Point processes for numerical integration

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

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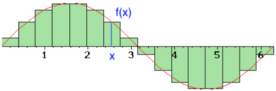

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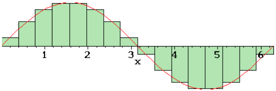

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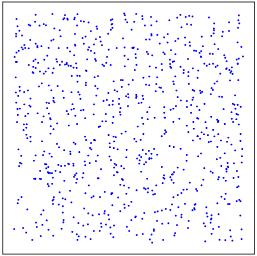

Fixed $\{\mathbf{z}_i\}_{i=1}^{N}$

N. S. Bakhvalov. On the optimality of linear methods for operator approximation in convex classes of functions. *USSR Computational Mathematics and Mathematical Physics*, 1971.

E. Novak and H. Woźniakowski. Tractability of multivariate problems. Vol. 1: Linear information. *European Mathematical Society (EMS)*, 2008.

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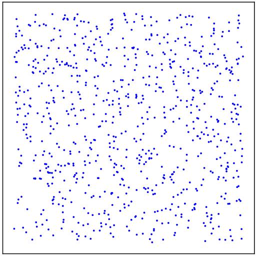

Fixed $\{\mathbf{z}_i\}_{i=1}^N$

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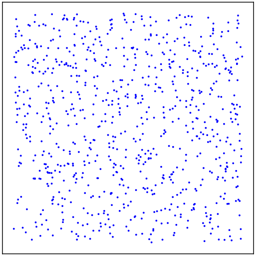

Random $\{\mathbf{z}_i\}_{i=1}^N$

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Numerical integration

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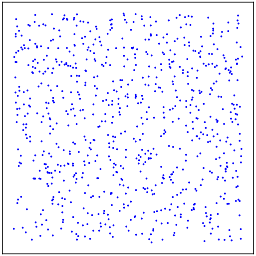
- The worst-case RMSE using random sets of N nodes is bounded from below by $O(N^{-k/d-1/2})$.



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

N. S. Bakhvalov. On the approximate calculation of multiple integrals. *Vestnik MGU, Ser. Math. Mech. Astron. Phys. Chem.*, 1959.

Monte Carlo method

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

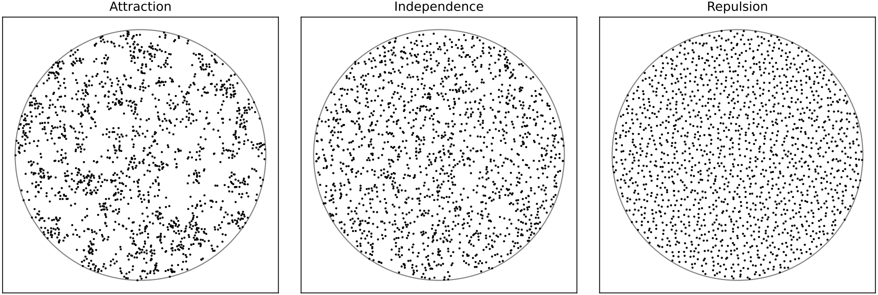
$$\mathbb{E}\left[\frac{1}{\rho}\sum_{\mathbf{z}\in\mathcal{X}\cap K} f(\mathbf{z})\right] = \int_K f(\mathbf{z})d\mathbf{z}.$$

Monte Carlo method

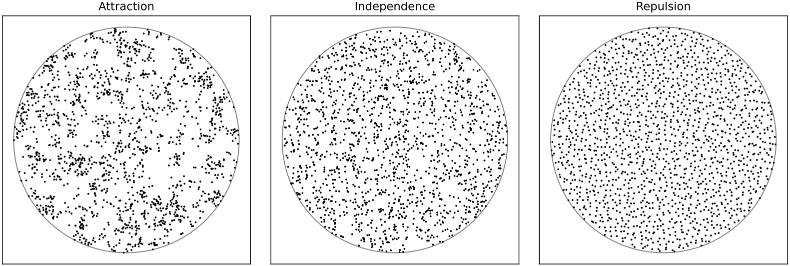
Let $\mathcal{X}$ be a stationary point process of intensity ρ

$$\mathbb{E}\Bigg[\underbrace{\frac{1}{\rho}\sum_{\mathbf{z}\in\mathcal{X}\cap K} f(\mathbf{z})}_{:=\widehat{I}_{\mathcal{X}}(f)}\Bigg] = \int_K f(\mathbf{z})d\mathbf{z}.$$

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


Attraction
Independence
Repulsion

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

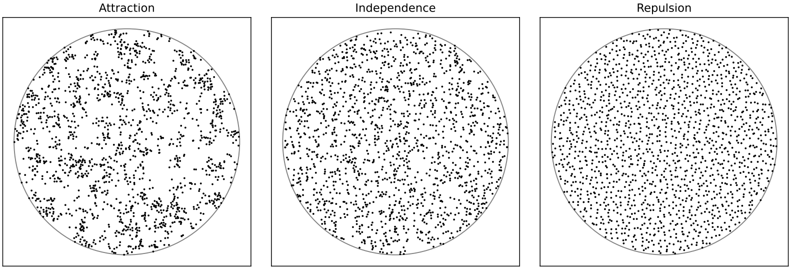


Monte Carlo with a homogeneous Poisson point process (PPP):

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

A. B. Owen. Monte Carlo theory, methods and examples. *Online book*, 2013.

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



Monte Carlo with a determinantal point processes (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. Monte Carlo with determinantal point processes. *The Annals of Applied Probability*, 2020.

J.-F. Coeurjolly, A. Mazoyer, and P.-O. Amblard. Monte Carlo integration of non-differentiable functions on $[0, 1]^i$, $i = 1, \ldots, d$, using a single determinantal point pattern defined on $[0, 1]^d$. *Electronic Journal of Statistics*, 2021.

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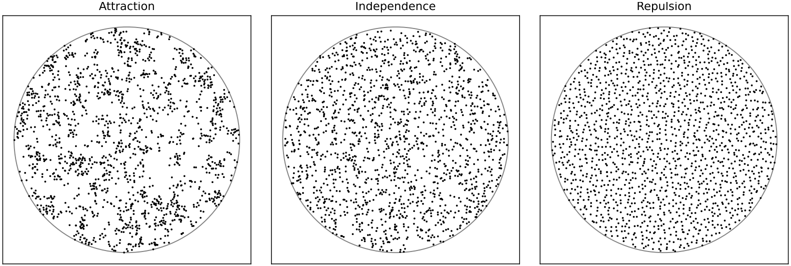


Monte Carlo with a determinantal point processes (DPP) :

- $\mathbb{V}\mathrm{ar}[\widehat{I}_{\mathcal{X}}(f)]^{1/2} = O(N^{-1/2-1/(2d)})$.
- Sampling from the DPP is expensive : at least $O(N^3)$.

R. Bardenet and A. Hardy. Monte Carlo with determinantal point processes. *The Annals of Applied Probability*, 2020.

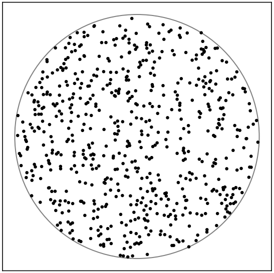
G. Gautier, R. Bardenet, and M. Valko. On two ways to use determinantal point processes for Monte Carlo integration. *Advances in Neural Information Processing Systems*, 2019.

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. Repelled point processes with application to numerical integration. *Preprint*, 2023.

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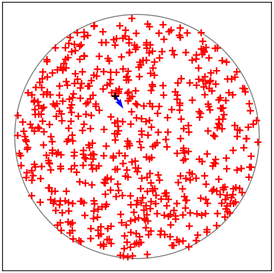
$\mathcal{X}$ a stationary point process of intensity ρ of $\mathbb{R}^d$.

- Force :

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

- Repulsion operator:

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



Sample

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

Chatterjee, Sourav, Ron Peled, Yuval Peres, and Dan Romik. Gravitational Allocation to Poisson Points. *Annals of Mathematics,* 2010.

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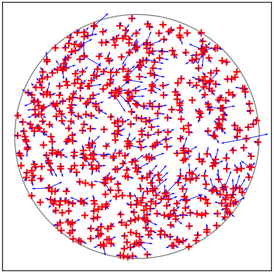

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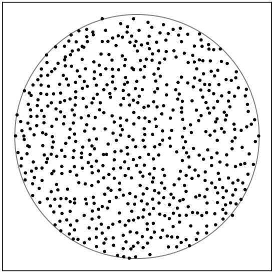
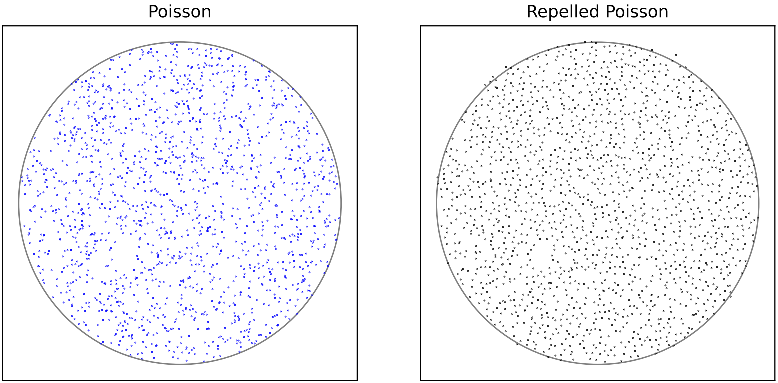


Repelled sample

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

Example



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

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

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

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- For $\varepsilon > 0$ small enough, $f \in C^2(\mathbb{R}^d)$: $\mathbb{V}ar[\widehat{I}_{\Pi_\varepsilon \mathcal{P}}(f)]^{\frac{1}{2}} < \mathbb{V}ar[\widehat{I}_{\mathcal{P}}(f)]^{\frac{1}{2}}$.

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. Repelled point processes with application to numerical integration. *Preprint*, 2023.

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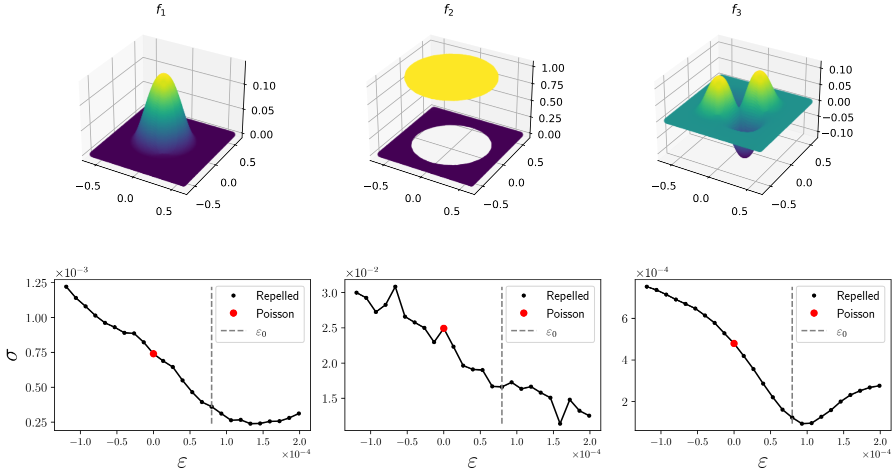
- $\varepsilon_0 = 1/(2d\kappa_d\rho)$.
- The computational complexity is $O(N^2)$ (parallalizable).

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

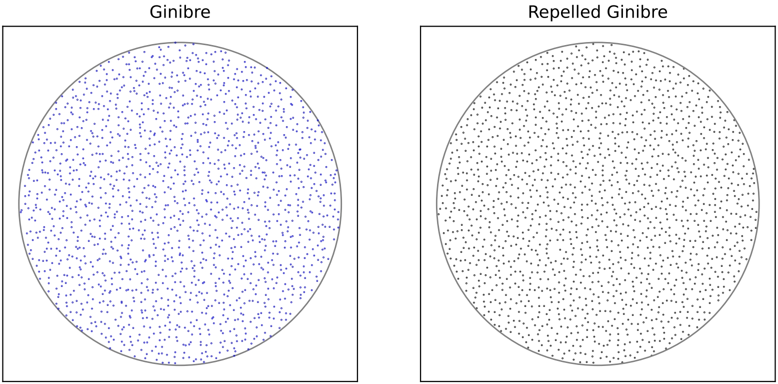
Experiments



Variance for Poisson ($d = 3$)

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

Experiments



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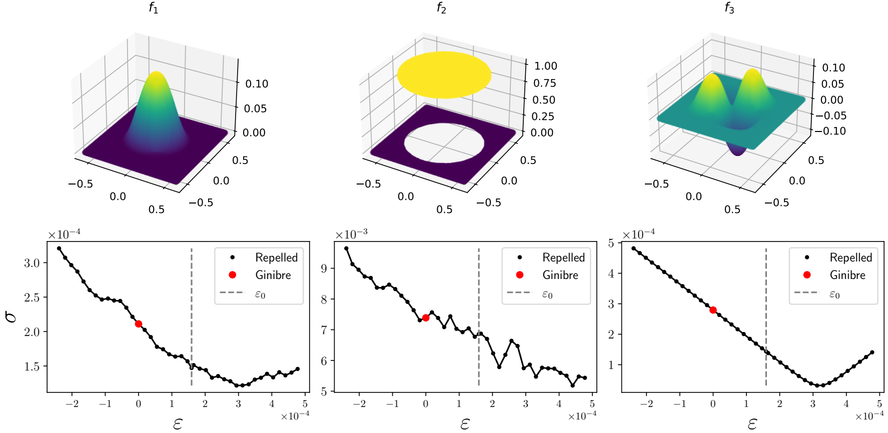

Variance for Ginibre ($d = 2$)

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

Code availability

CI passing | codecov 55% | python >=3.8,<3.10

1. Open-source Python toolbox called MCRPPy.
2. Available on GitHub.
3. Tutorial Jupyter notebook.

MCRPPy

https://github.com/dhawat/MCRPPy

https://github.com/dhawat/MCRPPy/tree/main/notebooks

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

- Variance:

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

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

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

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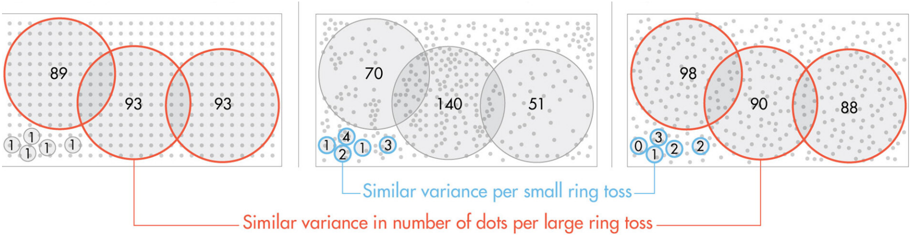

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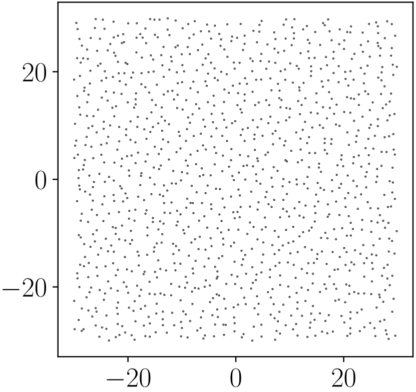
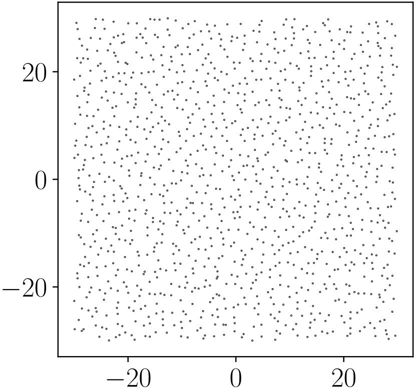
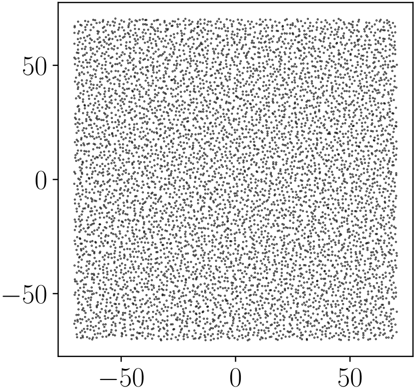
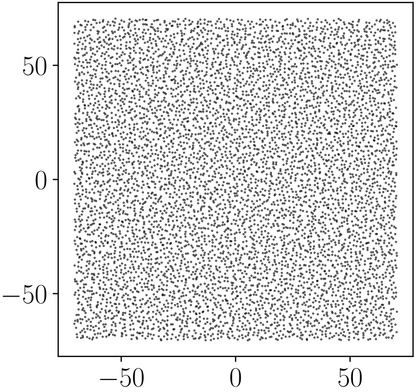
Hyperuniformity





Hyperuniformity





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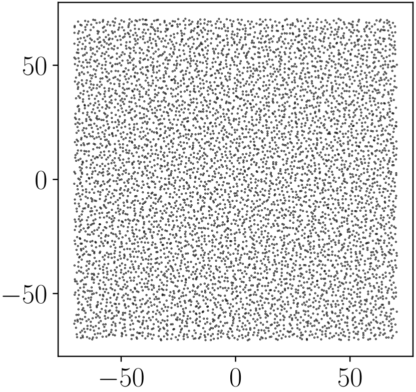

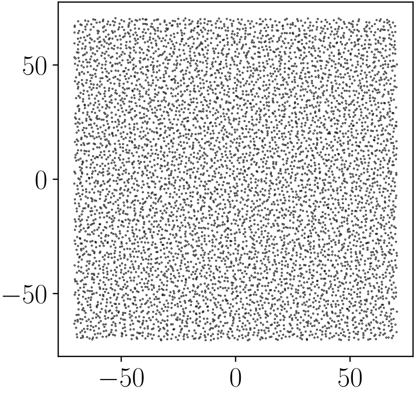

Independent thinning of Ginibre

✔ Ginibre

Hyperuniformity using the structure factor

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

- Structure factor S of $\mathcal{X}$ of intensity ρ

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

- $\mathcal{X}$ is hyperuniform iff

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

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

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

Hyperuniformity class

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

α	$\mathbb{V}\mathrm{ar}\left[\sum_{\mathbf{z}\in\mathcal{X}} \mathbb{1}_{B(0,R)}(\mathbf{z})\right]$	Class
> 1	$O(R^{d-1})$	I
1	$O(R^{d-1}\log(R))$	II
$]0,1[$	$O(R^{d-\alpha})$	III

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$]0,1[$	$O(R^{d-\alpha})$	III

- By appropriately rescaling $\mathcal{X}$, we get an unbiased Monte Carlo method $\widehat{I}_{\mathcal{X}}$ s.t. for f an indicator function we have

Class	$\mathbb{V}\mathrm{ar}[\widehat{I}_{\mathcal{X}}(f)]^{1/2}$
I	$O(N^{-1/2-1/(2d)})$
II	$O(N^{-1/2-1/(2d)}\log(N))$
III	$O(N^{-1/2-\alpha/(2d)})$

D. Hawat. Point processes for numerical integration. *Ph.D. thesis*, 2023.

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

Given a realization of $\mathcal{X}$ in $W = [-L/2, L/2]^d$:

- Estimator of S:

$$\widehat{S}_{\mathrm{SI,s}}(\mathbf{k}) \triangleq \frac{1}{\mathcal{X}(W)} \left| \sum_{z \in \mathcal{X} \cap W} e^{-i\langle \mathbf{k}, \mathbf{z} \rangle} \right|^2, \quad \mathbf{k} \in \mathbb{A}_L^{res}.$$

- Allowed wavevectors:

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

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

M. A. Klatt et al. Universal hidden order in amorphous cellular geometries. *Nature Communications*, 2019.

M. A. Klatt, G. Last, and D. Yogeshwaran. Hyperuniform and rigid stable matchings. *Random Structures Algorithms*, 2020.

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

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

- $S(\mathbf{k}) = \lim_{L\to\infty} \mathbb{E}\underbrace{\Big[\frac{1}{\rho|W|} \Big| \sum_{\mathbf{z}\in\mathcal{X}\cap W} e^{-i\langle \mathbf{k},\mathbf{z}\rangle} \Big|^2 \Big]}_{\widehat{S}_{\mathrm{SI}}(\mathbf{k})} - \rho \underbrace{\Big(\prod_{j=1}^{d} \frac{\sin(k_j L/2)}{k_j \sqrt{L}/2} \Big)^2}_{\epsilon_0(\mathbf{k},\mathbf{L})}.$
- $\epsilon_0(\mathbf{k},\mathbf{L}) = \begin{cases} 0 & \text{if } \mathbf{k} \in \mathbb{A}_{\mathbf{L}} \\ \rho L^d & \text{as } \|\mathbf{k}\|_2 \to 0 \\ 2^{2d} \prod_{j=1}^{d} \frac{1}{L k_j^2} & \text{as } \|\mathbf{k}\|_2 \to \infty \end{cases}$
- $\mathbb{A}_{\mathbf{L}} = \{(k_1, \dots, k_d) \in (\mathbb{R}^d)^*, \exists j \in \{1,\dots,d\}, n \in \mathbb{Z}^* \text{ s.t. } k_j = \frac{2\pi n}{L}\}.$

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.

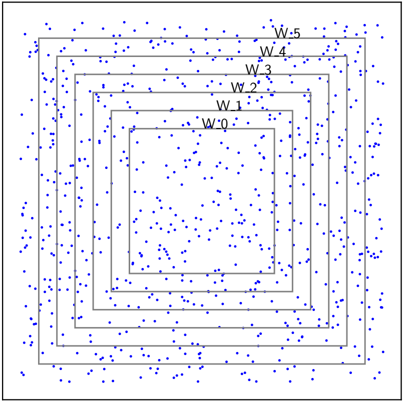
T. Rajala, S. Olhede, J. Grainger, and D. Murrell. What is the Fourier transform of a spatial point process? *IEEE Transactions on Information Theory*, 2023.

Multiscale hyperuniformity test

- Given: Realizations of $\mathcal{X}$ in the window W of lenghtside L (e.g., $W = [-L/2, L/2]^d$).
- Need: Check if $S(\mathbf{0}) = 0$.
- Problem: We don't have an estimator of $S(\mathbf{0})$.
- We have: $S(\mathbf{k}) = \lim_{L \to \infty} \mathbb{E}\left[\widehat{S}(\mathbf{k})\right]$ for $\mathbf{k} \in \mathbb{A}_L$, with $\|\mathbf{k}_{min}\|_2 \sim \frac{C}{L}$.

Multiscale hyperuniformity test

- Consider an increasing sequence of window $\{W_m\}_m$ with $W_\infty = \mathbb{R}^d$.
- Let $\mathbf{k}_m^{\min}$ the minimum wavevector in $\mathbb{A}_{L_m}$, $\mathbf{k}_m^{\min} \xrightarrow[m\to\infty]{} \mathbf{0}$.



Multiscale hyperuniformity test

- Consider an increasing sequence of window $\{W_m\}_m$ with $W_\infty = \mathbb{R}^d$.
- Let $\mathbf{k}_m^{\min}$ the minimum wavevector in $\mathbb{A}_{L_m}$, $\mathbf{k}_m^{\min} \xrightarrow[m\to\infty]{} \mathbf{0}$.
- Take

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

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

C. Rhee and P.W. Glynn. Unbiased estimation with square root convergence for SDE models. *Operations Research*, 2015.

Multiscale hyperuniformity test

- Consider an increasing sequence of window $\{W_m\}_m$ with $W_\infty = \mathbb{R}^d$.
- Let $\mathbf{k}_m^{\min}$ the minimum wavevector in $\mathbb{A}_{L_m}$, $\mathbf{k}_m^{\min} \xrightarrow[m\to\infty]{} \mathbf{0}$.
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with $Y_m = 1 \wedge \widehat{S}_m(\mathbf{k}_m^{\min})$ for $m \geq 1$, $Y_0 = 0$, and M an unbounded $\mathbb{N}$-r.v.

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 $\sup_m \mathbb{E}[\widehat{S}_m^2(\mathbf{k}_m^{\min})] < \infty$, then $\mathbb{E}[Z] \neq 0$.*

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.

Multiscale hyperuniformity test

Need: Check if $\mathbb{E}[Z] = 0$, with $Z = \sum_{j=1}^{M} \frac{Y_j - Y_{j-1}}{\mathbb{P}(M \geq j)}$

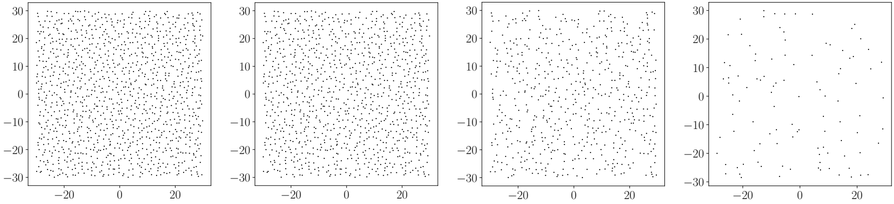
Test:

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

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

Code availability

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/
https://for-a-few-dpps-more.github.io/structure-factor/
https://github.com/For-a-few-DPPs-more/structure-factor/tree/main/notebooks

Conclusion

Repelled point processes [1] :

- Repulsion operator.
- Variance reduction of the repelled Poisson point process.
- Python toolbox `MCRPPy`.

Hyperuniform point processes [2] :

- Estimators of the structure factor.
- Statistical test of hyperuniformity.
- Python toolbox `structure-factor`.

[1] D. Hawat, R. Bardenet, and R. Lachièze-Rey. Repelled point processes with application to numerical integration. *Preprint,* 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.

THANK YOU !

Paper:

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.
3. D. Hawat, G. Gautier, R. Bardenet, and R. Lachieze-Rey. Estimation de la fonction de structure d'un processus ponctuel pour l'étude d'hyperuniformité. *XXVIIIème Colloque Francophone de Traitement du Signal et des Images GRETSI,* 2022.

Software:

1. `MCRPPy`. Python package available on GitHub, 2023.
2. `structure-factor`. Python package available on GitHub and PyPI, 2022.