# Exploring the hyperuniformity of a point process using its structure factor with Python

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# Numerical integration



- **Monte Carlo integration:**

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

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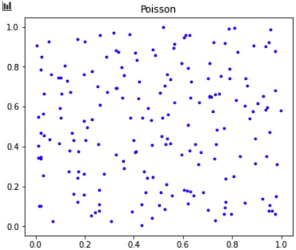


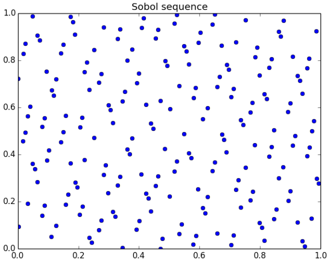
# Numerical integration



- **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:** $O(log(N)^d/N)$



# Hyperuniformity



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

- Variance:

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

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

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

# Structure Factor



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

- Structure factor:

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

- Pair correlation function

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

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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.*

# 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 class



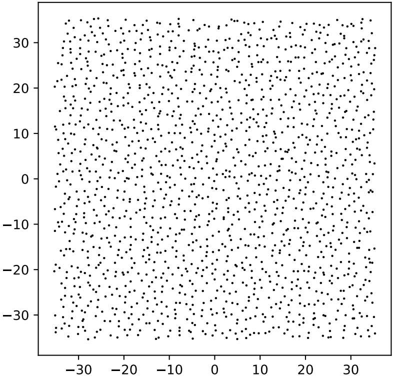
$\mathcal{X}$ is hyperuniform with $|S(\mathbf{k})| \sim c\|\mathbf{k}\|_2^\alpha$ in the neighborhood of 0 then,

| $\alpha$ | $\mathrm{Var}\left[\mathrm{Card}(\mathcal{X} \cap B(0, R))\right]$ | 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.*

# Ginibre ensemble

## Hyperuniformity



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

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 $\rho$ in $W = [-L/2, L/2]^d$.
- **Need**: Use $\mathcal{X}_N$ to approximate $S(\mathbf{k}) = 1 + \rho \int_{\mathbb{R}^d} (g(\mathbf{r}) - 1) e^{-i\langle \mathbf{k}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r}$.

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

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

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

# Scattering intensity estimator



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

# Tapered estimator



## General case

- Tapered estimator:

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

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

## General case

- Tapered estimator:

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

- 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:

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

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# 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.*

# Idea



- **Given**: $\mathcal{X}_N = \{\mathbf{x}_i\}_1^N$ a realization of a **stationary** and **isotropic** process $\mathcal{X}$ of intensity $\rho$ in $W = B(\mathbf{0}, R)$.
- **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** and **isotropic** process $\mathcal{X}$ of intensity $\rho$ in $W = B(\mathbf{0}, R)$.
- **Need**: Use $\mathcal{X}_N$ to approximate $S(k) = 1 + \rho \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty (g(r) - 1) r^{d/2} J_{d/2-1}(kr) \mathrm{d}r$
- **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. $\lim_{L\to\infty} \alpha_t(\mathbf{r}, W) = 1$, $\|t\|_2 = 1$ and $t$ is **radial**:

$$S(k) = 1 + \lim_{R\to\infty} \frac{(2\pi)^{d/2}}{k^{d/2-1}} \int_0^\infty \alpha_t(r, W)(g(r) - 1) r^{d/2} J_{d/2-1}(kr) \mathrm{d}r$$
$$= \lim_{L\to\infty} \mathbb{E}[\widehat{S}(t, k)] - \underbrace{\rho \mathcal{F}_s(\alpha_t)(k, W)}_{\epsilon_t(k,R)}$$

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

# Bartlett's isotropic estimator



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

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

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

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M. S. Bartlett, *The spectral analysis of two-dimensional point processes, 1964*.

# Package



1. Open-source Python toolbox called structure_factor[1]

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

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

# Package



1. Open-source Python toolbox called `structure_factor`[1]
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4. Jupyter notebook tutorial [4]

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[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

# Online simulation



https://colab.research.google.com/github/
For-a-few-DPPs-more/structure-factor/blob/main/notebooks/
tutorial_structure_factor.ipynb

# 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:

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

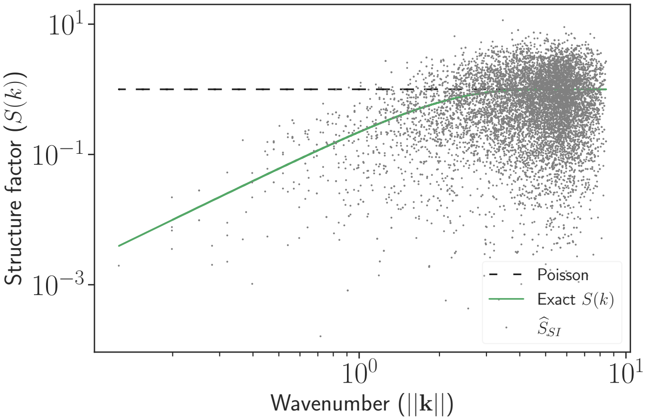
  2. Undirectly debiased:

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

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

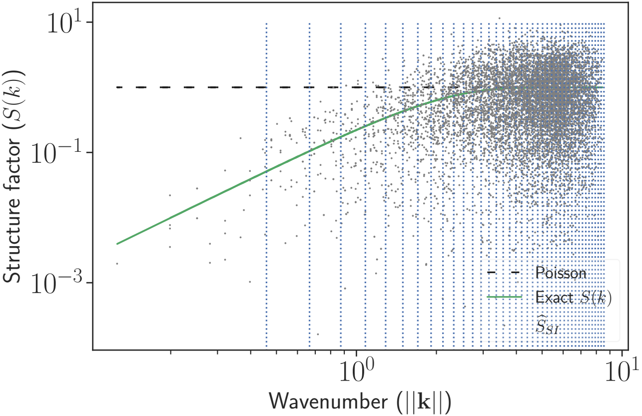
# Regularisation





# Regularisation

## Tests



# Regularisation

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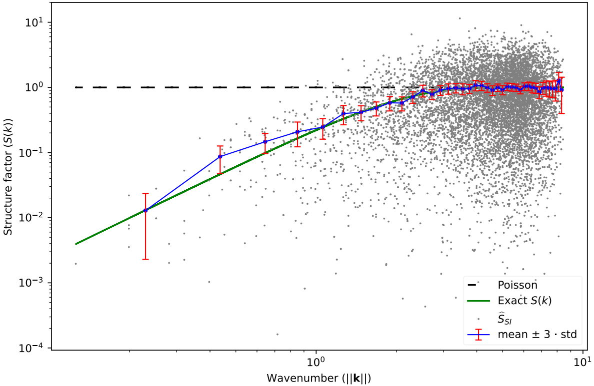
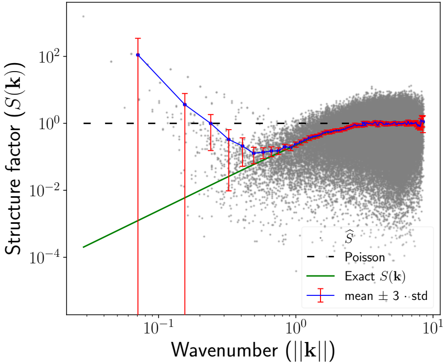


# Scattering intensity



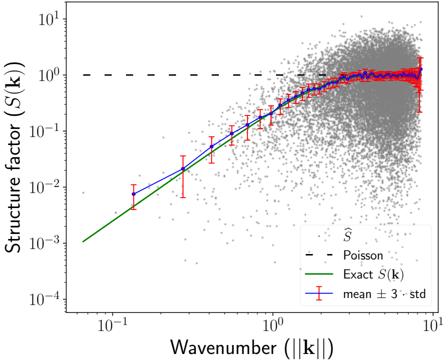



Scattering intensity on arbitrary wavevectors

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

# Scattering intensity






Scattering intensity on allowed wavevectors

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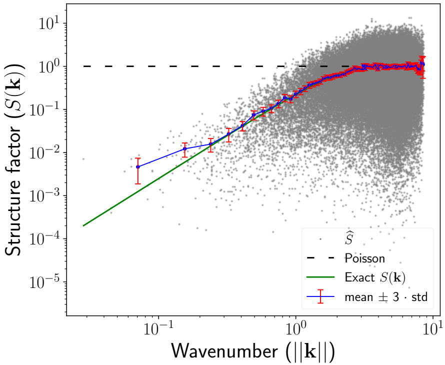
# Scattering intensity



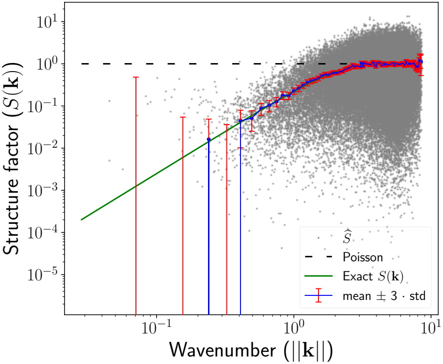



Scattering intensity directly debiased

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

# Sinusoidal tapers



Consider a centered rectangular window $W = \prod_{j=1}^{d} [-L_j/2, L_j/2]$

- Tapers:

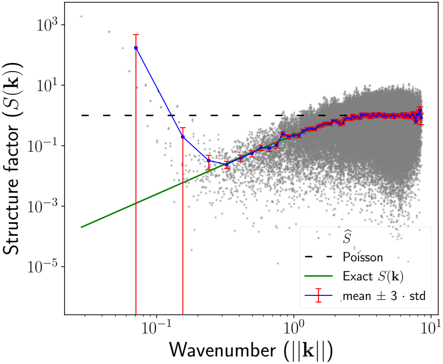
$$t(\mathbf{x}, \mathbf{p}^q, W) = \frac{\mathbb{1}_W(\mathbf{x})}{\sqrt{|W|}} \prod_{j=1}^{d} \sqrt{2} \sin\left(\frac{\pi p_j^q}{L_j}(x_j + L_j/2)\right)$$

- Fourier transform:

$$\frac{1}{\sqrt{|W|}} \prod_{j=1}^{d} \sqrt{2} i^{(p_j^q + 1)} \left[ \frac{\sin((k_j - \frac{\pi p_j^q}{L_j})\frac{L_j}{2})}{k_j - \frac{\pi p_j^q}{L_j}} - (-1)^{p_j^q} \frac{\sin((k_j + \frac{\pi p_j^q}{L_j})\frac{L_j}{2})}{k_j + \frac{\pi p_j^q}{L_j}} \right]$$

# Tapered estimator






Tapered estimator

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# Tapered estimator

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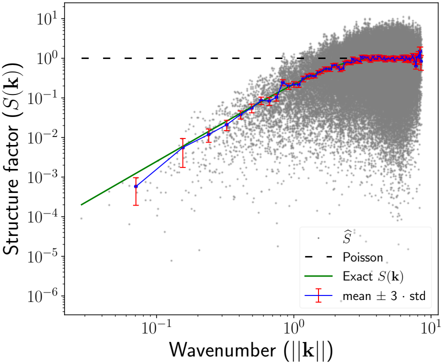


Tapered estimator directly debiased

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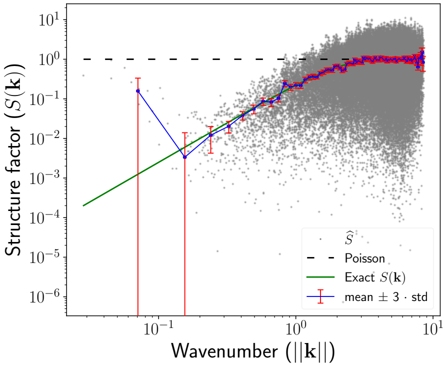
# Tapered estimator



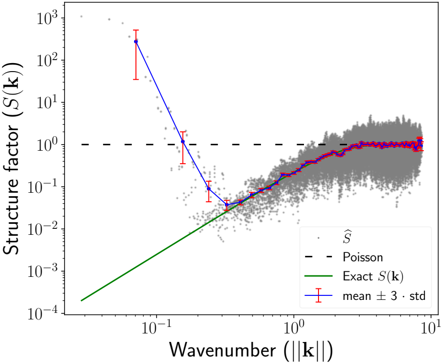



Tapered estimator undirectly debiased

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

# Multitapered estimator






Multitapered estimator

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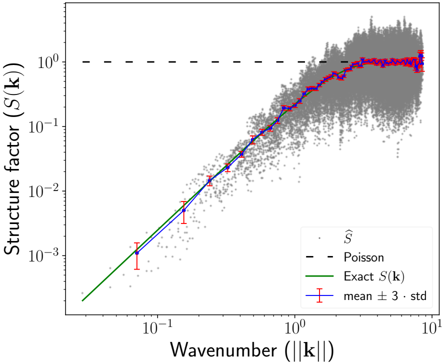


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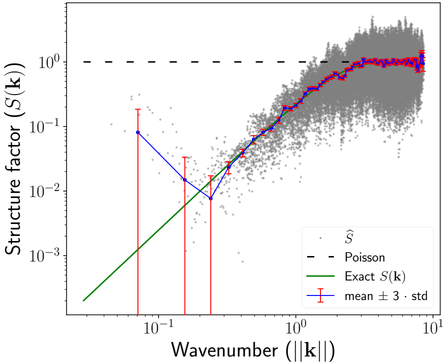


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# Estimator assuming isotropy and stationarity

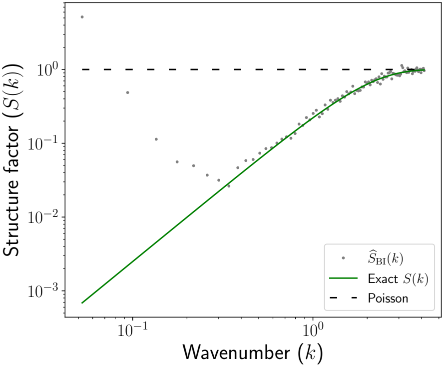


- Bartlett's isotropic estimator

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

# Bartlett's isotropic estimator

## Tests

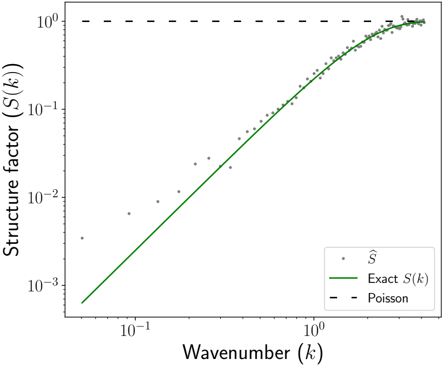



Bartlett's isotropic estimator on arbitrary wavenumbers

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

# Bartlett's isotropic estimator






Bartlett's isotropic estimator on allowed wavenumbers

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 | $0.32 \pm 0.02$ |
| $\widehat{S}_{\mathrm{DDT}}(t_0)$ | 0.32 | $0.33 \pm 0.03$ |
| $\widehat{S}_{\mathrm{DDT}}(t_1)$ | 0.34 | $0.35 \pm 0.06$ |
| $\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$ | 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

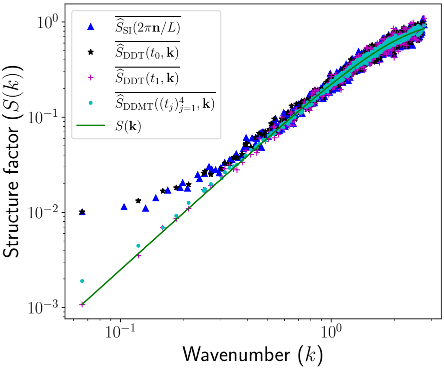


| Estimators | $T$-score | $p$-value |
|---|---|---|
| $\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$, $\widehat{S}_{\mathrm{SI}}(2\pi\mathbf{n}/L)$ | $-29.53$ | $3 \times 10^{-33}$ |
| $\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$, $\widehat{S}_{\mathrm{DDT}}(t_0)$ | $-22.40$ | $10^{-27}$ |
| $\widehat{S}_{\mathrm{DDMT}}((t_q)_1^4)$,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

# Integrated mean square error



| Estimator | $\widehat{\mathrm{iVar}}$ | $\mathrm{CI}[\widehat{\mathrm{iMSE}}]$ |
|---|---|---|
| $\widehat{S}_{\mathrm{BI}}$ | $3.9 \times 10^{-3}$ | $\mathbf{4.0 \times 10^{-3}} \pm 3 \times 10^{-4}$ |
| $\widehat{S}_{\mathrm{HO}}$ | $0.37$ | $0.38 \pm 0.09$ |
| $\widehat{S}_{\mathrm{HBC}}$ | $0.03$ | $0.03 \pm 0.01$ |
| | Ginibre ensemble | |

Sample integrated variance and MSE across 50 samples from the Ginibre point processes.

# Integrated mean square error

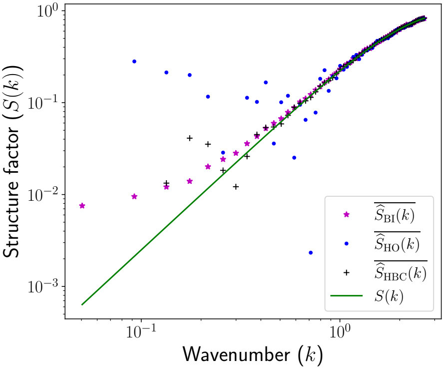
## Comparison of the estimators

| Estimators | $T$-score | $p$-value |
|---|---|---|
| $\widehat{S}_{\mathrm{BI}}$ vs. $\widehat{S}_{\mathrm{HO}}$ | $-12.24$ | $7 \times 10^{-17}$ |
| $\widehat{S}_{\mathrm{BI}}$ vs. $\widehat{S}_{\mathrm{HBC}}$ | $-25.51$ | $2 \times 10^{-30}$ |
| | Ginibre ensemble | |

Paired $t$-tests for the estimators that assume isotropy.

# Integrated mean square error

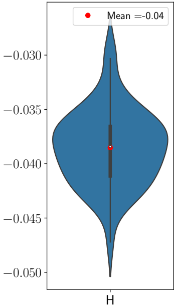
## Comparison of the estimators



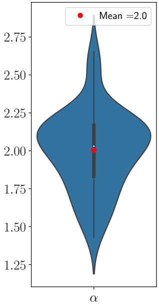

Means of the estimators across 50 samples from the Ginibre ensemble.

# Hyperuniformity

## Comparison of the estimators




(a) H index




(b) Power decay

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

# THANK YOU

Github

Documentation

Paper (Draft)

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

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

https://dhawat.github.io/assets/pdfs/draft_paper.pdf