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

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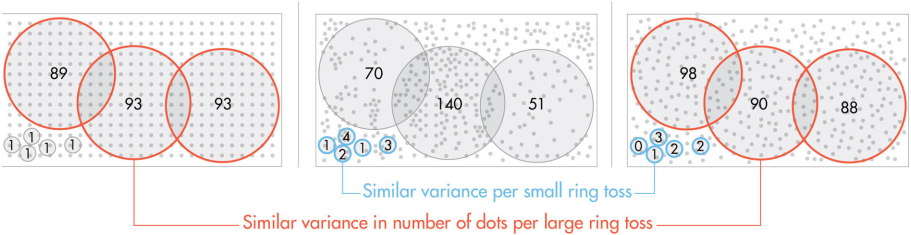
Contents

Hyperuniformity

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

- Variance:

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

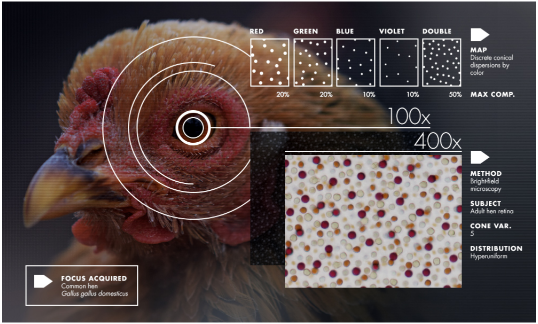


S. Torquato, *Hyperuniform States of Matter, 2018.*

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

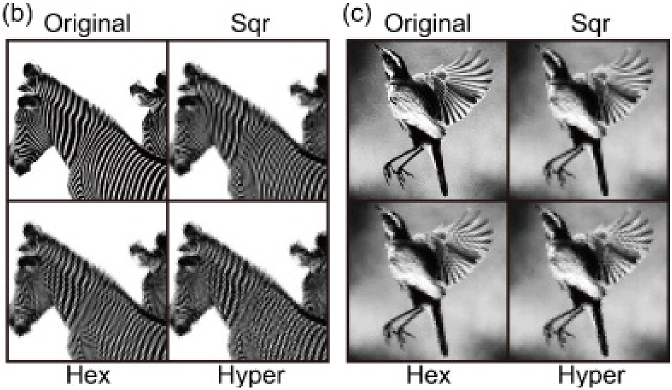
Bird's-Eye

Motivations



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



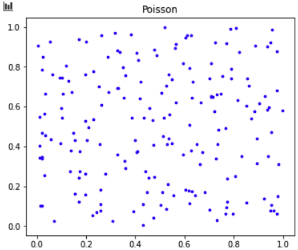
Ming-Jie Sun, Xin-Yu Zhao, and Li-Jing Li, *Imaging using hyperuniform sampling with a single-pixel camera,* 2018.

Numerical integration

- **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:** $O(1/\sqrt{N})$

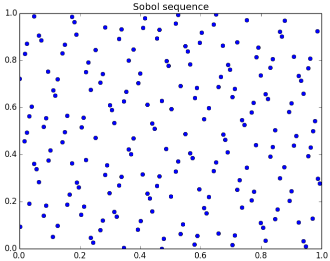


Numerical integration

- **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 $\mathcal{X}$ be a stationary point process of $\mathbb{R}^d$ 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

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- $\mathcal{X}$ is hyperuniform iff

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

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

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

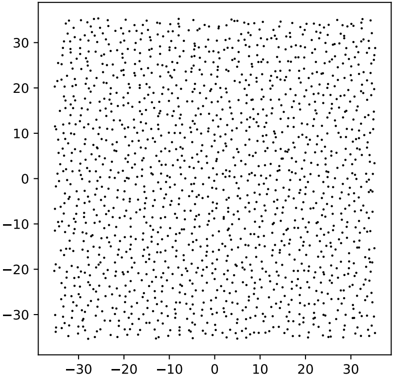
Hyperuniformity class

$\mathcal{X}$ 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. 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

Scattering intensity

$\mathcal{X}_N = \{\mathbf{x}_i\}_1^N$ a realization of a **stationary** process $\mathcal{X}$ of intensity ρ in $W = [-L/2, L/2]^d$.

- Estimator:

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

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

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

2- M.A. Klatt and G. Last and D. Yogeshwaran, *Hyperuniform and Rigid Stable Matchings, 2020.*

Idea

- **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

- **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:** $t_0(\mathbf{x}, W) = \frac{1}{\sqrt{|W|}} \mathbb{1}_W(\mathbf{x})$.
-

$$S(\mathbf{k}) = \lim_{L \to \infty} \mathbb{E}\underbrace{\left[\frac{1}{\rho|W|} \Big| \sum_{\mathbf{x} \in \mathcal{X} \cap W} e^{-i\langle \mathbf{k}, \mathbf{x} \rangle} \Big|^2 \right]}_{\widehat{S}_{\mathrm{SI}}(\mathbf{k})} - \rho \underbrace{\left(\prod_{j=1}^{d} \frac{\sin(k_j L/2)}{k_j \sqrt{L}/2} \right)^2}_{\epsilon_0(\mathbf{k}, \mathbf{L})}$$

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

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

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

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.*

Estimator assuming stationarity

- Tapered estimator:

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

- Debiased tapered estimator:
  1. Directly debiased:

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

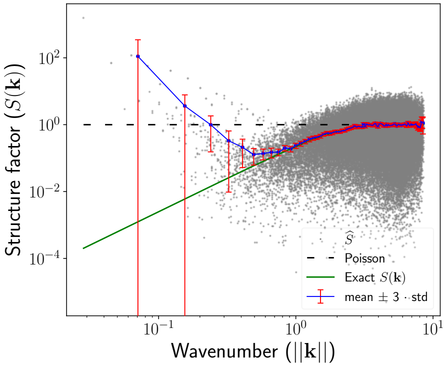
  2. Undirectly debiased:

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

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

Scattering intensity

Tests: Estimators

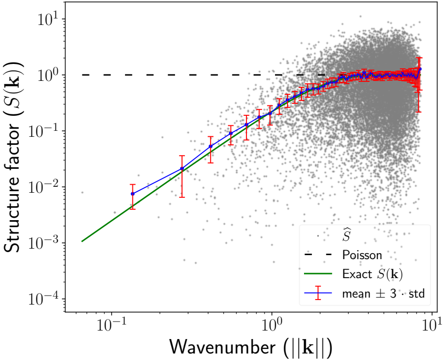


Scattering intensity on arbitrary wavevectors

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

Scattering intensity

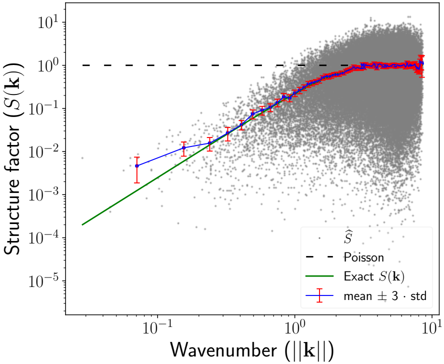
Tests: Estimators



Scattering intensity on allowed wavevectors

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

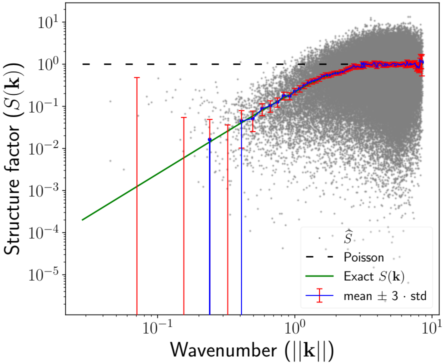
Scattering intensity



Scattering intensity directly debiased

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

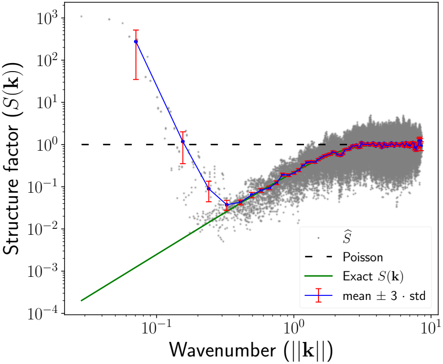
Scattering intensity



Scattering intensity undirectly debiased

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

Multitapered estimator



Multitapered estimator

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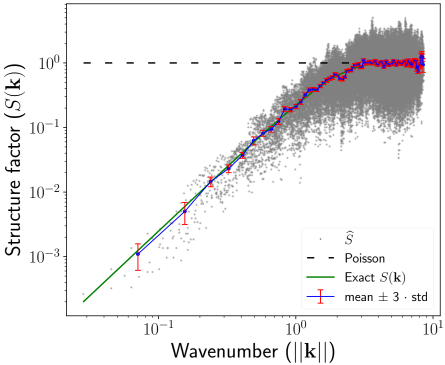

Multitapered estimator directly debiased

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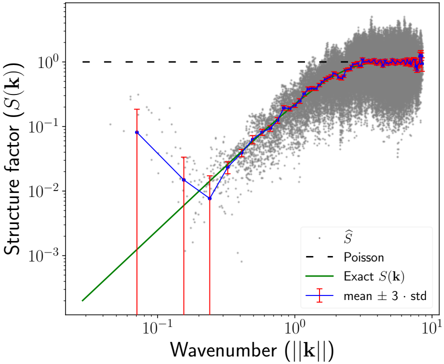
Multitapered estimator



Multitapered estimator undirectly debiased

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

Integrated mean square error

Estimators	$\widehat{\mathrm{iVar}}$	$\mathrm{CI}[\widehat{\mathrm{iMSE}}]$
$\widehat{S}_{\mathrm{SI}}(2\pi\mathbf{n}/L)$	0.32	0.32 ± 0.02
$\widehat{S}_{\mathrm{DDT}}(t_0)$	0.32	0.33 ± 0.03
$\widehat{S}_{\mathrm{DDT}}(t_1)$	0.34	0.35 ± 0.06
$\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$	0.08	$\mathbf{0.08} \pm 0.007$
	Ginibre ensemble	

Sample integrated variance and MSE for the variants of the scattering intensity across 50 samples from the Ginibre ensemble.

Integrated mean square error

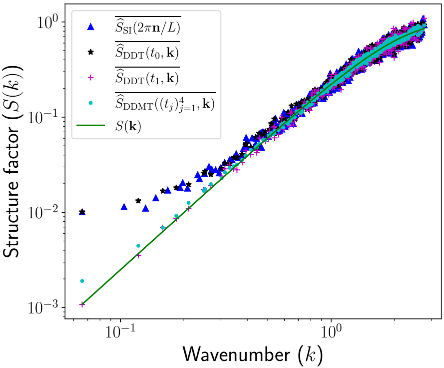
Comparison of the estimators

Estimators	T-score	p-value
$\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$, $\widehat{S}_{\mathrm{SI}}(2\pi\mathbf{n}/L)$	-29.53	3×10^{-33}
$\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$, $\widehat{S}_{\mathrm{DDT}}(t_0)$	-22.40	10^{-27}
$\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$, $\widehat{S}_{\mathrm{DDT}}(t_1)$	-12.18	9×10^{-17}
	Ginibre ensemble	

Paired t-tests for the variants of the scattering intensity.

Integrated mean square error

Comparison of the estimators



Means of the estimators across 50 samples from the Ginibre ensemble.

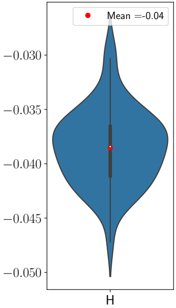
Effective hyperuniformity

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

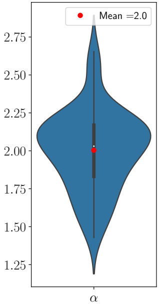
- $\widehat{S}(0)$ is a linear extrapolation of the estimated structure factor $\widehat{S}$ in $k = 0$.
- k_{peak} is the location of the first dominant peak value of $\widehat{S}$.

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

Hyperuniformity



(a) H index



(b) Power decay

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

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

THANK YOU

Github

Documentation

Preprint

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

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

https://arxiv.org/abs/2203.08749