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

1 Definition

2 Estimation of the structure factor

3 Hyperuniformity test

4 Numerical experiment

5 Code availability

Hyperuniformity using the structure factor

Structure Factor

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

- Structure factor S

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

Structure Factor

- Structure factor S

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

- Pair correlation function g

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

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

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

- $\mathcal{X}$ is hyperuniform iff

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

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

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

Hyperuniformity class

- $\mathcal{X}$ 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. Coste. *Order, Fluctuations, Rigidities*, 2021.

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

Estimation of the structure factor

Scattering intenisty

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

Scattering intenisty

- $S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k})$
- Box window : $W = [-L/2, L/2]^d$

Scattering intenisty

- $S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k})$
- Box window : $W = [-L/2, L/2]^d$
- $S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\left[\frac{1}{\rho|W|}\left|\sum_{\mathbf{x}\in\mathcal{X}\cap W} e^{-i\langle\mathbf{k},\mathbf{x}\rangle}\right|^2\right] - \rho\left(\prod_{j=1}^{d} \frac{\sin(k_j L/2)}{k_j\sqrt{L}/2}\right)^2$

Scattering intenisty

- $S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k})$
- Box window : $W = [-L/2, L/2]^d$
- $S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\Big[\frac{1}{\rho|W|}\Big|\sum_{\mathbf{x}\in\mathcal{X}\cap W} e^{-i\langle\mathbf{k},\mathbf{x}\rangle}\Big|^2\Big] - \underbrace{\rho\Big(\prod_{j=1}^{d}\frac{\sin(k_j L/2)}{k_j\sqrt{L}/2}\Big)^2}_{\epsilon_0(\mathbf{k},\mathbf{L})}$
- $\epsilon_0(\mathbf{k},\mathbf{L}) \leq \begin{cases} 0 & \text{if } \exists j \text{ s.t. } k_j = \frac{2\pi n}{L} \text{ with } n \in \mathbb{Z}^* \\ \rho L^d & \text{as } \|\mathbf{k}\|_2 \to 0 \\ 2^{2d}\prod_{j=1}^{d}\frac{1}{Lk_j^2} & \text{as } \|\mathbf{k}\|_2 \to \infty \end{cases}$

Scattering intenisty

- $S(\mathbf{k}) = 1 + \rho \mathcal{F}(g-1)(\mathbf{k})$
- Box window : $W = [-L/2, L/2]^d$
- $S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\Big[\underbrace{\frac{1}{\rho|W|} \Big| \sum_{\mathbf{x}\in\mathcal{X}\cap W} e^{-i\langle \mathbf{k},\mathbf{x}\rangle} \Big|^2}_{\widehat{S}_{\mathrm{SI}}(\mathbf{k})} \Big] - \rho \underbrace{\Big(\prod_{j=1}^{d} \frac{\sin(k_j L/2)}{k_j \sqrt{L}/2} \Big)^2}_{\epsilon_0(\mathbf{k},\mathbf{L})}$
- **Allowed wavevectors:**
  $\mathbb{A}_{\mathbf{L}} = \{(k_1, \cdots, k_d) \in (\mathbb{R}^d)^*, \exists j \in \{1, \cdots, d\}, n \in \mathbb{Z}^* \text{ s.t. } k_j = \frac{2\pi n}{L}\}$
- Minimum wavenumber: $\|\mathbf{k}_{min}\|_2 = \frac{2\pi}{L}$

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

Scattering intenisty

- $S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k})$
- Box window : $W = [-L/2, L/2]^d$
- $$S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\Big[\underbrace{\frac{1}{\rho|W|}\Big|\sum_{\mathbf{x}\in\mathcal{X}\cap W} e^{-i\langle \mathbf{k},\mathbf{x}\rangle}\Big|^2}_{\widehat{S}_{\mathrm{SI}}(\mathbf{k})}\Big] - \rho\underbrace{\Big(\prod_{j=1}^{d}\frac{\sin(k_j L/2)}{k_j\sqrt{L}/2}\Big)^2}_{\epsilon_0(\mathbf{k},\mathbf{L})}$$
- **Allowed wavevectors:** $\mathbb{A}_{\mathbf{L}} = \{(k_1, \cdots, k_d) \in (\mathbb{R}^d)^*, \exists j \in \{1, \cdots, d\}, n \in \mathbb{Z}^* \text{ s.t. } k_j = \frac{2\pi n}{L}\}$
- Minimum wavenumber: $\|\mathbf{k}_{min}\|_2 = \frac{2\pi}{L}$

T. A. Rajala, S. C. Olhede, and D. J. Murrell. *What is the fourier transform of a spatial point process?* 2020.

Isotropic case

Bartlett's isotropic estimator

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

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

Bartlett's isotropic estimator

- $S(k) = 1 + \rho \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty (g(r) - 1) r^{d/2} J_{d/2-1}(kr)\, dr.$
- Ball window : $W = B(0, R)$

Bartlett's isotropic estimator

- $S(k) = 1 + \rho \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty (g(r) - 1) r^{d/2} J_{d/2-1}(kr)\, dr.$
- Ball window : $W = B(0, R)$
- $S(k) = \lim_{R\to\infty} \mathbb{E}\left[1 + \frac{(2\pi)^{\frac{d}{2}}}{\rho |W| \omega_{d-1}} \sum_{\mathbf{x},\mathbf{y}\in\mathcal{X}\cap W}^{\neq} \frac{J_{d/2-1}(k\|\mathbf{x}-\mathbf{y}\|_2)}{(k\|\mathbf{x}-\mathbf{y}\|_2)^{d/2-1}}\right] + \epsilon_1(k, R)$
- $\epsilon_1(k, R) = \begin{cases} 0 & \text{if } k = \frac{x}{R} \text{ with } J_{d/2}(x) = 0, \\ O(R^d) & \text{as } k \to 0, \\ O\left(\frac{1}{k^d (Rk)^{2/3}}\right) & \text{as } k \to \infty. \end{cases}$

Bartlett's isotropic estimator

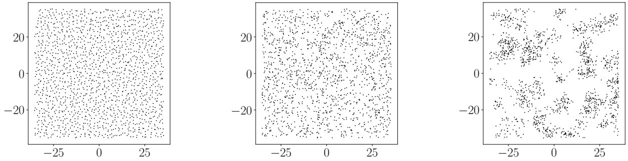
- $S(k) = 1 + \rho \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty (g(r) - 1) r^{d/2} J_{d/2-1}(kr)\, dr.$
- Ball window : $W = B(0, R)$
- $S(k) =$

$$\lim_{R\to\infty} \mathbb{E}\Big[\underbrace{1 + \frac{(2\pi)^{\frac{d}{2}}}{\rho|W|\omega_{d-1}} \sum_{\mathbf{x},\mathbf{y}\in\mathcal{X}\cap W}^{\neq} \frac{J_{d/2-1}(k\|\mathbf{x}-\mathbf{y}\|_2)}{(k\|\mathbf{x}-\mathbf{y}\|_2)^{d/2-1}}}_{\widehat{S}_{\mathrm{BI}}(k)} \Big] + \epsilon_1(k, R)$$

- Allowed wavenumbers: $\mathbb{A}_R = \left\{ k = \frac{x}{R} \in \mathbb{R}^*, \text{ s.t. } J_{d/2}(x) = 0 \right\}$
- Minimum wavenumber: $k_{min} = \frac{x_0}{R}$

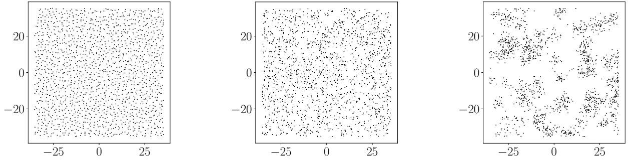
Preprint: D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey. *On estimating the structure factor of a point process, with applications to hyperuniformity, 2022.*

Comparison of the estimators



(a) Ginibre $S(0) = 0$ (b) Poisson $S(0) = 1$ (c) Thomas $S(0) > 1$

Comparison of the estimators



(a) Ginibre $S(0) = 0$ (b) Poisson $S(0) = 1$ (c) Thomas $S(0) > 1$

Table: Sample integrated variance and MSE

Estimators	$\widehat{\mathrm{iVar}}$	$\mathrm{CI}[\widehat{\mathrm{iMSE}}]$	$\widehat{\mathrm{iVar}}$	$\mathrm{CI}[\widehat{\mathrm{iMSE}}]$	$\widehat{\mathrm{iVar}}$	$\mathrm{CI}[\widehat{\mathrm{iMSE}}]$
$\widehat{S}_{\mathrm{SI}}$	0.32	0.32 ± 0.02	1.31	1.34 ± 0.06	69.51	70.71 ± 17.95
$\widehat{S}_{\mathrm{BI}}$	3.9×10^{-3}	$\mathbf{4.0 \times 10^{-3}} \pm 3 \times 10^{-4}$	0.057	$\mathbf{0.058} \pm 9 \times 10^{-3}$	11.25	$\mathbf{11.65} \pm 4.71$
	Ginibre		Poisson		Thomas	

Multiscale hyperuniformity test

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

- Need: Check if $S(\mathbf{0}) = 0$
- Problem: We don't have an unbiased estimator of $S(\mathbf{0})$
- On allowed wavevectors we have:
  $S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\left[\widehat{S}_{\mathrm{SI}}(\mathbf{k})\right]$, $S(k) = \lim_{R\to\infty} \mathbb{E}\left[\widehat{S}_{\mathrm{BI}}(k)\right]$
- How one can construct unbiased estimators when only biased estimators are available?

Coupled sum estimator

- Need: estimate $\mathbb{E}[Y] := \bar{Y}$
- Able to generate a sequence of r.v. $(Y_m)_m$ s.t. $\bar{Y} = \lim_{m\to\infty} \mathbb{E}[Y_m]$

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

Coupled sum estimator

- Need: estimate $\mathbb{E}[Y] := \bar{Y}$
- Able to generate a sequence of r.v. $(Y_m)_m$ s.t. $\bar{Y} = \lim_{m\to\infty} \mathbb{E}[Y_m]$
- Consider an $\mathbb{N}$-r.v. M s.t., $\mathbb{P}(M \geq j) > 0$ for all j, and let $Y_0 = 0$

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

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

Coupled sum estimator

- Need: estimate $\mathbb{E}[Y] := \bar{Y}$
- Able to generate a sequence of r.v. $(Y_m)_m$ s.t. $\bar{Y} = \lim_{m\to\infty} \mathbb{E}[Y_m]$
- Consider an $\mathbb{N}$-r.v. M s.t., $\mathbb{P}(M \geq j) > 0$ for all j, and let $Y_0 = 0$

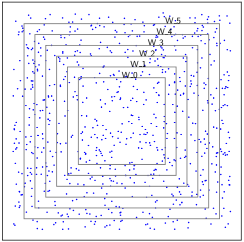
$$Z_m = \sum_{j=1}^{m\wedge M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}, \quad m \geq 1$$

- $\mathbb{E}[Z_m] = \mathbb{E}[Y_m]$ and $Z_m \xrightarrow[m\to\infty]{\text{a.s.}} Z := \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$.
- If $Y_m \xrightarrow[m\to\infty]{L^2} Y$ + some hypotheses, then $\mathbb{E}[Z] = \bar{Y}$

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

Multiscale hyperuniformity test

- Consider an increasing sequence of sets $(\mathcal{X} \cap W_m)_{m \geq 1}$, with $\{W_m\}_m \uparrow$ and $W_\infty = \mathbb{R}^d$
- $\mathbf{k}_m^{\min}$ minimum allowed wavevector associated to W_m, $\mathbf{k}_m^{\min} \xrightarrow[m \to \infty]{} \mathbf{0}$



Multiscale hyperuniformity test

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

Multiscale hyperuniformity test

- Consider an increasing sequence of sets $(\mathcal{X} \cap W_m)_{m\geq 1}$, with $\{W_m\}_m \uparrow$ and $W_\infty = \mathbb{R}^d$
- $\mathbf{k}_m^{\min}$ minimum allowed wavevector associated to W_m, $\mathbf{k}_m^{\min} \xrightarrow[m\to\infty]{} \mathbf{0}$
- Take $Y_m = 1 \wedge \widehat{S}_m(\mathbf{k}_m^{\min})$
- $Z = \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$ with 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 $\mathbb{E}[Z] = 0$, with $Z = \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$

Test:

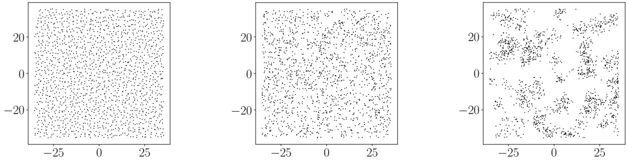
- M a Poisson r.v. of parameter λ
- i.i.d. pairs $(\mathcal{X}_a, M_a)_{a=1}^{A}$ of realizations of $(\mathcal{X}, M)$
- Asymptotic confidence interval $CI[\mathbb{E}[Z]]$ of level ζ

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

  with $\mathbb{P}(-z < \mathcal{N}(0,1) < z) = \zeta$
- Assessing whether 0 lies in $CI[\mathbb{E}[Z]]$

Point processes

Numerical experiment



(a) Ginibre $S(0) = 0$ (b) Poisson $S(0) = 1$ (c) Thomas $S(0) > 1$

Multiscale hyperuniformity test

$$\mathcal{X} \text{ is hyperuniform} \iff \mathbb{E}[Z] = 0$$

Table: Multiscale hyperuniformity test

	$\bar{Z}_{50}$	$CI[\mathbb{E}[Z]]$	$\bar{Z}_{50}$	$CI[\mathbb{E}[Z]]$
Ginibre	0.015	$[-0.021, 0.051]$	0.007	$[-0.003, 0.011]$
Poisson	0.832	$[0.444, 1.220]$	0.781	$[0.560, 1.001]$
Thomas	0.928	$[0.788, 1.068]$	1	$[0.999, 1]$
$\widehat{S}$	$\widehat{S}_{\mathrm{SI}}$		$\widehat{S}_{\mathrm{BI}}$	

Multiscale hyperuniformity test

$$\mathcal{X} \text{ is hyperuniform} \iff \mathbb{E}[Z] = 0$$

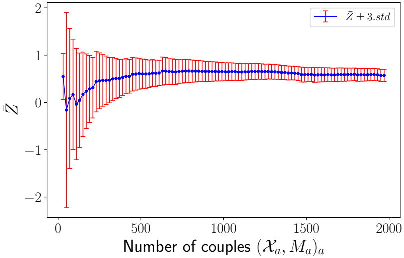


Figure: $CI[\mathbb{E}[\bar{Z}]]$ for a Poisson point process with the scattering intensity, as a function of the number of realizations of Z.

Thinning HU process

- $\mathcal{X}$ a point process of intensity ρ
- $\mathcal{X}_p$ an independent p-thinning with $p \in (0, 1)$

J. Kim and S. Torquato. *Effect of imperfections on the hyperuniformity of many-body systems*, 2018.

M. A. Klatt, G. Last, and N. Henze. *A genuine test for hyperuniformity*, 2022.

Thinning HU process

- $\mathcal{X}$ a point process of intensity ρ
- $\mathcal{X}_p$ an independent p-thinning with $p \in (0, 1)$
- Intensity: $\rho_p = p \times \rho$

Thinning HU process

- $\mathcal{X}$ a point process of intensity ρ
- $\mathcal{X}_p$ an independent p-thinning with $p \in (0, 1)$
- Intensity: $\rho_p = p \times \rho$
- Pair correlation function: $g_p(\mathbf{r}) = g(\mathbf{r})$

Thinning HU process

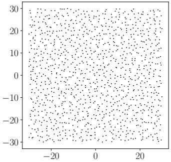
- $\mathcal{X}$ a point process of intensity ρ
- $\mathcal{X}_p$ an independent p-thinning with $p \in (0, 1)$
- Intensity: $\rho_p = p \times \rho$
- Pair correlation function: $g_p(\mathbf{r}) = g(\mathbf{r})$
- Structure factor: $S_p(\mathbf{k}) = pS(\mathbf{k}) + 1 - p$

Thinning HU process

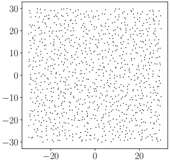
- $\mathcal{X}$ a point process of intensity ρ
- $\mathcal{X}_p$ an independent p-thinning with $p \in (0, 1)$
- Intensity: $\rho_p = p \times \rho$
- Pair correlation function: $g_p(\mathbf{r}) = g(\mathbf{r})$
- Structure factor: $S_p(\mathbf{k}) = pS(\mathbf{k}) + 1 - p$
- $\mathcal{X}$ is hyperuniform $\implies S_p(\mathbf{0}) = 1 - p$

Multiscale hyperuniformity test

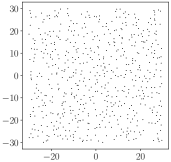
Numerical experiment



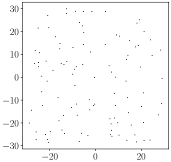
Ginibre, $S(0) = 0$



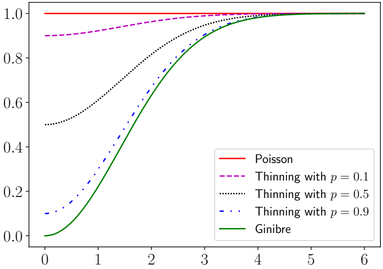
$p = 0.9,\ S(0) = 0.1$



$p = 0.5,\ S(0) = 0.5$



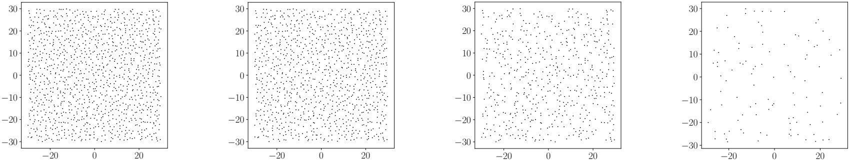
$p = 0.1,\ S(0) = 0.9$



Structure factor

Multiscale hyperuniformity test

Numerical experiment



Ginibre, $S(0) = 0$ $\quad$ $p = 0.9,\ S(0) = 0.1$ $\quad$ $p = 0.5,\ S(0) = 0.5$ $\quad$ $p = 0.1,\ S(0) = 0.9$

Table: Multiscale hyperuniformity test obtained using $\widehat{S}_{\mathrm{BI}}$ on the thinned Ginibre process.

	$\bar{Z}_A$	$CI[\mathbb{E}[Z]]$
Ginibre	0.0057	$[-0.0042, 0.0156]$
Thinning $p = 0.9,\ S(\mathbf{0}) = 0.1$	0.0865	$[0.0411, 0.1318]$
Thinning $p = 0.5,\ S(\mathbf{0}) = 0.5$	0.5722	$[0.4227, 0.7217]$
Thinning $p = 0.1,\ S(\mathbf{0}) = 0.9$	0.611	$[0.2082, 1.0137]$

Properties and limitations

- Validity for any class of hyperuniform point process ☺

Properties and limitations

- Validity for any class of hyperuniform point process ☺
- Code availability 😉

Properties and limitations

- Validity for any class of hyperuniform point process ☺
- Code availability 😉
- Need many realisations of the point process ☹

Code availability

Python Package

Code availability

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
- Statistical test of hyperuniformity
- Python toolbox `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.*

THANK YOU

Code availability

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.*