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

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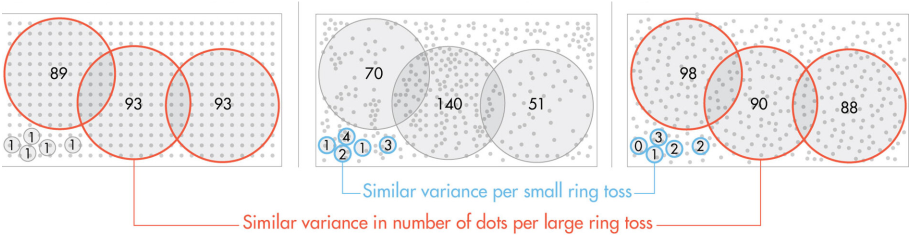
Hyperuniformity

Hyperuniformity

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.

Hyperuniformity using the 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 of $\mathcal{X}$

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

- $\mathcal{X}$ is hyperuniform iff

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

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

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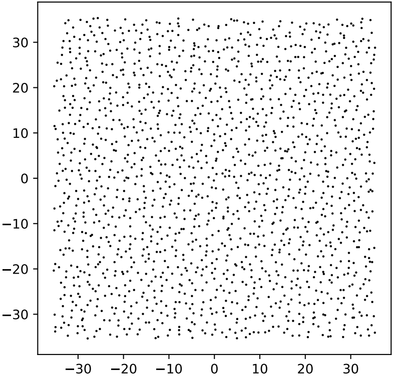
Example: Ginibre point process

- $\rho_{\text{Ginibre}} = 1/\pi$
- $S_{\text{Ginibre}}(k) = 1 - \exp(-k^2/4)$
- $S(0) = 0$



Multiscale hyperuniformity test

- Given: Realizations $\{\mathcal{X}_W\}$ of $\mathcal{X}$ in the window W of lenghtside L (e.g., $W = [-L/2, L/2]^d$)
- Need: Check if $S(\mathbf{0}) = 0$ using $\{\mathcal{X}_W\}$
- Problem: We don't have an unbiased estimator of $S(\mathbf{0})$

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- How one can construct an unbiased estimator 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*.

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- Consider an $\mathbb{N}$-r.v. M s.t., $\mathbb{P}(M \geq j) > 0$ for all j, and let $Y_0 = 0$

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

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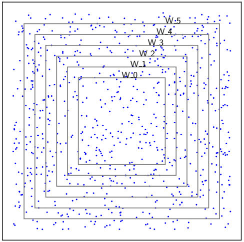
- $\mathbb{E}[Z_m] = \mathbb{E}[Y_m]$ and $Z_m \xrightarrow[m\to\infty]{\text{a.s.}} Z := \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$.
- If $Y_m \xrightarrow[m\to\infty]{L^2} Y$ + some hypotheses, then $\mathbb{E}[Z] = \bar{Y}$

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 wavevector of $\mathbb{A}_{W_m}$, $\mathbf{k}_m^{\min} \xrightarrow[m\to\infty]{} \mathbf{0}$



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- 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 $Y_0 = 0$

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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 $CI[\mathbb{E}[Z]]$

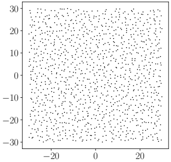
Thinning HU process

- $\mathcal{X}$ a stationary point process
- $\mathcal{X}_p$ an independent p-thinning with $p \in (0, 1)$
- Structure factor: $S_p(\mathbf{k}) = pS(\mathbf{k}) + 1 - p$
- $\mathcal{X}$ is hyperuniform $\implies S_p(\mathbf{0}) = 1 - p$

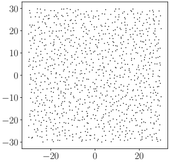
J. Kim and S. Torquato. *Effect of imperfections on the hyperuniformity of many-body systems*, 2018.

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

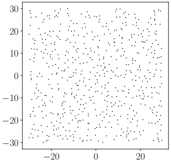
Multiscale hyperuniformity test



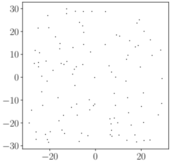
Ginibre, $S(0) = 0$



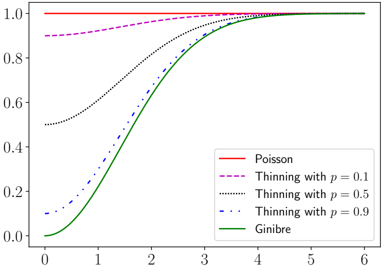
$p = 0.9$, $S(0) = 0.1$



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

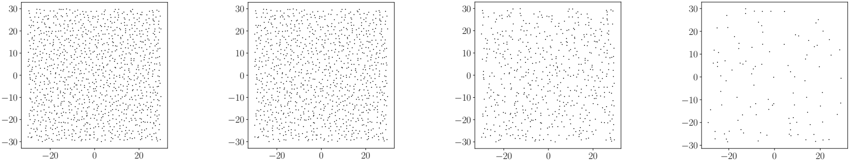


$p = 0.1$, $S(0) = 0.9$



Structure factor

Multiscale hyperuniformity test



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

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	$[0.2082, 1.0137]$

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

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- Statistical test of hyperuniformity using biased estimators of the structure factor
- Python toolbox `structure-factor`

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THANK YOU

Github

Documentation

Preprint

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

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