Point processes for numerical integration

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Numerical integration

Let f be a continuous function supported on a compact $K \subset \mathbb{R}^d$.

- **Need:** approximate $\int_K f(\mathbf{z}) \, \mathrm{d}\mathbf{z}$.

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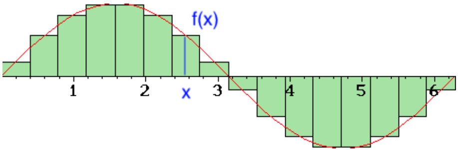

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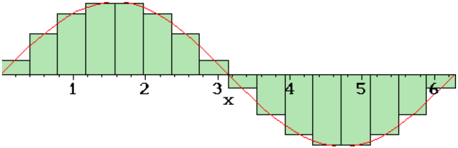
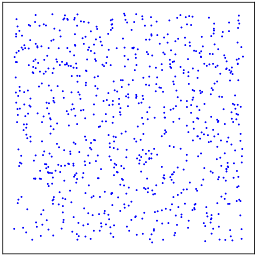


Numerical integration

- For any $\{\mathbf{z}_i\}_{i=1}^N \subset K$ and $\{w_i\}_{i=1}^N \subset \mathbb{R}$, there exists $f \in \mathcal{F}^k$ s.t.

$$\Big| \int_K f(\mathbf{z}) \, \mathrm{d}\mathbf{z} - \sum_{i=1}^{N} w_i f(\mathbf{z}_i) \Big| \geq \frac{C_1}{N^{k/d}}.$$



Fixed $\{\mathbf{z}_i\}_{i=1}^N$

N. Bakhvalov. *Vestnik MGU, Ser. Math. Mech. Astron. Phys. Chem.*, 1959.

N. Bakhvalov. *USSR Comp. Math. and Mathematical Physics*, 1971.

Numerical integration

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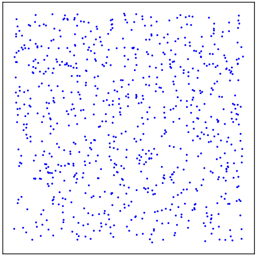
- For $\{\mathbf{z}_i\}_{i=1}^N$ random elements of K and $\{w_i\}_{i=1}^N \subset \mathbb{R}$, there exists $f \in \mathcal{F}^k$ s.t.

$$\mathbb{E}\Big[\Big| \int_K f(\mathbf{z})\, \mathrm{d}\mathbf{z} - \sum_{i=1}^N w_i f(\mathbf{z}_i) \Big|\Big] \geq \frac{C_2}{N^{k/d+1/2}}.$$



Random $\{\mathbf{z}_i\}_{i=1}^N$

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- For $\{\mathbf{z}_i\}_{i=1}^N$ random elements of K and $\{w_i\}_{i=1}^N \subset \mathbb{R}$, there exists $f \in \mathcal{F}^k$ s.t.

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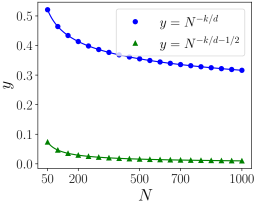

$k = 1$ and $d = 6$

N. Bakhvalov. *Vestnik MGU, Ser. Math. Mech. Astron. Phys. Chem.*, 1959.

N. Bakhvalov. *USSR Comp. Math. and Mathematical Physics*, 1971.

Monte Carlo method

Let $\mathcal{X}$ be a stationary point process of intensity ρ

$$\int_K f(\mathbf{z})\, \mathrm{d}\mathbf{z} = \mathbb{E}\left[\sum_{\mathbf{z}\in\mathcal{X}\cap K} \rho^{-1} f(\mathbf{z})\right].$$

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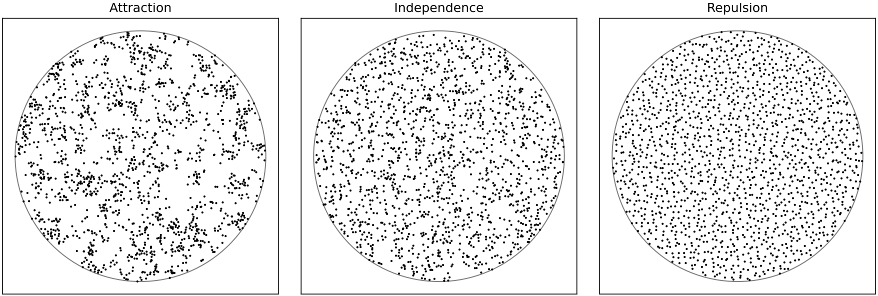
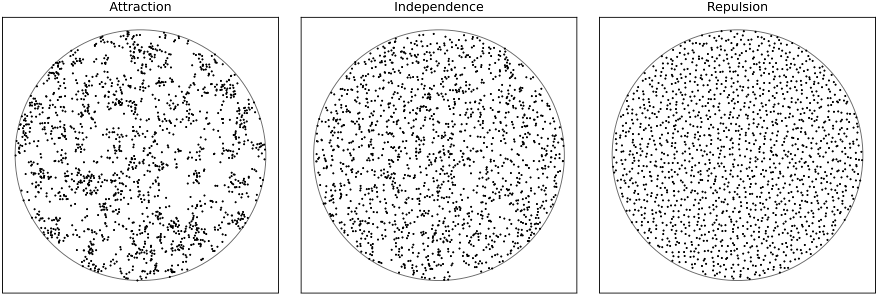
- Monte Carlo method: $\widehat{I}_{\mathcal{X}}(f) = \sum_{\mathbf{z}\in\mathcal{X}\cap K} \rho^{-1} f(\mathbf{z})$.
- Number of points: $\mathcal{X}(K)$ (random).
- $N := \mathbb{E}[\mathcal{X}(K)] = \rho|K|$.

$$\widehat{I}_{\mathcal{X}}(f) = \sum_{\mathbf{z} \in \mathcal{X} \cap K} \rho^{-1} f(\mathbf{z}) \approx \int_K f(\mathbf{z}) \, \mathrm{d}\mathbf{z}$$





Monte Carlo with a homogeneous Poisson point process (PPP):

- Sampling from a PPP is fast.
- $\mathbb{V}\mathrm{ar}[\widehat{I}_{\mathcal{X}}(f)]^{1/2} = c(d, f)N^{-1/2}$.

A. B. Owen. *Online book*, 2013.

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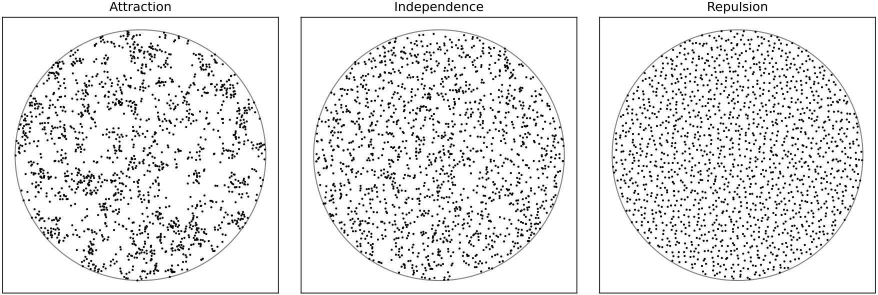

Monte Carlo with a determinantal point process (DPP) :

- $\mathbb{V}\mathrm{ar}[\widehat{I}_{\mathcal{X}}(f)]^{1/2} = O(N^{-1/2-1/(2d)})$.
- Sampling from DPPs is expensive.

R. Bardenet and A. Hardy. *The Annals of Applied Probability*, 2020.

J.-F. Coeurjolly, A. Mazoyer, and P.-O. Amblard. *Electronic Journal of Statistics*, 2021.

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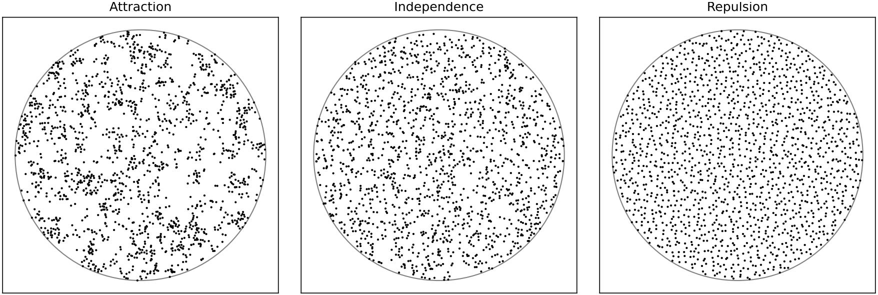

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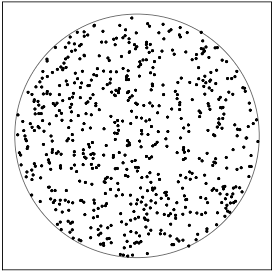
G. Gautier, R. Bardenet, and M. Valko. *Adv. in Neural Info. Processing Systems*, 2019.

Repelled point processes:

"D. Hawat, R. Bardenet, and R. Lachièze-Rey. Repelled point processes with application to numerical integration. Preprint, 2023."

Construction

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



Sample

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

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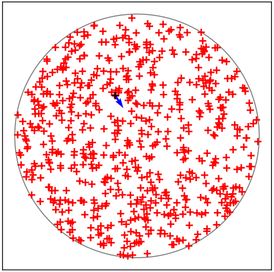
$\mathcal{X}$ a stationary point process of intensity ρ of $\mathbb{R}^d$.

- **Force:**

$$F_{\mathcal{X}}(\mathbf{a}) := \sum_{\substack{\mathbf{z}\in\mathcal{X}\setminus\{\mathbf{a}\} \\ \|\mathbf{a}-\mathbf{z}\|_2\uparrow}} \frac{\mathbf{a}-\mathbf{z}}{\|\mathbf{a}-\mathbf{z}\|_2^d}.$$



Sample

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint,* 2023.

Chatterjee, Sourav, Ron Peled, Yuval Peres, and Dan Romik. *Ann. of Mathematics,* 2010.

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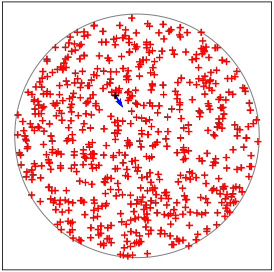
- **Repulsion operator:**

$$\Pi_\varepsilon : \mathcal{X} \longmapsto \{\mathbf{a}+\varepsilon F_{\mathcal{X}}(\mathbf{a}) : \mathbf{a}\in\mathcal{X}\}.$$



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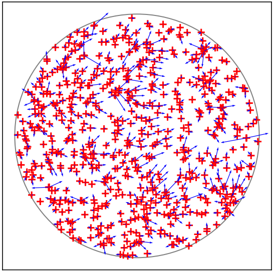

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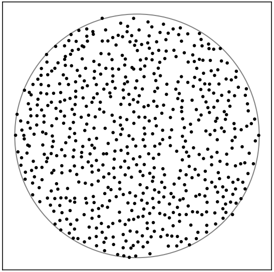
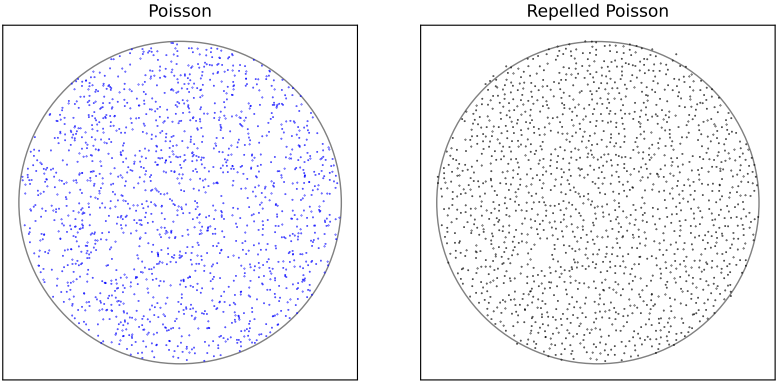


Repelled sample

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

Example



D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

Main theoretical results

Let $\mathcal{P} \in \mathbb{R}^d$ be a PPP of intensity $\rho > 0$, $d \geq 3$, and $\varepsilon \in \mathbb{R}$.

- $\Pi_\varepsilon \mathcal{P}$ is a simple, stationary, isotropic point process of intensity ρ.

Proposition

For any two distinct points $\mathbf{x}, \mathbf{y}$ *of* $\mathbb{R}^d$*, the random vector* $F_{\mathcal{P}}(\mathbf{x}) - F_{\mathcal{P}}(\mathbf{y})$ *is continuous, i.e., for any* $\mathbf{c} \in \mathbb{R}^d$,

$$\mathbb{P}\left(F_{\mathcal{P}}(\mathbf{x}) - F_{\mathcal{P}}(\mathbf{y}) = \mathbf{c}\right) = 0.$$

Moreover, $\Pi_\varepsilon \mathcal{P}$ *is a stationary and isotropic point process of intensity* ρ*.*

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

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- For any $\varepsilon \in (-1, 1)$, the moments of $\Pi_\varepsilon \mathcal{P}$ exist.

Proposition

For any positive integer m and $R > 0$, we have

$$\mathbb{E}\left[\left(\sum_{\mathbf{z} \in \Pi_\varepsilon \mathcal{P}} \mathbb{1}_{B(\mathbf{0},R)}(\mathbf{z})\right)^m\right] < \infty.$$

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

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- For any $\varepsilon \in (-1, 1)$, the moments of $\Pi_\varepsilon \mathcal{P}$ exist.
- For $\varepsilon > 0$ small enough and $f \in C^2(\mathbb{R}^d)$, $\mathbb{V}\mathrm{ar}[\widehat{I}_{\Pi_\varepsilon \mathcal{P}}(f)] < \mathbb{V}\mathrm{ar}[\widehat{I}_{\mathcal{P}}(f)]$.

Theorem

For any function $f \in C^2(\mathbb{R}^d)$ of compact support K, we have

$$\mathbb{V}\mathrm{ar}\left[\widehat{I}_{\Pi_\varepsilon \mathcal{P}}(f)\right] = \mathbb{V}\mathrm{ar}\left[\widehat{I}_{\mathcal{P}}(f)\right](1 - 2d\kappa_d \rho \varepsilon) + O(\varepsilon^2),$$

where κ_d is the volume of the unit ball of $\mathbb{R}^d$.

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

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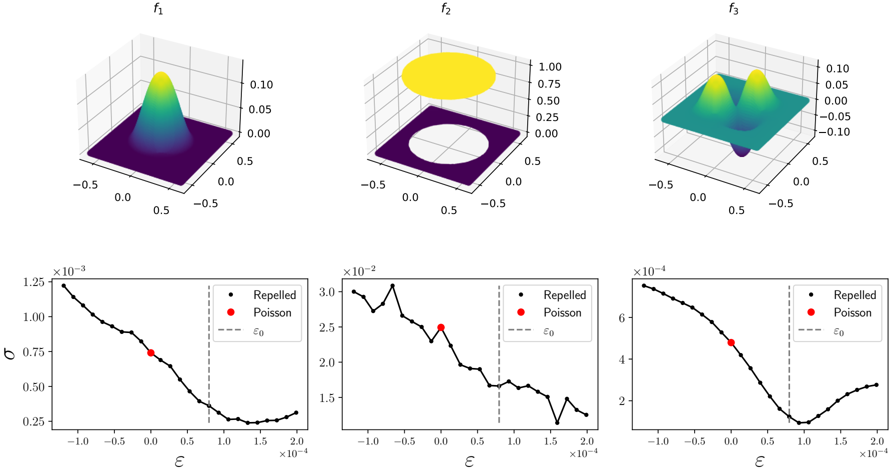
D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

Experiments



Variance for Poisson $(d = 3)$

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

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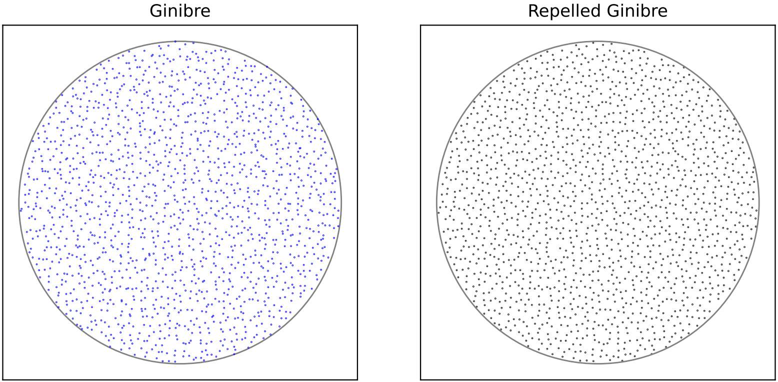

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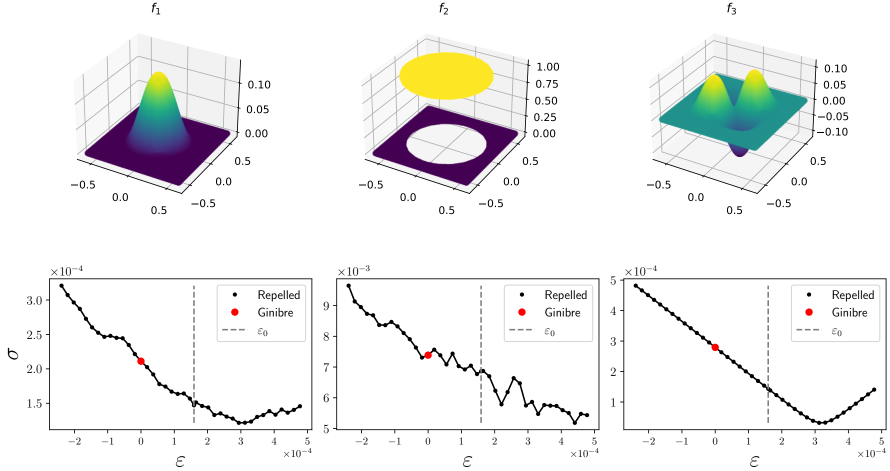

Variance for Ginibre ($d = 2$)

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

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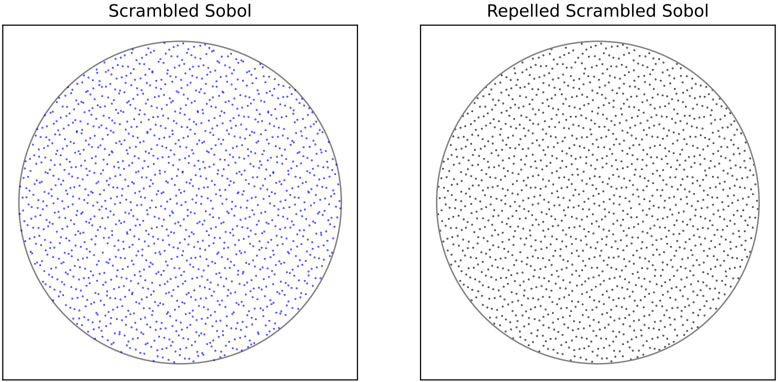

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

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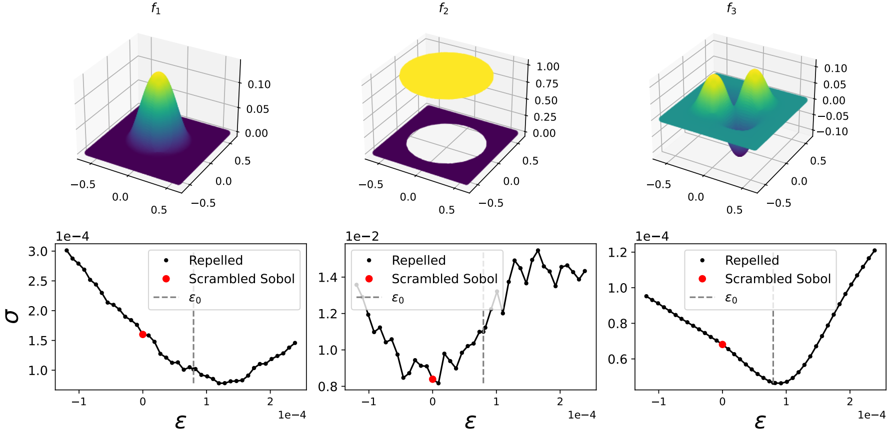

Variance for Scrambled Sobol ($d = 3$)

D. Hawat, R. Bardenet, and R. Lachièze-Rey. *Preprint*, 2023.

Diagnosing hyperuniformity:

"D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey. On estimating the structure factor of a point process, with applications to hyperuniformity. Statistics and Computing, 2023."

Hyperuniformity

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

$$\lim_{R\to\infty} \frac{\mathbb{V}\mathrm{ar}\left[\sum_{\mathbf{z}\in\mathcal{X}} \mathbb{1}_{B(\mathbf{0},R)}(\mathbf{z})\right]}{|B(\mathbf{0},R)|} = 0.$$

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

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

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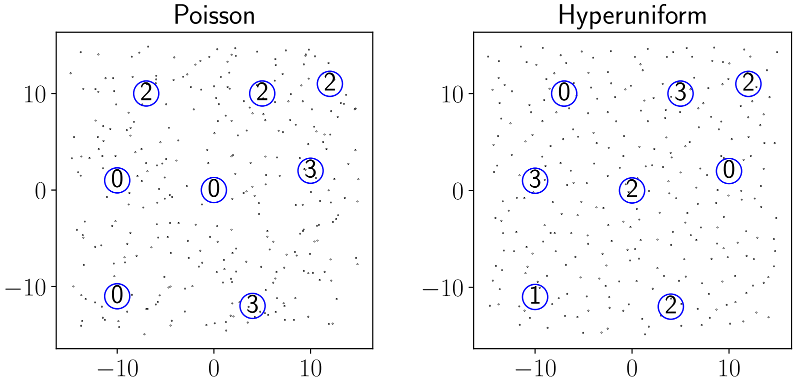

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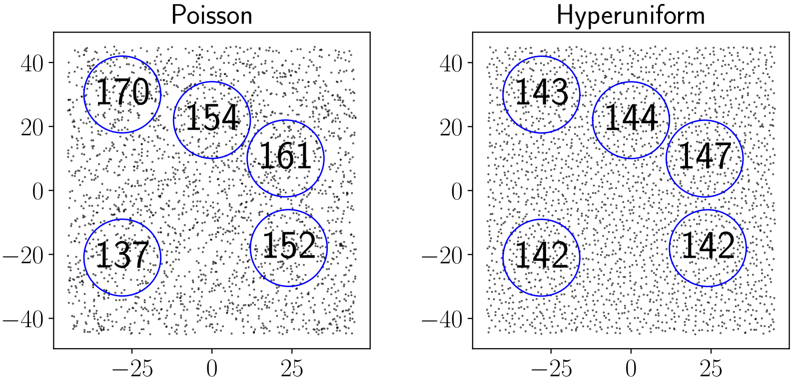

Hyperuniformity using the structure factor

$\mathcal{X}$ a stationary point process of intensity ρ

- Structure factor 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. *Online survey*, 2021.

S. Torquato. *Physics Reports*, 2018.

Testing the hyperuniformity ($S(\mathbf{0}) = 0$)

- **Given:** Realization of $\mathcal{X}$ in a window W_L of lenghtside L (e.g., $W_L = [-L/2, L/2]^d$).

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$$\widehat{S}(\mathbf{k}) := \frac{1}{\rho|W_L|}\left|\sum_{z\in\mathcal{X}\cap W_L} e^{-i\langle \mathbf{k},\mathbf{z}\rangle}\right|^2, \quad \mathbf{k} \in \mathbb{A}_L.$$

- **We have:**
  1. $\|\mathbf{k}_L^{\min}\|_2 := \min_{\mathbf{k}\in\mathbb{A}_L} \|\mathbf{k}\|_2 = \frac{C}{L}$.
  2. For $\mathbf{k} \in \mathbb{A}_L$, $S(\mathbf{k}) = \lim_{W_L\uparrow\mathbb{R}^d} \mathbb{E}\left[\widehat{S}(\mathbf{k})\right]$.

S. Torquato. *Physics Reports*, 2018.

M. A. Klatt et al. *Nature Communications*, 2019.

M. A. Klatt, G. Last, and D. Yogeshwaran. *Random Structures Algorithms*, 2020.

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M. A. Klatt, G. Last, and N. Henze. *Preprint*, 2022.

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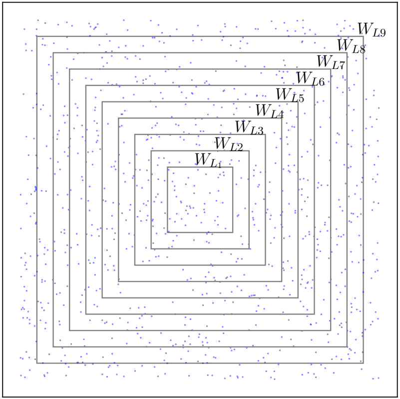
C. Rhee and P.W. Glynn. *Operations Research*, 2015.

Multiscale hyperuniformity test

- **Let:**
  1. $\{W_{L_m}\}_{m\geq 1}$ an increasing sequence of windows s.t., $W_{L_\infty} = \mathbb{R}^d$.
  2. $\widehat{S}_m$ an estimator of S based on the points of $\mathcal{X} \cap W_{L_m}$.
  3. $\mathbf{k}_{L_m}^{\min}$ a minimum allowed wavevector for the estimator $\widehat{S}_m$.



Multiscale hyperuniformity test

- **Let:**
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- **Define:**

$$Z = \sum_{m=1}^{M} \frac{Y_m - Y_{m-1}}{\mathbb{P}(M \geq m)},$$

with $Y_m = 1 \wedge \widehat{S}_m(\mathbf{k}_{L_m}^{\min})$, $Y_0 = 0$, and M an unbounded $\mathbb{N}$-r.v.

D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey. *Statistics and Computing*, 2023.

Multiscale hyperuniformity test

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Proposition

Assume that $M \in L^p$ for some $p \geq 1$. Then $Z \in L^p$ and we have

1. *If $\mathcal{X}$ is hyperuniform, then $\mathbb{E}[Z] = 0$.*
2. *If $\mathcal{X}$ is not hyperuniform and $\sup_m \mathbb{E}[\widehat{S}_m^2(\mathbf{k}_{L_m}^{\min})] < \infty$, then $\mathbb{E}[Z] \neq 0$.*

D. Hawat, G. Gautier, R. Bardenet, R. Lachièze-Rey. *Statistics and Computing*, 2023.

Multiscale hyperuniformity test

Proposition

Assume that $M \in L^p$ *for some* $p \geq 1$. *Then* $Z := \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)} \in L^p$ *and*

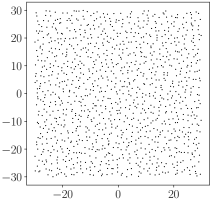
1. *If* $\mathcal{X}$ *is hyperuniform, then* $\mathbb{E}[Z] = 0$.
2. *If* $\mathcal{X}$ *is not hyperuniform and* $\sup_m \mathbb{E}[\widehat{S}^2_m(\mathbf{k}^{\min}_{L_m})] < \infty$, *then* $\mathbb{E}[Z] \neq 0$.

- i.i.d. pairs $(\mathcal{X}_a, M_a)_{a=1}^{A}$ of realizations of $(\mathcal{X}, M)$.
- Asymptotic confidence interval of level ζ

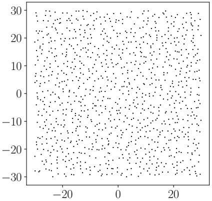
$$CI[\mathbb{E}[Z]] = \left[\bar{Z}_A - z\bar{\sigma}_A A^{-1/2}, \bar{Z}_A + z\bar{\sigma}_A A^{-1/2}\right],$$

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

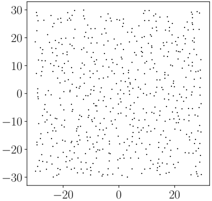
Multiscale hyperuniformity test



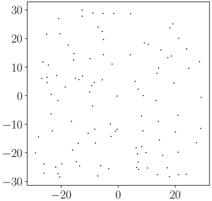
$S(\mathbf{0}) = 0$



$S(\mathbf{0}) = 0.1$



$S(\mathbf{0}) = 0.5$



$S(\mathbf{0}) = 0.9$

	$\bar{Z}_A$	$CI[\mathbb{E}[Z]]$
Ginibre, $S(\mathbf{0}) = 0$	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	$[0.2082, 1.0137]$

Table: Multiscale hyperuniformity test

Python **toolbox**

CI passing | codecov 71% | docs passing | docs latest | pypi v2.2.1 | python >=3.7.1,<3.10 | Open in Colab

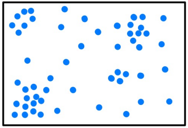
1. Open-source Python toolbox called `structure-factor`.
2. Available on GitHub and PyPI.
3. Detailed documentation.
4. Jupyter notebook tutorial.

structure-factor

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

Conclusion and perspectives

Repelled point processes

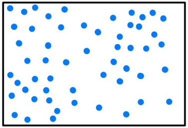


Sample

Apply the repulsion operator Π_ε

$\mathcal{O}(N^2)$ operations

$\boxed{\text{Reduce clustering}}$



Repelled sample

$$\mathrm{Var}\left[\sum_{x \in \Pi_\varepsilon \mathcal{P}} f(x)\right] < \mathrm{Var}\left[\sum_{x \in \mathcal{P}} f(x)\right]$$

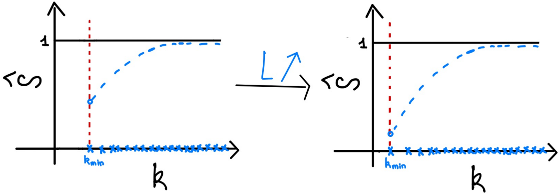
ε: positive, small

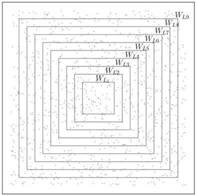
f: C^2-function of compact support

$\mathcal{P}$: homogeneous Poisson point process

Diagnosing hyperuniform point processes

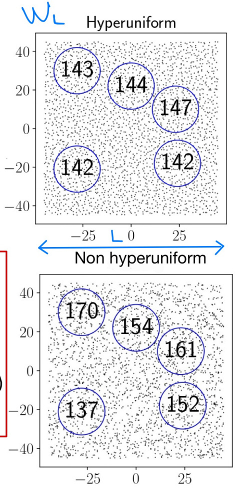
- X is hyperuniform $\Longleftrightarrow$ $S(0)=0$





- $Z = Z\left(\{\hat{S}, W_{L_m}, k_{L_m}\}_m, M\right)$

$$\begin{cases} \circ\ X \text{ hyperuniform} \Rightarrow \mathbb{E}[Z]=0 \\ \circ\ X \text{ not hyperuniform} + (H) \Rightarrow \mathbb{E}[Z]\neq 0 \end{cases}$$



THANK YOU!

Papers:

1. D. Hawat, R. Bardenet, and R. Lachieze-Rey. Repelled point processes with application to numerical integration, *Preprint, Axiv, HAL*, 2023.
2. D. Hawat, G. Gautier, R. Bardenet, and R. Lachièze-Rey. On estimating the structure factor of a point process, with applications to hyperuniformity. *Statistics and Computing*, 2023.

Softwares:

1. D. Hawat, R. Bardenet, and R. Lachieze-Rey. Python package `MCRPPy`. *GitHub*, 2023.
2. D. Hawat, G. Gautier, R. Bardenet, and R. Lachieze-Rey. Python package `structure-factor`. *GitHub and PyPI*, 2022.