Exploring the hyperuniformity of a point process using `structure_factor`

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Hyperuniform (HU) point processes could form a new family of Monte Carlo quadratures. By definition, HU point processes are more efficient than rejection sampling at estimating the volume of a set. There are many candidate HU processes in the physics literature, but rigorously proving that a point process is HU is usually difficult. It is thus desirable to have standardised numerical tests of hyperunifomity. We survey existing estimators of the structure factor and gather them all in a Python toolbox `structute_factor`, along with numerical diagnosis of hyperuniformity.

Hyperuniformity and structure factor

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

- The structure factor S of $\mathcal{X}$ is defined by

$$S(\mathbf{k}) = 1 + \rho\mathcal{F}(g-1)(\mathbf{k}),\ \mathbf{k} \in \mathbb{R}^d, \tag{1}$$

where $\mathcal{F}$ is the Fourier transform and g is the pair correlation function of $\mathcal{X}$.

Hyperuniformity

$$\mathcal{X} \text{ is hyperuniform} \iff \lim_{R\to\infty} \frac{\mathrm{Var}\left[\mathrm{Card}(\mathcal{X}\cap B(0,R))\right]}{\mathrm{Volume}(B(0,R))} = 0 \iff S(0) = 0$$

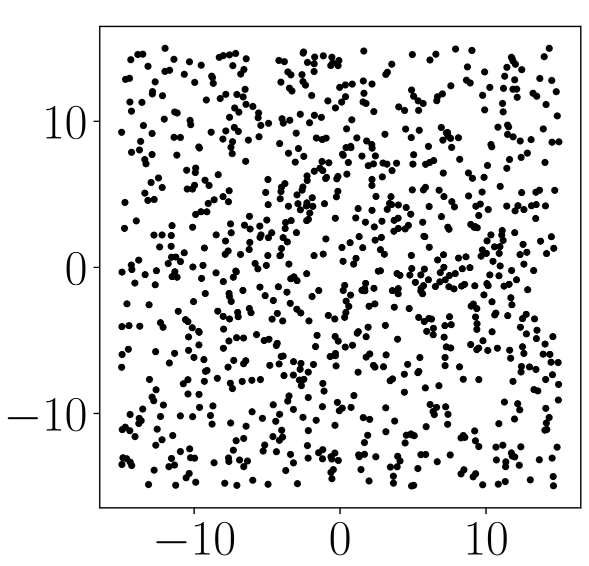

Figure: Poisson Point Process.

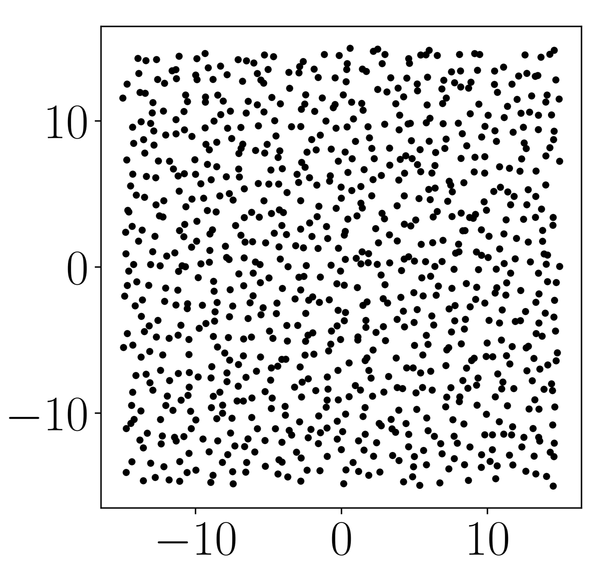

Figure: Ginibre Ensemble.

- The homogeneous Poisson point process is not hyperuniform,

$$g_{poisson}(r) = S_{poisson}(k) = 1.$$

- The Ginibre Ensemble is hyperuniform,

$$S_{\text{Ginibre}}(k) = 1 - \exp(-k^2/4),\ S_{\text{Ginibre}}(k) \sim k^2, \quad (k \to 0).$$

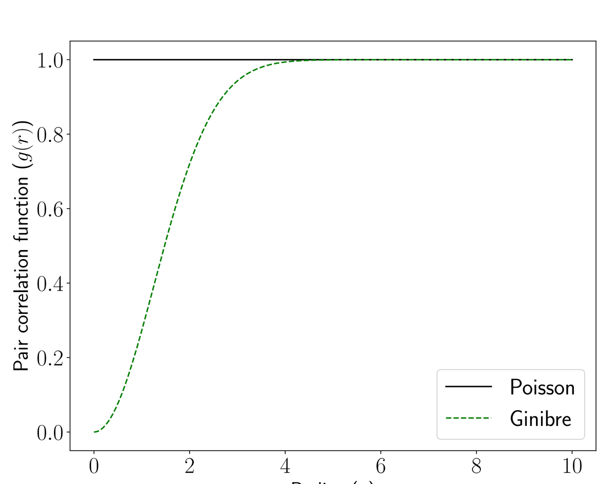

Figure: Pair correlation function.

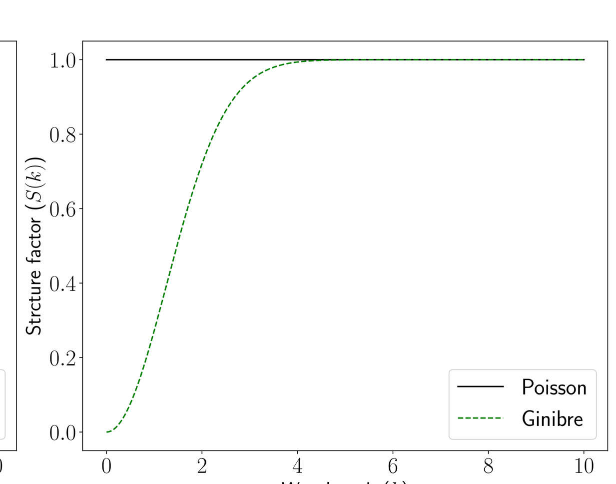

Figure: Structure Factor.

The scattering intensity estimator of S

- Let $W = [-L/2, L/2]^d$ and $\mathcal{X} \cap W = \{x_1, \dots, x_N\}$.

Scattering intensity

$$\widehat{S}_{\mathrm{SI}}\left(\frac{2\pi}{L}\mathbf{k}\right) \triangleq \frac{1}{N}\left|\sum_{j=1}^{N} e^{\frac{-2i\pi}{L}\langle \mathbf{k}, x_j\rangle}\right|^2,\ \mathbf{k} \in (\mathbb{Z}^d)^*$$

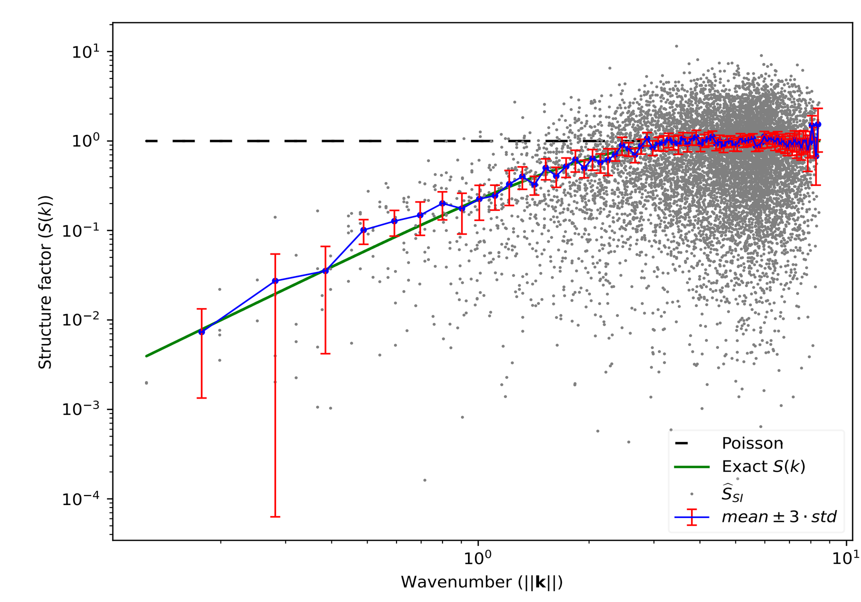

Figure: Scattering intensity of the Ginibre Ensemble as a function of $\|\mathbf{k}\|$.

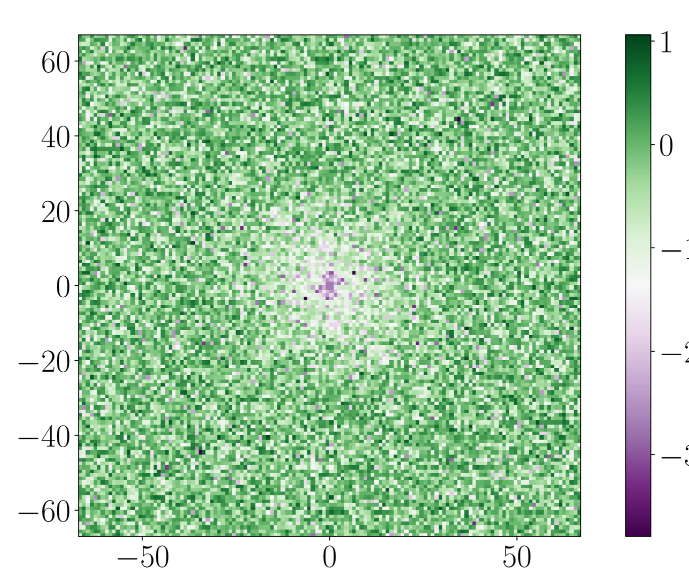

Figure: Scattering intensity of the Ginibre Ensemble as a function of $\mathbf{k} \in \mathbb{Z}^2$.

Estimating S using the Hankel transform

- The structure factor S of an isotropic point process can be formulated using the Hankel transform $\mathcal{H}_\gamma$

$$S(\|\mathbf{k}\|) = 1 + \rho\frac{(2\pi)^{d/2}}{\|\mathbf{k}\|^{d/2-1}}\mathcal{H}_{d/2-1}(\tilde{g}-1)(\|\mathbf{k}\|), \quad \tilde{g}: x \mapsto g(x)x^{d/2-1}.$$

- Estimating the pair correlation function using the two estimators `pcf.ppp`, and `pcf.fv` of the R package `spatstat`.
- Estimating the Hankel transform using Ogata quadrature or the Discrete Hankel transform.

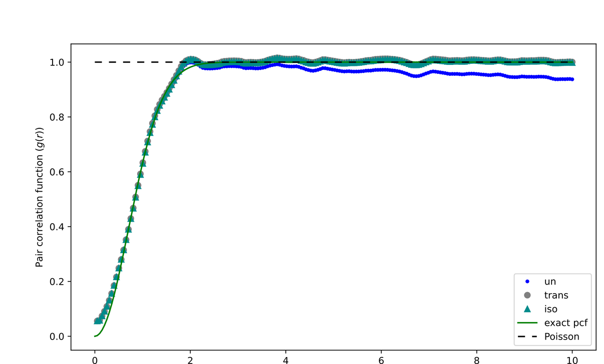

Figure: Approximated pair correlation function of the Ginibre using pcf.ppp.

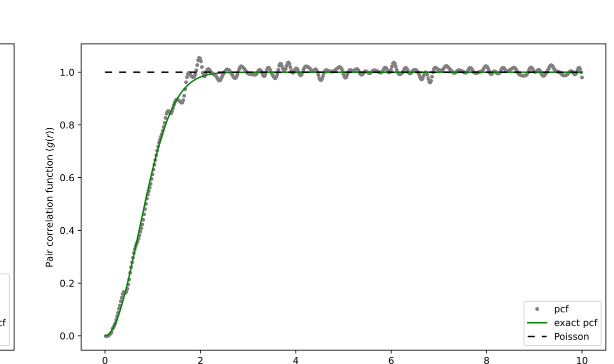

Figure: Approximated pair correlation function of the Ginibre using pcf.fv.

Estimator using Ogata quadrature

$$\widehat{S}_{\mathrm{HO}}(k) = 1 + 2\pi^2\rho\sum_{j=1}^{N} w_{0j} J_0\Big(f(\xi_{0j})\Big)\big(\hat{g}_k(f(\xi_{0j})) - 1\big),$$

where, $\{\xi_{0j}\}_{j\geq 1}$ are the positive zeros of the Bessel function $J_0(\pi x)$, $\{w_{0j}\}_{j\geq 1}$ is a specific set of weights and f is a Tanh-Sinh function.

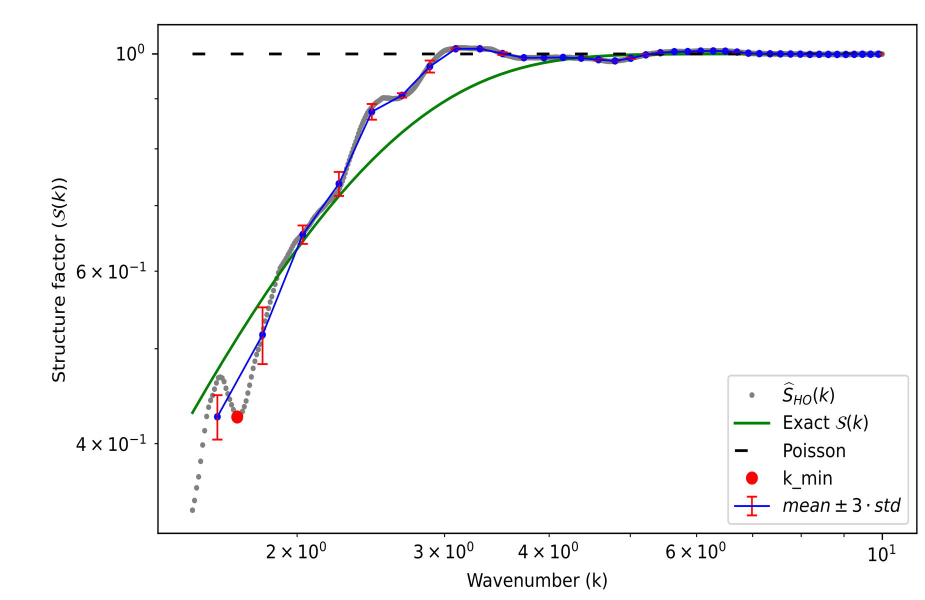

Figure: Approximated structure factor of the Ginibre using $\widehat{S}_{\mathrm{HO}}$.

Estimator using the Discrete Hankel Transform

$$\widehat{S}_{\mathrm{HBC}}(k_m) = 1 + 2\pi\rho\alpha\sum_{j=1}^{N-1}\beta_{0j}J_0\left(\frac{\eta_{0m}\eta_{0j}}{\eta_{0N}}\right)(\hat{g}(r_j) - 1),$$

for specific set of wavenumbers k_m, with $\{\eta_{0j}\}_{j\geq 1}$ the positive zeros of the Bessel function $J_0(x)$, $\{r_j\}_{j\geq 1}$ a specific set of radius and $\{\beta_{0j}\}_{j\geq 1}$ a specific set of weights.

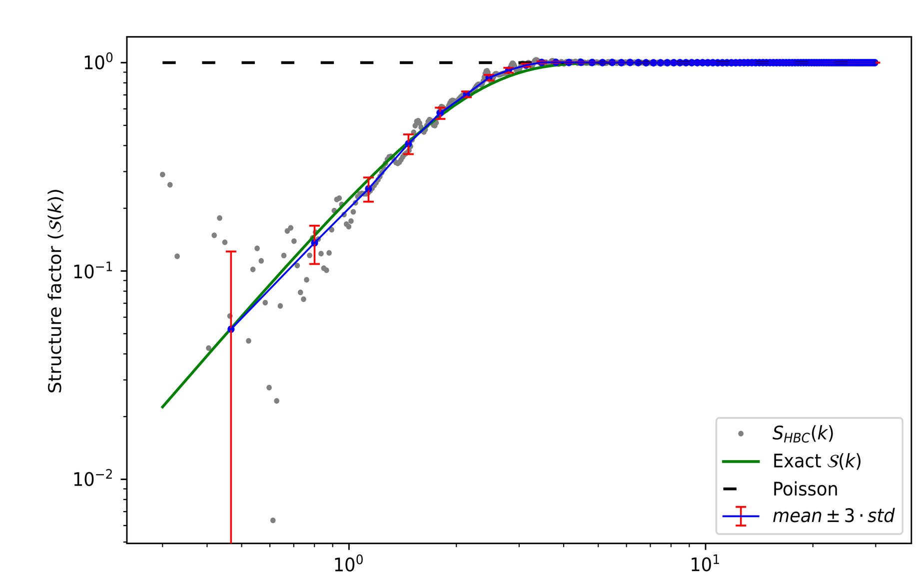

Figure: Approximated structure factor of the Ginibre using $\widehat{S}_{\mathrm{HBC}}$.

Hyperuniformity tests

- **Test of effective hyperuniformity:**

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

  - $\widehat{S}(0)$ 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 $\widehat{S}$.

- **Test of hyperuniformity's class:**

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

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

The Python toolbox `structure_factor`

- Python toolbox.

```
In [1]: !pip install structure_factor
```

- Implement all the above estimators.
- Open source available on Github.
- Documentation available online.

Github QR-code

Personal webpage QR-code

References

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