Estimating the hyperuniformity exponent of point processes

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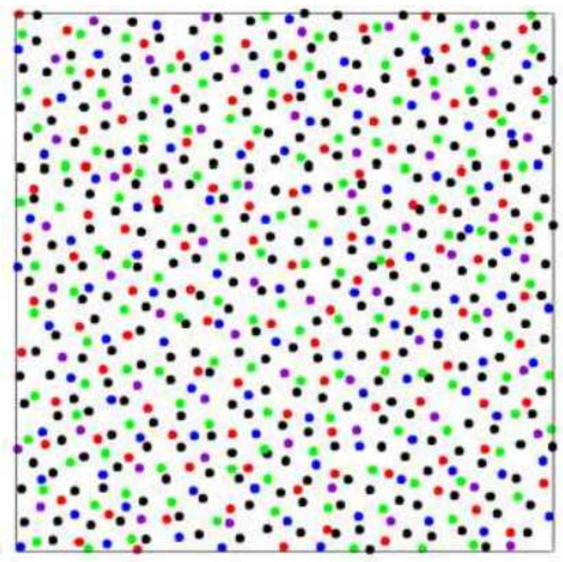
Stochastic Geometry in Action
University of Bath, September 10-13, 2024

A striking feature of nature?

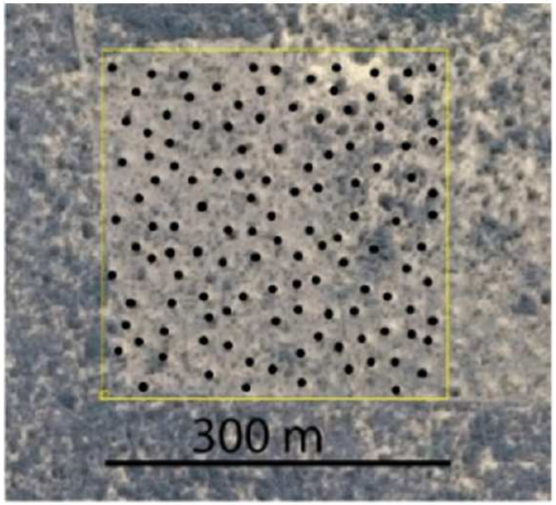


(Jiao et al. 2014)

Avian photoreceptors

(Huang et al. 2021)

Swimming algae



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Termite mounds

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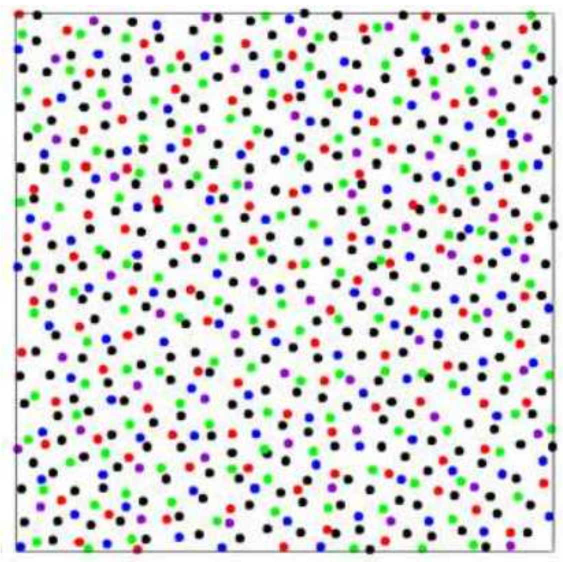

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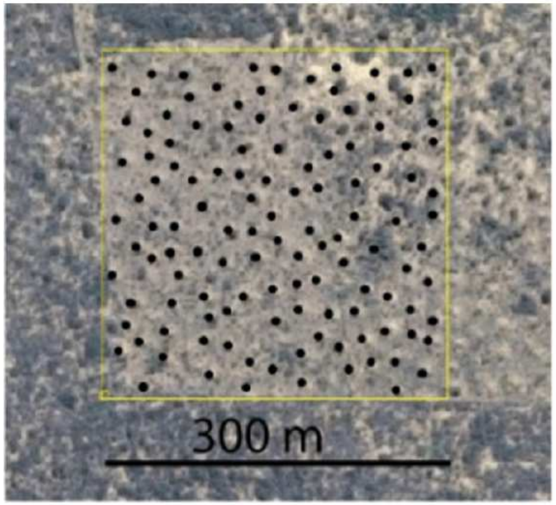

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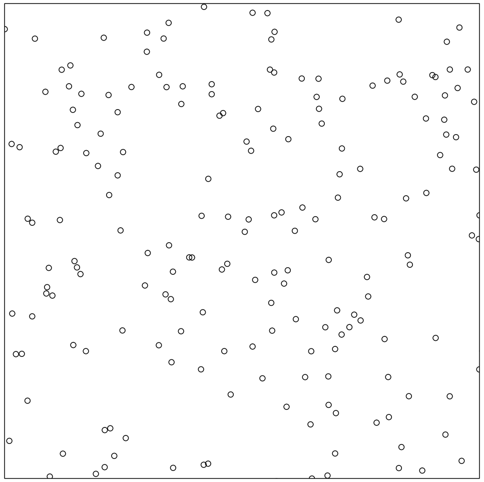
Patterns more "regular" with respect to Poisson model



Examples in physics

- Cristals (Torquato and Stillinger 2003),
- Plasmas Plasmas (Jancovici 1981),
- Gas (Torquato, Scardicchio, and Zachary 2008),
- Fuilds (Lei and Ni 2019),
- Ices (Martelli, Torquato, Giovambattista, and Car 2017),
- Engineering/materials (Gorsky et al. 2019)
- ...

MODELS
All crystals [27], many quasicrystals [32, 33], stealthy and other hyperuniform disordered ground states [62, 63, 65, 68, 143], perturbed lattices [134, 137–139, 145], g_2-invariant disordered point processes [27], one-component plasmas [35, 146], hard-sphere plasmas [147, 148], random organization models [56], perfect glasses [68], and Weyl-Heisenberg ensembles [136].
Some quasicrystals [33], classical disordered ground states [68, 143], zeros of the Riemann zeta function [34, 71], eigenvalues of random matrices [14], fermionic point processes [34], superfluid helium [61, 144], maximally random jammed packings [36, 38, 39, 41, 43], perturbed lattices [137]. density fluctuations in early Universe [17, 18, 145], and perfect glasses [68].
Classical disordered ground states [135], random organization models [52, 54], perfect glasses [68], and perturbed lattices [139].

Hyperuniformity

Hyperuniform point processes

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- Φ is said hyperuniform if

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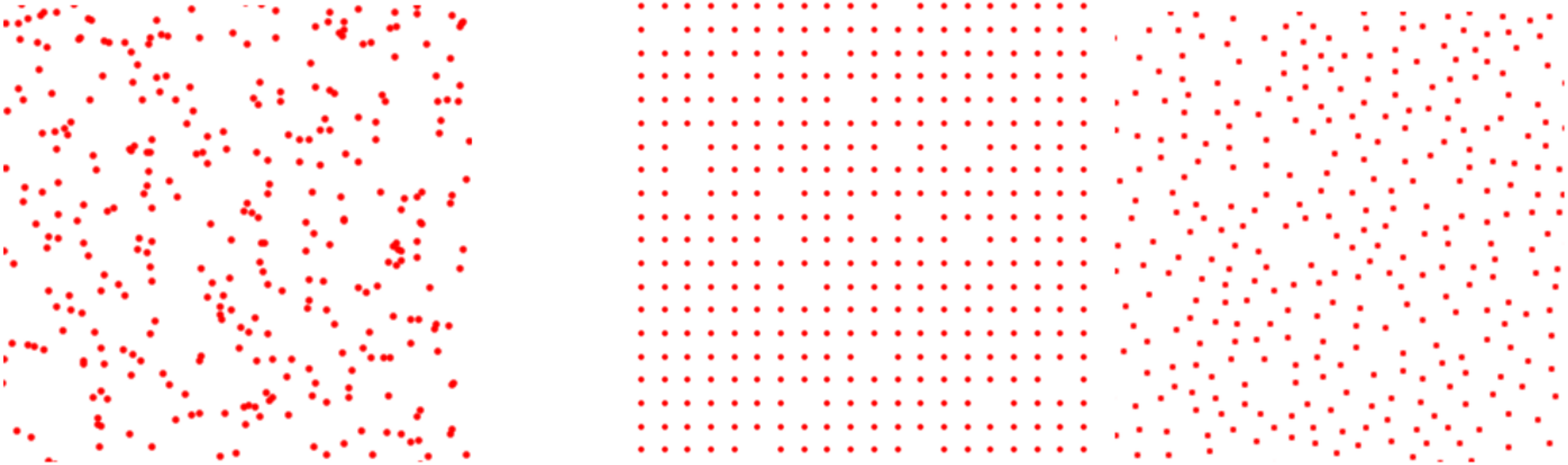
where $B_0(R)$ is a ball of radius R in $\mathbb{R}^d$.
- Remember, for Poisson point process $\mathbf{\Phi}$ (complete independent configuration of points) $\mathbf{Var}[\mathbf{\Phi}(B_0(R))] \sim R^d$.
- Hyperuniformity $\equiv$ sub-Poissonian growth in number variance.

Can you recognize hyperuniformity?



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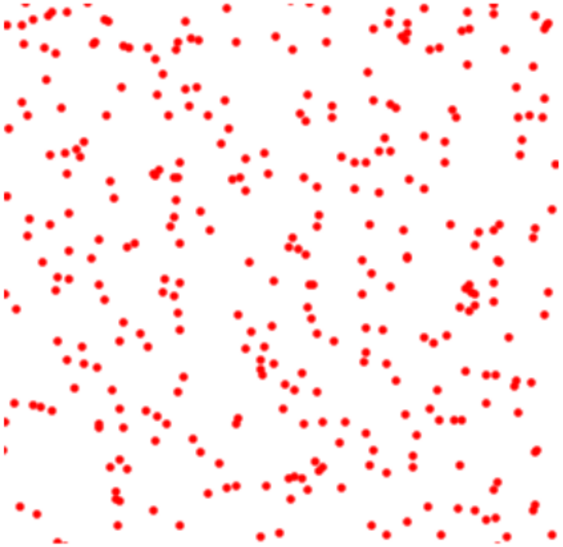
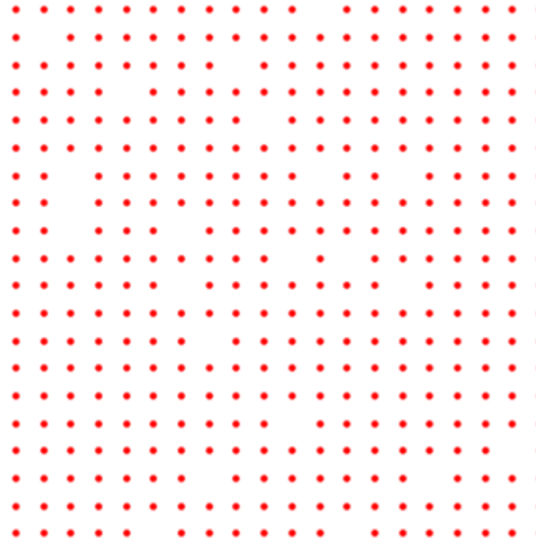
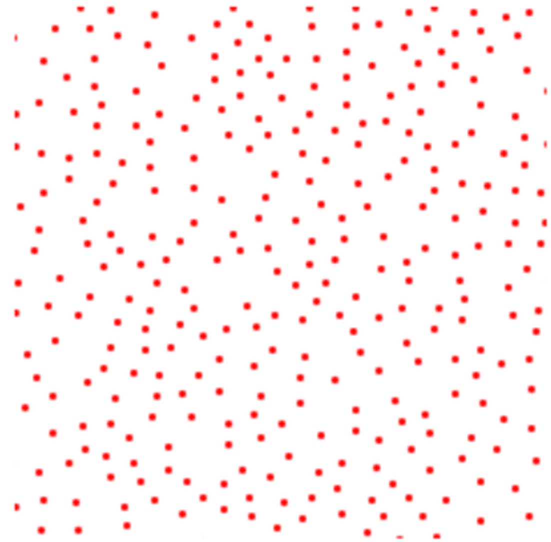


(a) Perturbed Ginibre: hyperuniform.



(b) Thinned URL: not hyperuniform.



(c) Matérn-III (RSA): not hyperuniform.

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- Are there any point processes exhibiting degree $\alpha > 1$?
- No, when counting the points! We need finer tools to capture large-scale fluctuations.
- The reason lies in the indicator function $1(x \in B_0(R))$ used in

$$\mathbf{Var}[\Phi(B_0(R))] = \mathbf{Var}\Big[\sum_{x\in\Phi} 1(x \in B_0(R))\Big] = \mathbf{Var}\Big[\sum_{x\in\Phi} 1\left(\frac{x}{R} \in B_0(1)\right)\Big]$$

which introduces an unavoidable boundary effect of the order of the "surface volume", of all orders R^{d-1}.

Hyperuniformity cases

- By using sufficiently smooth functions $\boldsymbol{f(x)}$ instead of $\mathbf{1}(\boldsymbol{x} \in \boldsymbol{B_0(R)})$, we can observe the variance rate

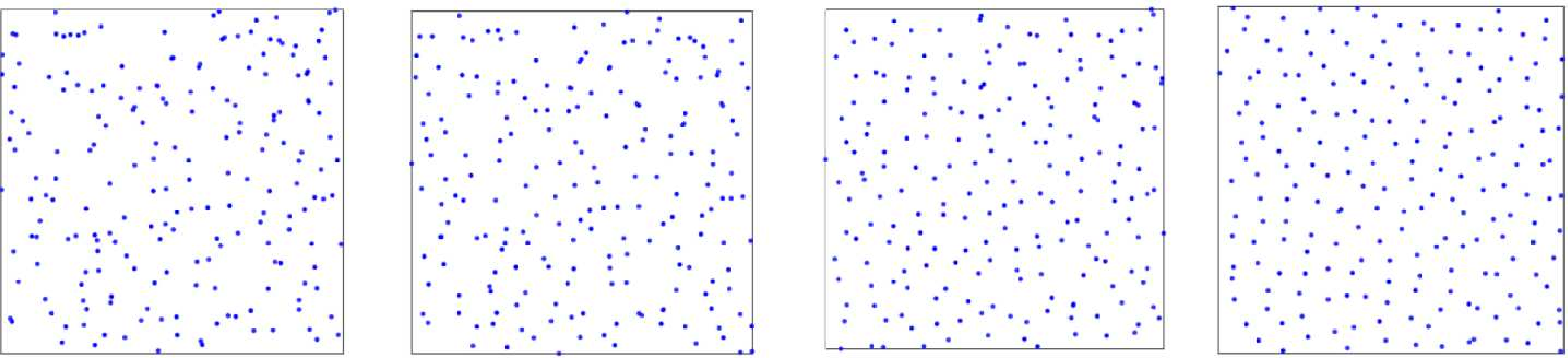
$$\mathbf{Var}\left[\sum_{x\in\Phi} f\left(\frac{x}{R}\right)\right] = O(R^{d-\alpha})$$

for hyperuniform point processes of degree $\boldsymbol{\alpha \geq 0}$.

Examples: perturbed lattices

$$\Phi_\alpha = \{y + U + U_y + V_y | y \in \mathbb{Z}^2\}$$

where U, $(U_y)_{y\in\mathbb{Z}^2}$ are i.i.d. uniform on $[-1/2, 1/2]^2$, and $(V_y)_{y\in\mathbb{Z}^2}$ are i.i.d. with characteristic function φ s.t. $1 - |\varphi(k)|^2 \sim_0 |k|^\alpha$.
(for $V_y \equiv 1$ — cloaked lattice (Klatt, Kim, and Torquato 2020)).



(a) $\alpha = 0.5$ (b) $\alpha = 1$ (c) $\alpha = 2$ (d) $\alpha = 4$

Figure: Different degrees α of hyperuniformity (Torquato 2018).

Hyperuniformity in frequency domain

- Bartlett spectrum (structure factor) S of point process Φ is a complex-valued function on $\mathbb{R}^d$

$$S(k) := 1 + \lambda \mathcal{F}[g - 1](k),$$

where

- $\lambda := \mathbb{E}[\Phi([0,1]^d)]$ intensity of Φ,
- $\mathcal{F}$ denotes the Fourier transform on $\mathbb{R}^d$,
- g is pair-correlation function of Φ (assumed $g - 1 \in L^1(\mathbb{R}^d)$), defined via second correlation function $\rho^{(2)}(dx, dy) = \mathbb{E}[\Phi(dx)\Phi(dy)] = \lambda^2 g(x-y)dxdy$, $x \neq y$.
- Equivalently, g represents (if it exists) the density of the mean measure under reduced Palm probability

$$\mathbb{E}^{0!}[\Phi(B)] = \lambda \int_B g(x)\,dx.$$

Hyperuniformity in frequency domain

- Fourier-Campbell formula: For all $f_1, f_2 \in L^2(\mathbb{R}^d)$:

$$\mathrm{Cov}\left[\sum_{x\in\Phi} f_1(x), \sum_{x\in\Phi} f_2(x)\right] = \lambda \int_{\mathbb{R}^d} \mathcal{F}[f_1](k)\overline{\mathcal{F}[f_2]}(k) S(k) dk.$$

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- Consequently,

$$\mathrm{Var}\left[\sum_{x\in\Phi} f\left(\frac{x}{R}\right)\right] = R^d \times \lambda \int_{\mathbb{R}^d} |\mathcal{F}[f](k)|^2 S(k/R) dk.$$

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- If $S(0) > 0$ then the RHS is $\sim R^d$, hence Φ is not hyperuniform.
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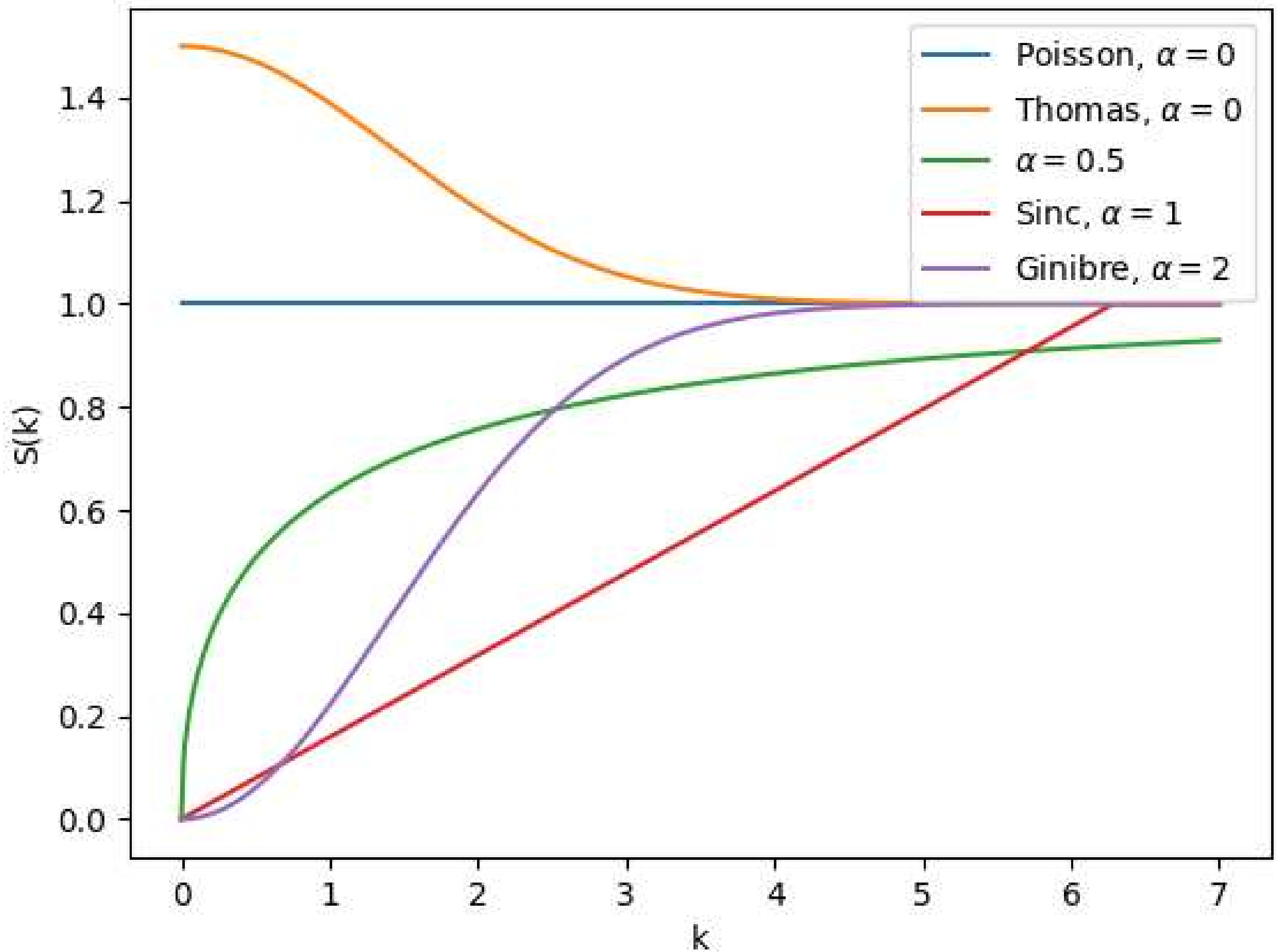
- If moreover f is sufficiently smooth then the RHS is $\sim R^{d-\alpha}$.

Structure function for theoretical point process models



Estimation of α

(on one realization)

Estimation of the degree α of hyperuniformity?

- State-of-the-art [Klatt, Last, Henze (2022), Hawat, Gautier, Bardenet, Lachièze-Rey (2023), ...]:
  1. Estimation of S with $\widehat{S}_R$. Example:

$$\widehat{S}_R(k) = \frac{1}{\#\{\Phi \cap [-R, R]^d\}} \left| \sum_{x \in \Phi \cap [-R,R]^d} e^{-ik.x} \right|^2 .$$

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- Idea: combine the two asymptotic regimes...

The key asymptotic result

- PROPOSITION: Assume: $S(k) \underset{|k|\to 0}{\sim} c|k|^{\alpha}$ ($\alpha \geq 0$, $c > 0$). Let f be a Schwartz function and $j \in (0,1)$ then

$$\mathbf{Var}\left[\sum_{x\in\Phi\cap[-R,R]^d} f(x/R^j)\right] \underset{R\to\infty}{\sim} R^{j(d-\alpha)}\lambda \int_{\mathbb{R}^d} |\mathcal{F}[f](k)|^2 c|k|^{\alpha} dk.$$

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- Remark: If $\int f = 0$,

$$\left(\sum_{x\in\Phi\cap[-R,R]^d} f(x/R^j)\right)^2 = R^{j(d-\alpha)} \times \mathcal{E}(R),$$

where $\mathbf{E}[\mathcal{E}(R)] = O(R)$.

Consistent estimator

- Consider

$$\mathcal{C} := \frac{1}{\log(R)} \log\left\{\left(\sum_{x\in\Phi\cap[-R,R]^d} f(x/R^j)\right)^2\right\} = (d-\alpha)j + \frac{\log(\mathcal{E}(R))}{\log(R)}.$$

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- Exploring the diversity in one realization of Φ: To reduce the variance of $\mathcal{C} = \mathcal{C}(R)$ for $R < \infty$, one can consider employing several "scales" j as well as several functions ("tapers") f...

Multi-scale, multi-tapers estimator

- For several scales $j \in J$, $0 < j < 1$
  and several smooth (Schwartz) function (tapers) f_i, $i \in I$ with $\int f_i = 0$,

  Least-square estimator of α:

  $$\widehat{\alpha} = d - \sum_{j \in J} \frac{\hat{w}_j}{\log(R)} \log \left(\sum_{i \in I} \left(\sum_{x \in \Phi \cap [-R,R]^d} f_i(x/R^j) \right)^2 \right),$$

  with weights:

  $$\forall j \in J,\ \hat{w}_j = \frac{|J| j - \sum_{j' \in J} j'}{|J| \left(\sum_{j' \in J} j'^2 \right) - \left(\sum_{j' \in J} j' \right)^2}.$$

  Two properties: $\sum_{j \in J} \hat{w}_j = 0$ and $\sum_{j \in J} j \hat{w}_j = 1$.

Consistency

- Observe:

$$\widehat{\alpha}(I,J,R)-\alpha=\sum_{j\in J}\frac{\hat{w}_j}{\log(R)}\log\left(\sum_{i\in I}\left(R^{\frac{\alpha-d}{2}j}\sum_{x\in\Phi\cap[-R,R]^d}f_i(x/R^j)\right)^2\right).$$

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- PROPOSITION: Assume:
  - $S(k) \sim c|k|^\alpha$ as $|k| \to 0$, where $\alpha \geq 0$ and $c > 0$.
  - for each $j \in J$, there exists $i_j \in I$ such that:

$$R^{\frac{\alpha-d}{2}j} \sum_{x\in\Phi\cap[-R,R]^d} f_{i_j}(x/R^j) \xrightarrow[R\to\infty]{Law} X_j,$$

  - $\mathbb{P}[X_j = 0] = 0$.

Then $\widehat{\alpha}(I,J,R) \to \alpha$ in probability as $R \to \infty$.

A key tool for asymptotic properties

- THEOREM:(Multivariate central limit theorem) Assume that
  - $S(k) \sim c|k|^{\alpha}$, as $|k| \to 0$ where $c > 0$ and $0 < \alpha < d$,
  - Φ is Brillinger mixing.[1]

  Then:

$$\left(R^{\frac{\alpha-d}{2}j} \sum_{x \in \Phi \cap [-R,R]^d} f_i(x/R^j) \right)_{i \in I, j \in J} \xrightarrow[R\to\infty]{Law} (\sqrt{c} N(i,j,\alpha))_{i \in I, j \in J},$$

where $(N(i,j,\alpha))_{i \in I, j \in J}$ is a Gaussian vector with zero mean and covariance matrix:

$$\Sigma(\alpha) := \left(1_{j_1 = j_2} \int_{\mathbb{R}^d} \mathcal{F}[f_{i_1}](k) \overline{\mathcal{F}[f_{i_2}]}(k) |k|^{\alpha} dk \right)_{(j_1,j_2) \in J^2, (i_1,i_2) \in I^2}.$$

[1] Remember mixing $\mathbb{P}_{\Phi \cap (B_1 \cup (x + B_2))} \xrightarrow{x \to \infty} \mathbb{P}_{\Phi \cap B_1} \times \mathbb{P}_{\Phi \cap B_2}$.
Brillinger mixing concerns the rate of convergence in the mixing process.

Transient confidence intervals

- Under the assumptions of the CLT, let:
  - $a \in (0,1)$,
  - for all $\beta \geq 0$ and $q \in (0,1)$, let $F^{-1}(q;\beta)$ be the quantile of order q of

$$\sum_{j \in J} w_j \log \left(\sum_{i \in I} N(i,j,\beta)^2 \right).$$

Then

$$\left[\widehat{\alpha} - \frac{F^{-1}(1-a/2;(\widehat{\alpha})_+)}{\log(R)},\ \widehat{\alpha} - \frac{F^{-1}(a/2;(\widehat{\alpha})_+)}{\log(R)} \right]$$

is an asymptotic confidence interval of order $1-a$.

Bias and variance

- Assume:
  - $S(k) \sim c|k|^{\alpha}| + c_1|k|^{\beta}$, with $\beta > \alpha \geq 0$ and $c, c_1 > 0$ constants.
  - Φ is Brillinger mixing,
  - $f_i = \psi_i(x) = e^{-\frac{1}{2}|x|^2} \prod_{l=1}^{d} H_{i_l}(x_l)$ where $H_n(y)$ are the Hermite polynomials and $I = \{i \in \mathbb{N}^d | \ |i|_\infty \leq N_I, \ \int \psi_i = 0\}$.

Then, there exists $R_0 > 0$ and $0 < C(\epsilon, J) < \infty$ such that for all $R \geq R_0$:

$$\mathbb{P}\left(\log(R)\left|\widehat{\alpha}(I, J, R) - \alpha\right| \geq \epsilon\right) \leq C(\epsilon, J)\left(\left(\frac{|I|}{R^{2j}}\right)^{\beta-\alpha} + \frac{1}{|I|}\right).$$

- Assume:
  - $S(k) \sim c|k|^{\alpha}| + c_1|k|^{\beta}$, with $\beta > \alpha \geq 0$ and $c, c_1 > 0$ constants.
  - Φ is Brillinger mixing,
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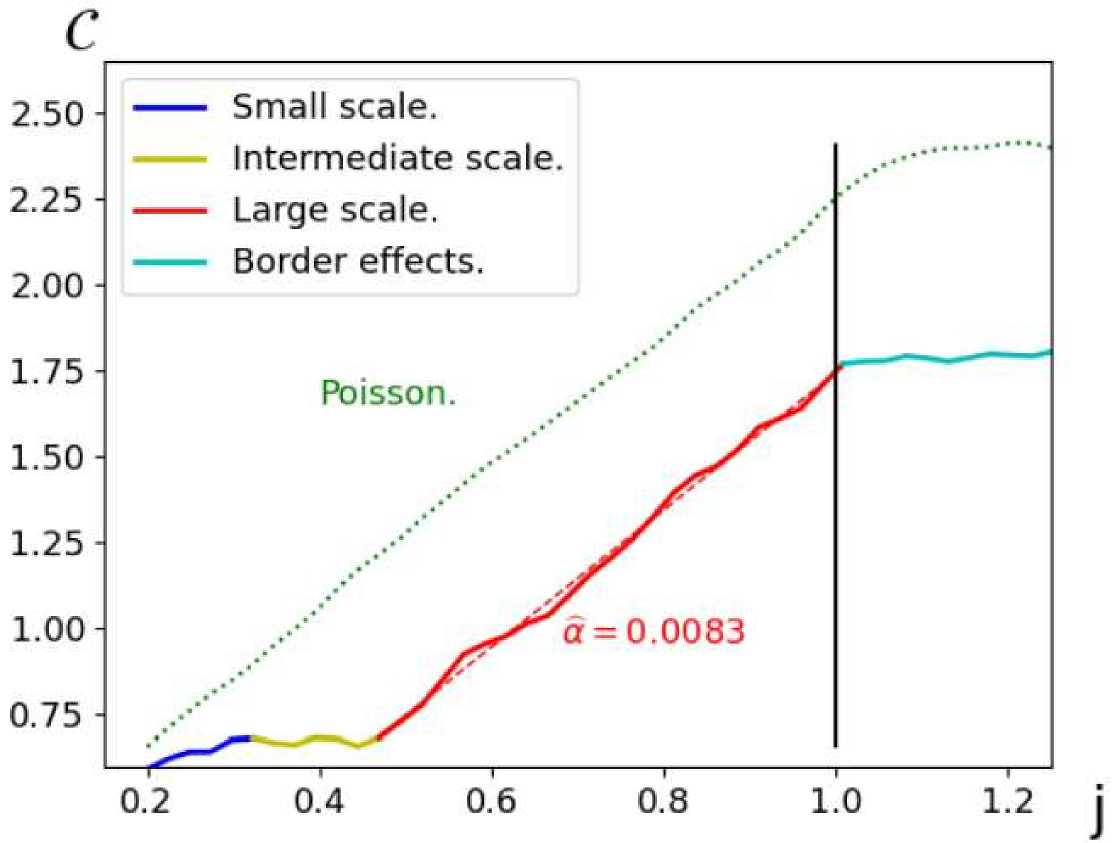
- Variance scales as $|I|^{-1}$, Bias can be high if $|I|$ is large for fixed R.

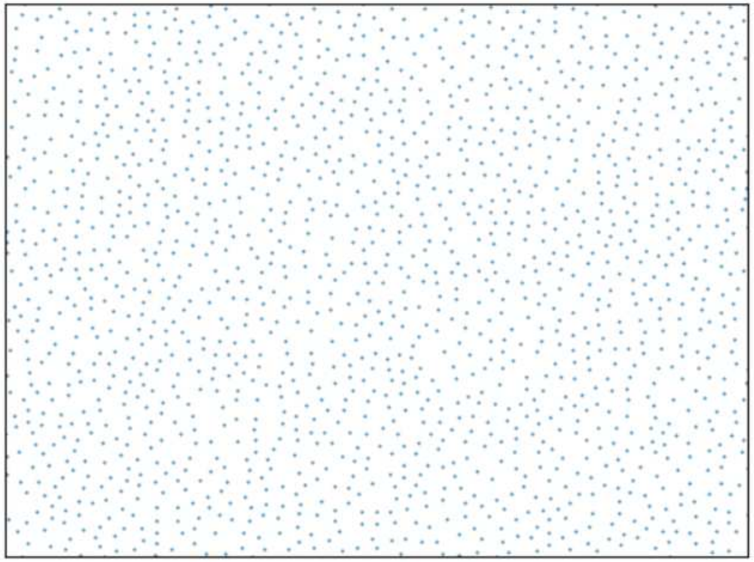
Examples / implementation issues

RSA — non-hyperuniform

$$\widehat{\alpha} = d - \text{ slope of } \mathcal{C}\text{, with}$$

$$\mathcal{C} : j \mapsto \frac{1}{\log(R)} \log \left(\sum_{i \in I} \left(\sum_{x \in \Phi \cap [-R,R]^d} f_i\left(x/R^j\right) \right)^2 \right).$$

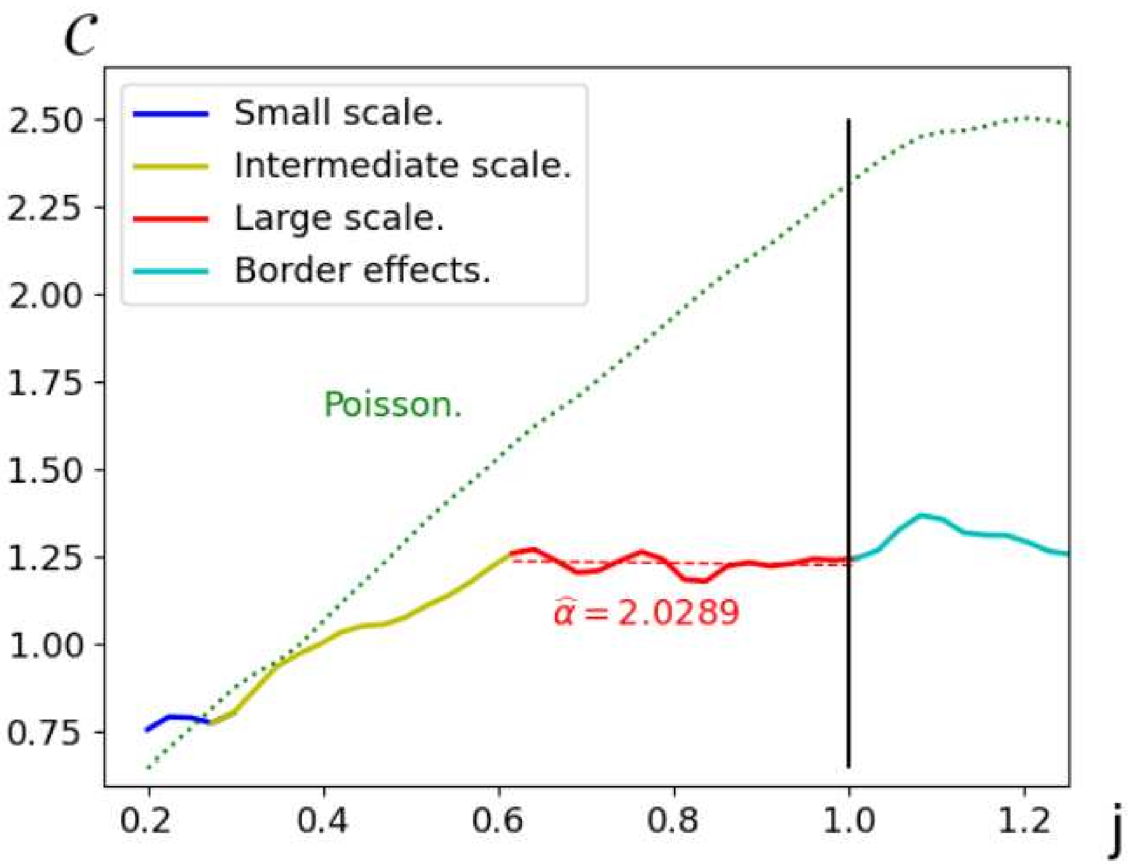


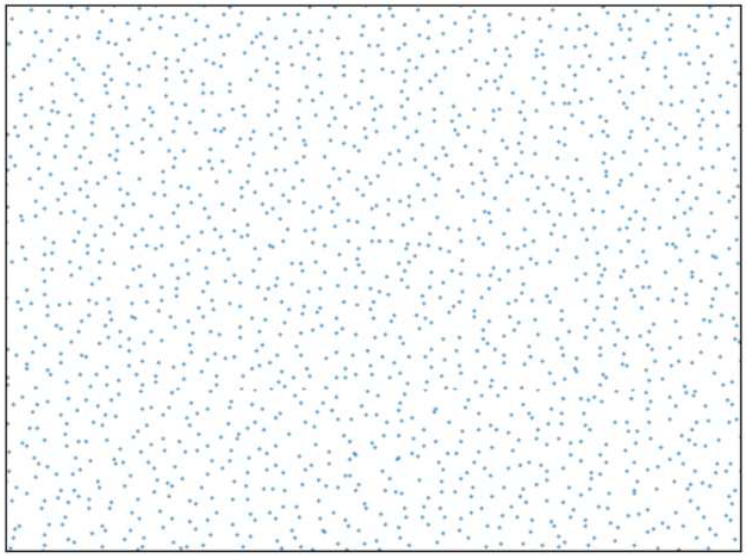


RSA

Matérn-III (RSA) model; 5000 points, $I = \{75 \text{ Hermite tapers}\}$.

Ginibre — strong hyperuniform

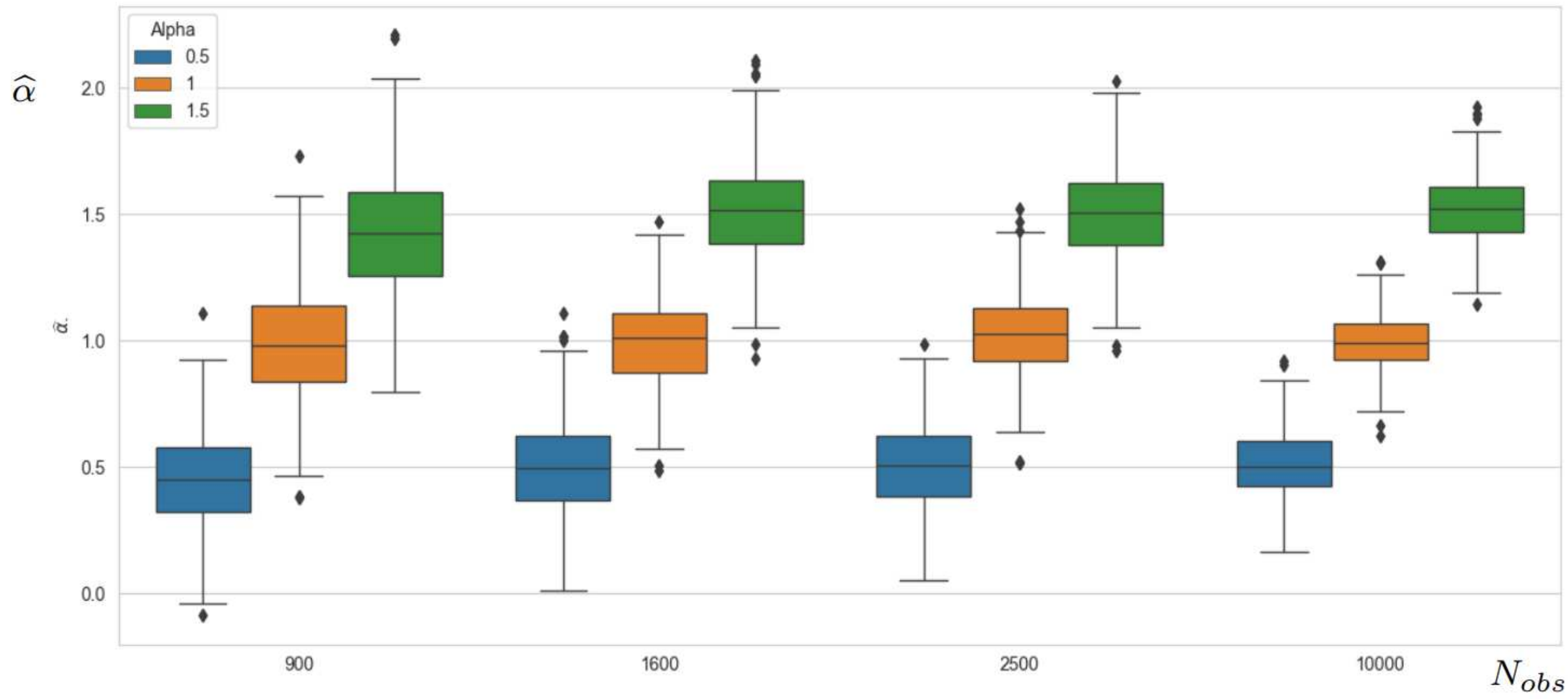




Ginibre

Ginibre model, 1600 points, $I = \{75$ Hermite tapers$\}$.

Benchmark on perturbed lattices

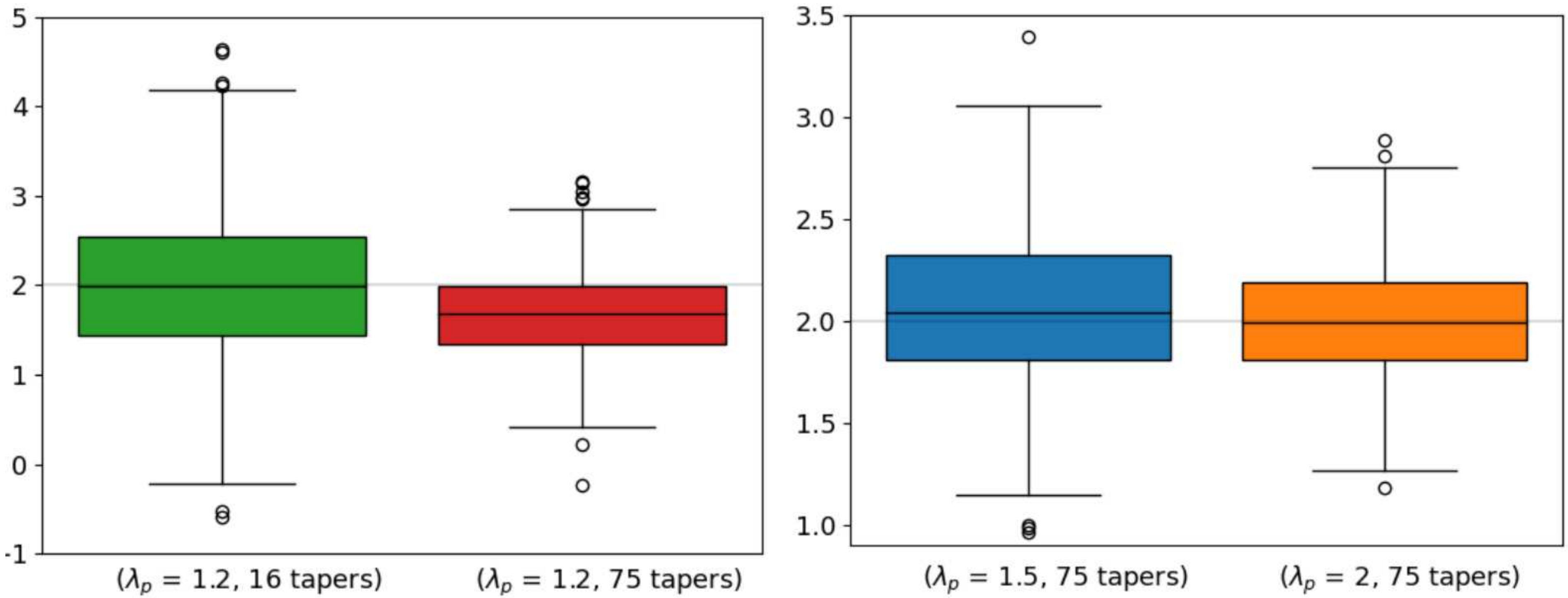


Perturbed lattices, $\alpha = 0.5, 1, 1.5$, N_{obs} number of points, $I = \{75$ Hermite tapers$\}$.

Coverage of 95%-confidence intervals:

α	Average number of points					
	900	1600	2500	3600	4900	6400
0.5	93.2%	93.4%	95.6%	89.9%	94.4%	95.2%
1	92%	93%	95.2%	88.6 %	90.6%	93.8%
1.5	84.2%	88%	91.2%	91.2%	95.2%	95.2%

Points of Poisson p.p. of intensity $\lambda_p > 1$ sequentially, mutual-nearest-neighbour matched to a lattice with intensity 1. Conjecture $\alpha = 2$.



Matching Poisson to lattice — Klatt, Last, Yogeshwaran (2020)

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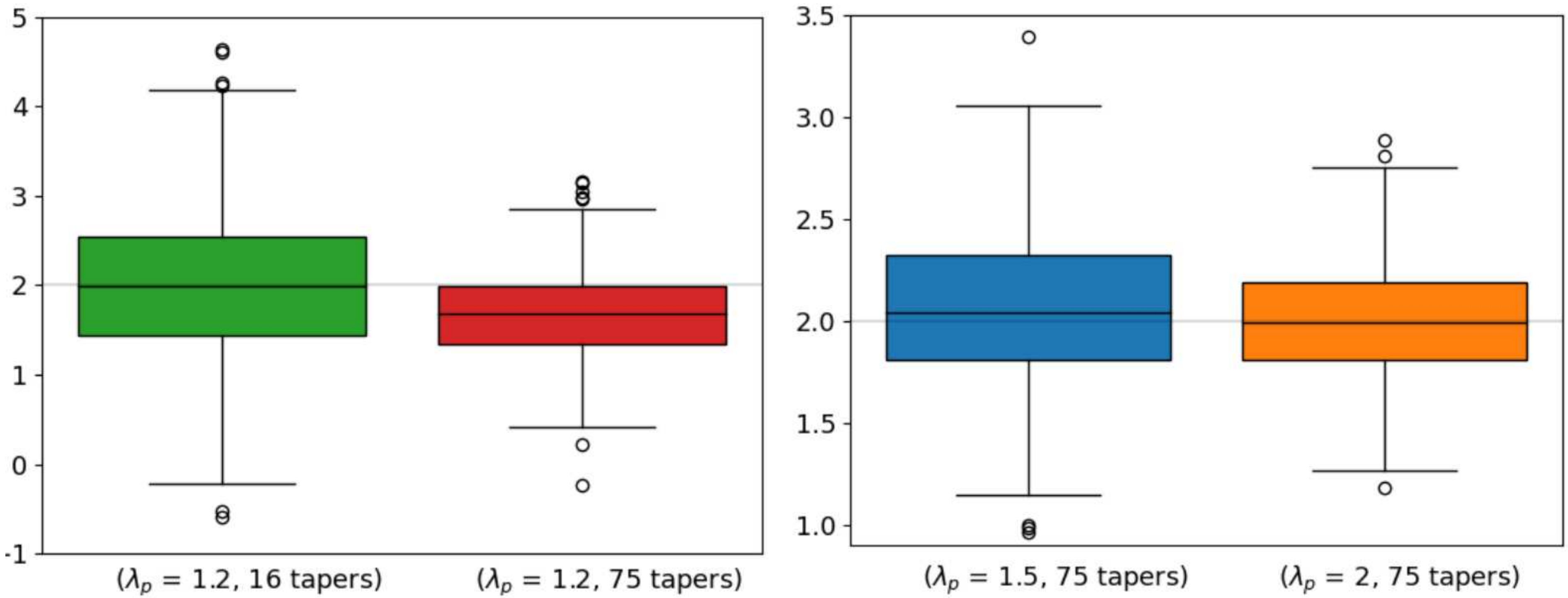
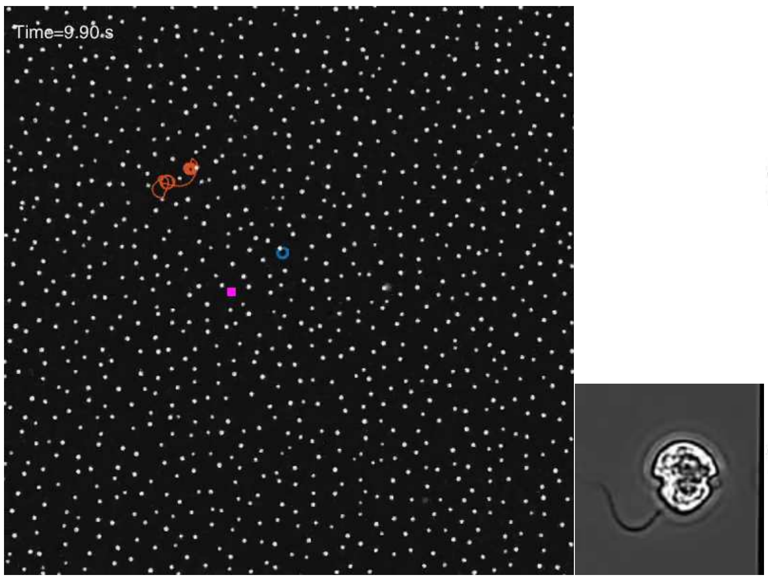
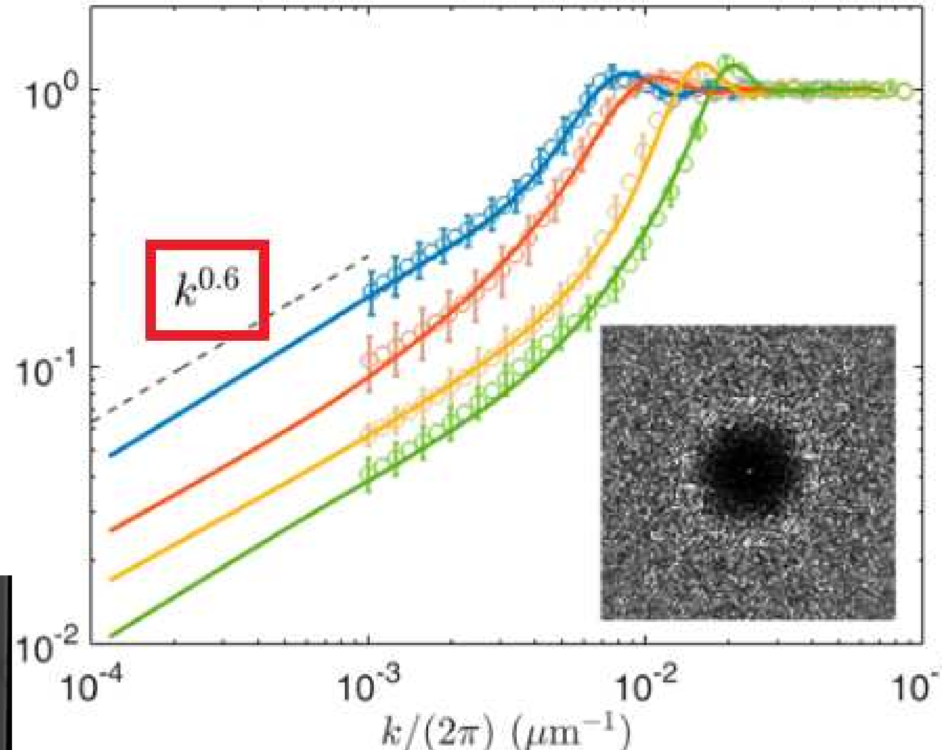


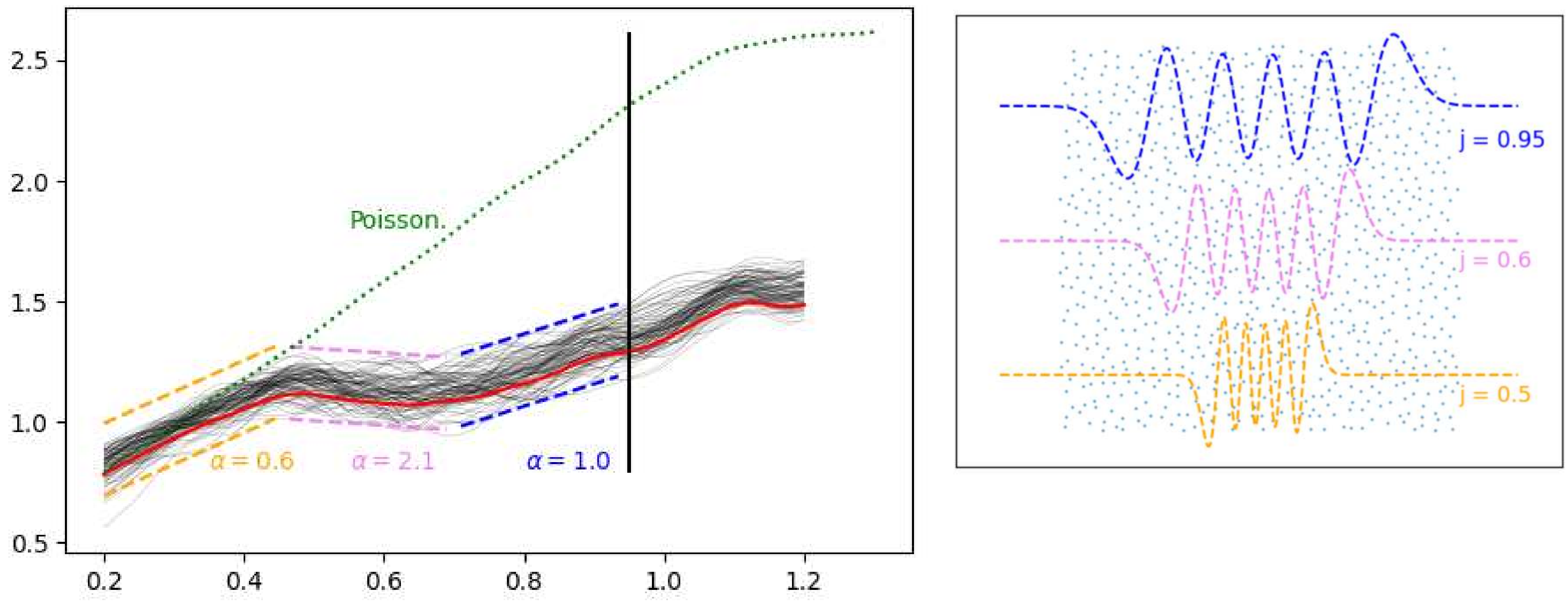
For $\boldsymbol{\lambda_p = 1.2}$ (in left figure) observe the bias-variance tradeoff in the choice of the number of tapers.

Real data — System of marine algae (Huang et al. 2021)





Marine algae — our estimation of α



Estimating α for an algae system (approximately 900 points).

Conclusions

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- Choice of the number of tapers: bias/variance trade-off.

Beyond hyperuniformity

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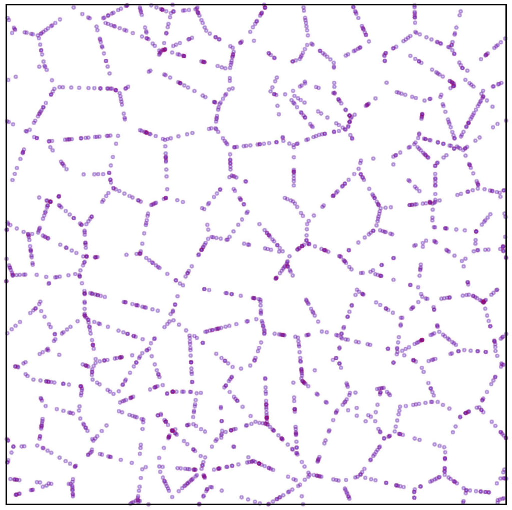
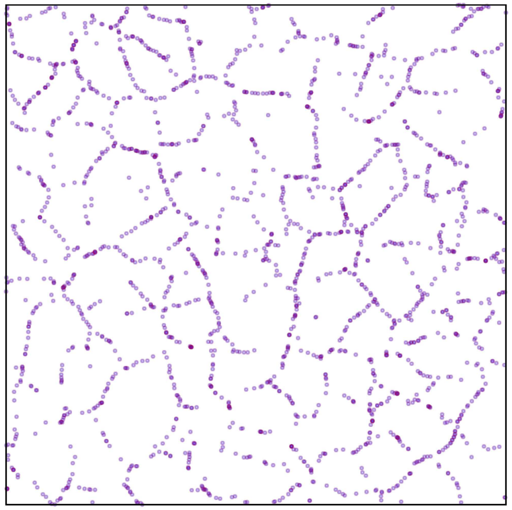
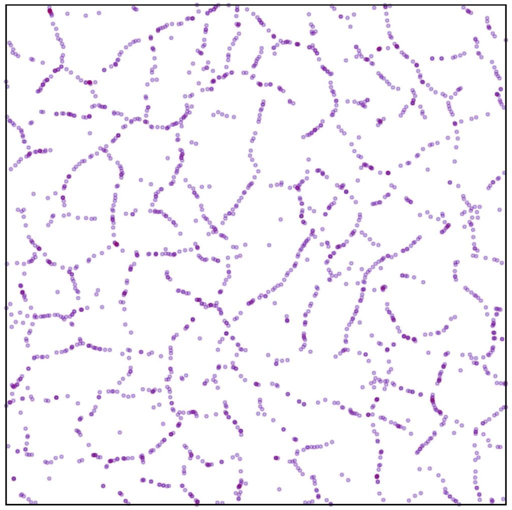
- Recall: Almost surely, any infinite realization of an ergodic point process alows one to fully characterize its distribution and thus (in principle) to sample from this distribution new realizations. $\Rightarrow$ Spatial averaging!

- But in practice, we have only a finite learning window. Can we get approximations of the unknown distribution?

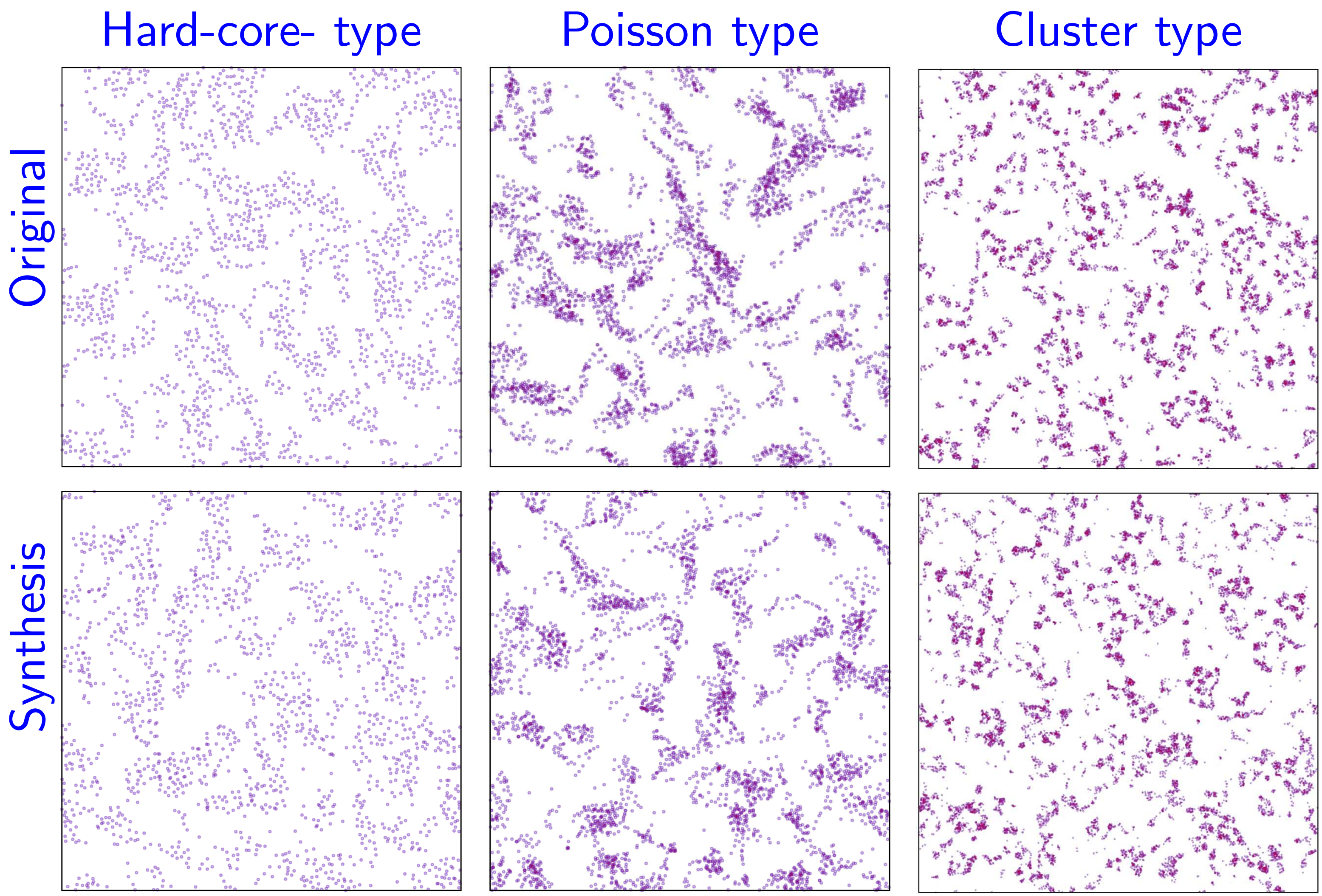

Original image


Synthesis 1


Synthesis 2

samples from "ergodic learning model"

Learning some "model-less" processes?



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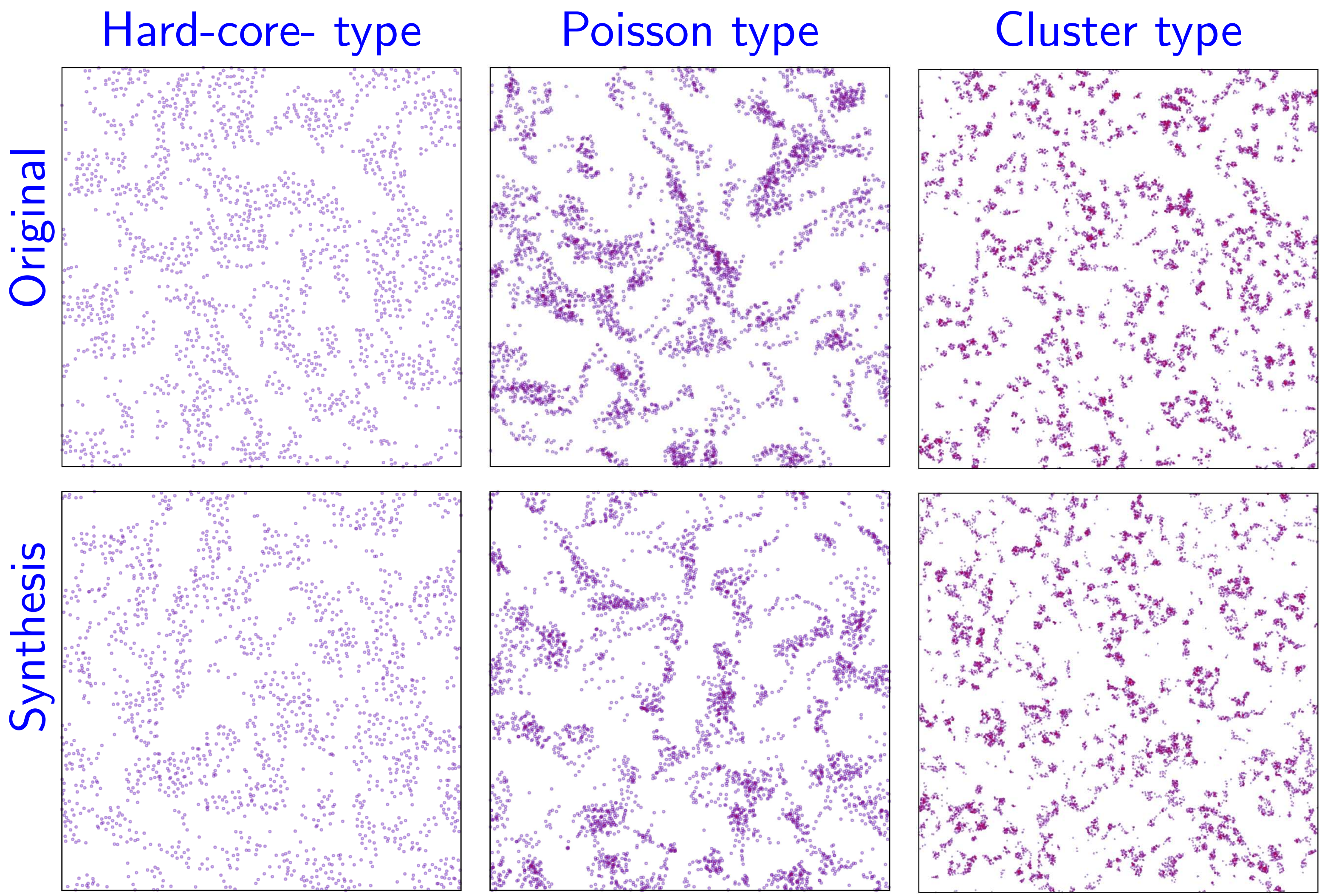

[Brochard, BB, Mallat, Zhang (2022)]; but that is for another talk.

For more details, see:

- Mastrilli, G., BB, Lavancier, F. (2024). Estimating the hyperuniformity exponent of point processes. arXiv:2407.16797
- Klatt, M. A., Last, G. and Henze, N. A genuine test for hyperuniformity. (2022) *arXiv:2210.12790*
- Hawat, D., Gautier, G., Bardenet, R. and Lachièze-Rey, R. On estimating the structure factor of a point process, with applications to hyperuniformity. (2023) *Statistics and Computing*
- Klatt M., Last, G. and Yogeshwaran, D. (2020). Hyperuniform and rigid stable matchings. *Random Structures & Algorithms*
- Brochard, A., BB, Mallat, S. and Zhang, S. (2022). Particle gradient descent model for point process generation. *Statistics and Computing*
- Torquato, S. Hyperuniform states of matter. (2018) *Physics Reports*
- Torquato, S. and Stillinger, F. H. Local density fluctuations, hyperuniformity, and order metrics. (2003) *Physical Review E.*
- ...

Thanks for your attention!