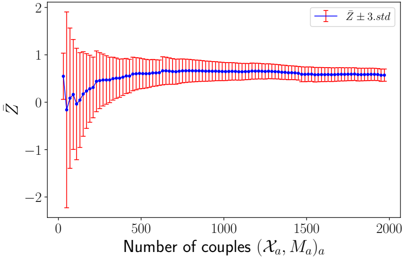
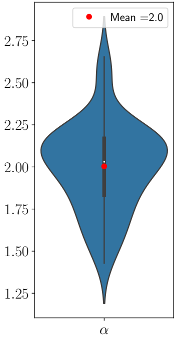


Figure: $CI[\mathbb{E}[\bar{Z}]]$ for a Poisson point process with the scattering intensity, as a function of the number of realizations of Z.

Hyperuniformity class

$\mathcal{X}$ is hyperuniform with $|S(\mathbf{k})| \sim c\|\mathbf{k}\|_2^\alpha$ in the neighborhood of zero



α of 50 samples from Ginibre using Bartlett's isotropic estimator

https://github.com/For-a-few-DPPs-more/structure-factor

Code availability

Python Package

1. Open-source Python toolbox called structure_factor[1]
2. Available on Github and PyPI [2]
3. Detailed documentation [3]
4. Jupyter notebook tutorial [4]

[1] https://github.com/For-a-few-DPPs-more/structure-factor

[2] https://pypi.org/project/structure-factor/

[3] https://for-a-few-dpps-more.github.io/structure-factor/

[4] https://github.com/For-a-few-DPPs-more/structure-factor/tree/main/notebooks

Conclusion

Conclusion

- Estimators of the structure factor, properties and performances
- Available diagnostics of hyperuniformity and limitations
- The first statistical test of hyperuniformity and limitations
- Python toolbox `structure-factor`

THANK YOU

Github

Documentation

Preprint

Github: `https://github.com/For-a-few-DPPs-more/structure-factor`

Documentation: `https://for-a-few-dpps-more.github.io/structure-factor/`

Preprint: D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey *On estimating the structure factor of a point process, with applications to hyperuniformity, 2022.*