

Statistical aspects of determinantal point processes

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Joint work with

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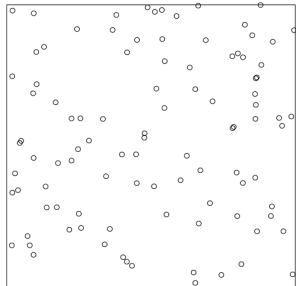
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- 1 Introduction
- 2 Definition, existence and basic properties
- 3 Simulation
- 4 Parametric models
- 5 Inference

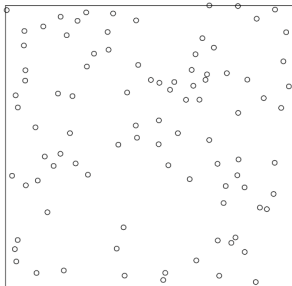
Introduction

- Determinantal point processes (DPP) form a class of repulsive point processes.
- They were introduced in their general form by O. Macchi in 1975 to model fermions (i.e. particles with repulsion) in quantum mechanics.
- Particular cases include the law of the eigenvalues of certain random matrices (Gaussian Unitary Ensemble, Ginibre Ensemble,...)
- Most theoretical studies have been published in the 2000's.
- The statistical aspects have so far been largely unexplored.

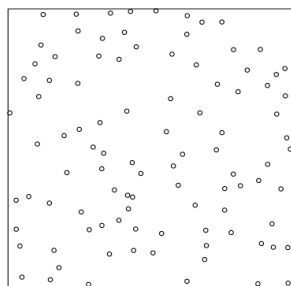
Examples



Poisson



DPP



DPP with
stronger repulsion

Statistical motivation

Do DPP's constitute a *tractable* and *flexible* class of models for *repulsive* point processes?

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These properties are unusual for Gibbs point processes which are commonly used to model inhibition (e.g. the Strauss process).

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- For any integer $n > 0$, denote $\rho^{(n)}$ the n 'th *order product density function* of X .

Intuitively,

$$\rho^{(n)}(x_1, \dots, x_n) dx_1 \cdots dx_n$$

is the probability that for each $i = 1, \dots, n$,
 X has a point in a region around x_i of volume dx_i .

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In particular $\rho = \rho^{(1)}$ is the *intensity function*.

Definition of a determinantal point process

For any function $C : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{C}$, denote $[C](x_1, \dots, x_n)$ the $n \times n$ matrix with entries $C(x_i, x_j)$.

Ex.: $[C](x_1) = C(x_1, x_1)$ $[C](x_1, x_2) = \begin{pmatrix} C(x_1, x_1) & C(x_1, x_2) \\ C(x_2, x_1) & C(x_2, x_2) \end{pmatrix}$.

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Definition

X is a *determinantal point process* with *kernel* C , denoted $X \sim \text{DPP}(C)$, if its product density functions satisfy

$$\rho^{(n)}(x_1, \dots, x_n) = \det[C](x_1, \dots, x_n), \quad n = 1, 2, \dots$$

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For existence, conditions on the kernel C are mandatory, e.g. C must satisfy: for all x_1, \dots, x_n , $\det[C](x_1, \dots, x_n) \geq 0$.

First properties

- From the definition, if C is continuous,

$$\rho^{(n)}(x_1, \dots, x_n) \approx 0 \quad \text{whenever} \quad x_i \approx x_j \quad \text{for some } i \neq j,$$

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$$g(x, y) := \frac{\rho^{(2)}(x, y)}{\rho(x)\rho(y)} = 1 - \frac{C(x, y)C(y, x)}{C(x, x)C(y, y)}$$

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- Thus $g \leq 1$ (i.e. repulsiveness).
- If $X \sim \text{DPP}(C)$, then $X_B \sim \text{DPP}_B(C_B)$
- Any smooth transformation or independent thinning of a DPP is still a DPP with explicit given kernel.
- There exists at most one $\text{DPP}(C)$.

Existence

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By Mercer's theorem, for any compact set $S \subset \mathbb{R}^d$, C restricted to $S \times S$, denoted C_S , has a spectral representation,

$$C_S(x, y) = \sum_{k=1}^{\infty} \lambda_k^S \phi_k^S(x) \overline{\phi_k^S(y)}, \quad (x, y) \in S \times S,$$

where $\lambda_k^S \geq 0$ and $\int_S \phi_k^S(x) \overline{\phi_l^S(x)} dx = \mathbf{1}_{\{k=l\}}$.

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Theorem (Macchi, 1975; Hough et al., 2009; our paper)

Under (C1), existence of DPP(C) is equivalent to that

$$\lambda_k^S \leq 1 \text{ for all compact } S \subset \mathbb{R}^d \text{ and all } k.$$

Density on a compact set S

Let $X_S \sim \text{DPP}_S(C_S)$ with $S \subset \mathbb{R}^d$ compact.

Recall that $C_S(x, y) = \sum_{k=1}^{\infty} \lambda_k^S \phi_k^S(x) \overline{\phi_k^S(y)}$.

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Theorem (Macchi, 1975)

Assuming $\lambda_k^S < 1$, for all k , then X_S is absolutely continuous with respect to the homogeneous Poisson process on S with unit intensity, and has density

$$f(\{x_1, \dots, x_n\}) = \exp(|S| - D) \det[\tilde{C}](x_1, \dots, x_n),$$

where $D = -\sum_{k=1}^{\infty} \log(1 - \lambda_k^S)$ and $\tilde{C} : S \times S \rightarrow \mathbb{C}$ is given by

$$\tilde{C}(x, y) = \sum_{k=1}^{\infty} \frac{\lambda_k^S}{1 - \lambda_k^S} \phi_k^S(x) \overline{\phi_k^S(y)}$$

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Theorem (Hough et al., 2006)

For $k \in \mathbb{N}$, let B_k be independent Bernoulli r.v.'s with means λ_k^S . Define

$$K(x, y) = \sum_{k=1}^{\infty} B_k \phi_k^S(x) \overline{\phi_k^S(y)}, \quad (x, y) \in S \times S.$$

Then $\text{DPP}_S(C_S) \stackrel{d}{=} \text{DPP}_S(K)$.

So simulating X_S is equivalent to simulate $\text{DPP}_S(K)$ with

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In step 3, the kernel K becomes a *projection kernel*, and w.l.o.g.

$$K(x, y) = \sum_{k=1}^n \phi_k^S(x) \overline{\phi_k^S(y)}$$

where $n = \#\{1 \leq k \leq M : B_k = 1\}$.

Simulation of determinantal projection processes

Denoting $\mathbf{v}(x) = (\phi_1^S(x), \dots, \phi_n^S(x))^T$, we have

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set $\mathbf{e}_1 = \mathbf{v}(X_n)/\|\mathbf{v}(X_n)\|$.

for $i = (n - 1)$ to 1 **do**

sample X_i from the distribution (given X_{i+1}, \dots, X_n) :

$$p_i(x) = \frac{1}{i} \left[\|\mathbf{v}(x)\|^2 - \sum_{j=1}^{n-i} |\mathbf{e}_j^* \mathbf{v}(x)|^2 \right], \quad x \in S$$

set $\mathbf{w}_i = \mathbf{v}(X_i) - \sum_{j=1}^{n-i} (\mathbf{e}_j^* \mathbf{v}(X_i)) \mathbf{e}_j$, $\mathbf{e}_{n-i+1} = \mathbf{w}_i/\|\mathbf{w}_i\|$

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Theorem

$\{X_1, \dots, X_n\}$ generated as above has distribution $\text{DPP}_S(K)$.

Illustration of simulation algorithm

Example: Let $S = [-1/2, 1/2]^2$ and

$$\phi_k(x) = e^{2\pi i k \cdot x}, \quad k \in \mathbb{Z}^2, \quad x \in S,$$

for a set of indices k_1, \dots, k_n in \mathbb{Z}^2 .

So the projection kernel writes

$$K(x, y) = \sum_{j=1}^n e^{2\pi i k_j \cdot (x-y)}$$

and $X_S \sim \text{DPP}_S(K)$ is homogeneous and has a.s. n points.

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Step 2. The next point is sampled w.r.t. the following density :

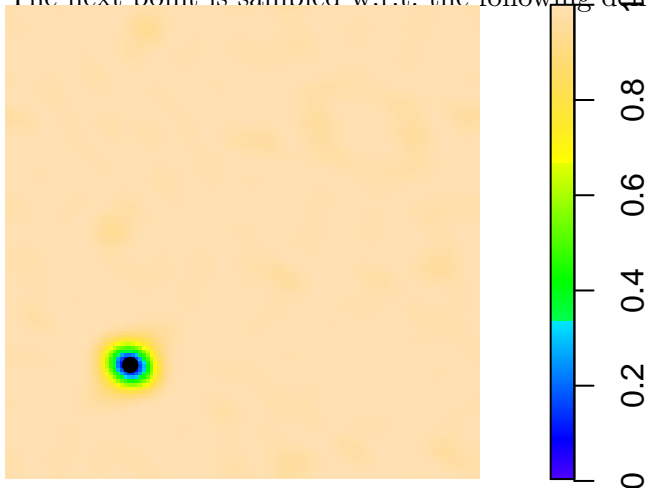


Illustration of simulation algorithm

Step 3. The next point is sampled w.r.t. the following density :

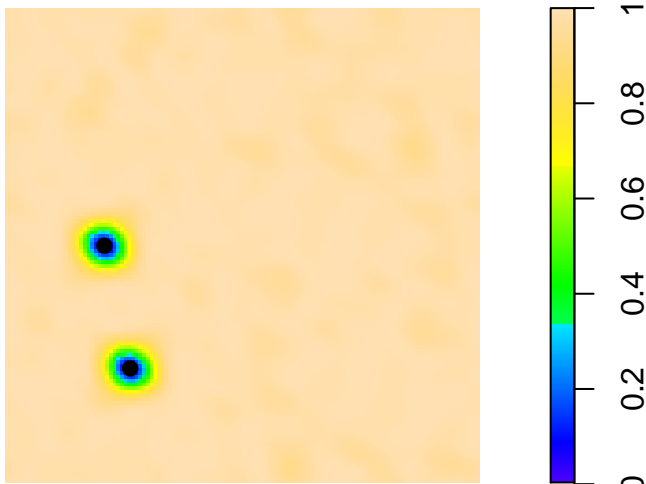


Illustration of simulation algorithm

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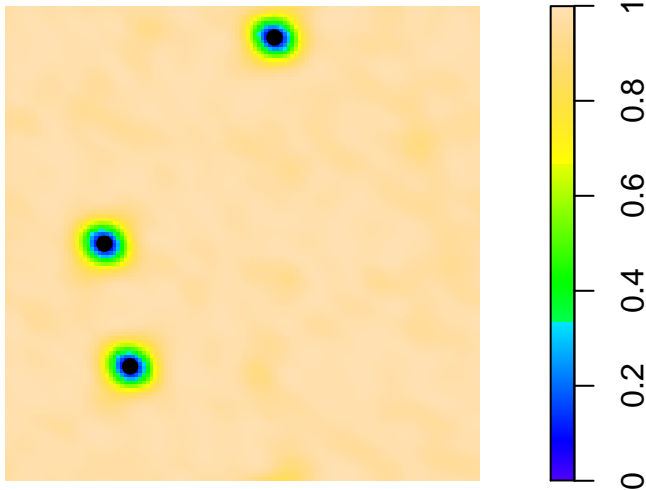


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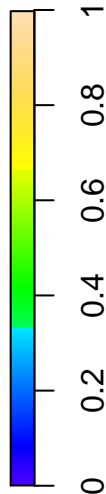
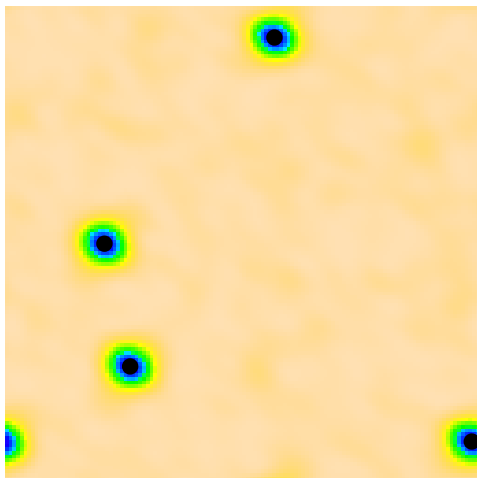


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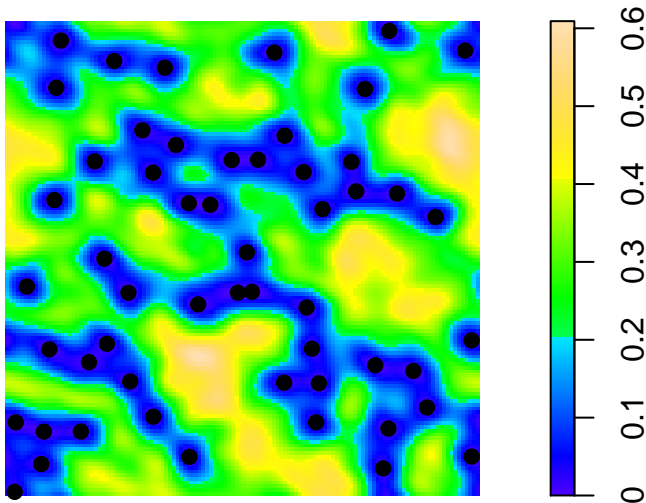
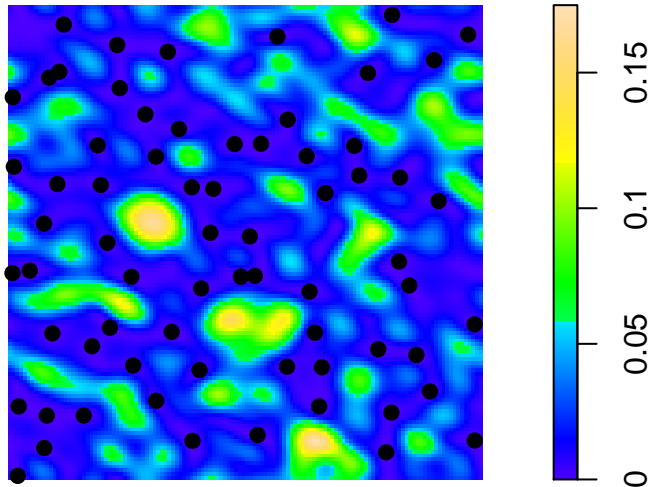


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Stationary models

We focus on a kernel C of the form

$$C(x, y) = C_0(x - y), \quad x, y \in \mathbb{R}^d.$$

(C1) C_0 is a continuous covariance function

Moreover, if $C_0 \in L^2(\mathbb{R}^d)$ we can define its Fourier transform

$$\varphi(x) = \int C_0(t) e^{-2\pi i x \cdot t} dt, \quad x \in \mathbb{R}^d.$$

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Theorem

Under (C1), if $C_0 \in L^2(\mathbb{R}^d)$, then existence of $DPP(C_0)$ is equivalent to

$$\varphi \leq 1.$$

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Under (C1), if $C_0 \in L^2(\mathbb{R}^d)$, then existence of DPP(C_0) is equivalent to

$$\varphi \leq 1.$$

To construct parametric families of DPP :

Consider parametric families of C_0 and rescale so that $\varphi \leq 1$.

→ This will induce a bound on the parameter space.

Several parametric families of covariance function are available, with closed form expressions for their Fourier transform.

- For $d = 2$, the circular covariance function with range α is given by

$$C_0(x) = \rho \frac{2}{\pi} \left(\arccos(\|x\|/\alpha) - \|x\|/\alpha \sqrt{1 - (\|x\|/\alpha)^2} \right) \mathbf{1}_{\|x\| < \alpha}.$$

DPP(C_0) exists iff $\varphi \leq 1 \Leftrightarrow \rho\alpha^2 \leq 4/\pi$.

\Rightarrow Tradeoff between the intensity ρ and the range of repulsion α .

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- Whittle-Matérn (includes Exponential and Gaussian) :

$$C_0(x) = \rho \frac{2^{1-\nu}}{\Gamma(\nu)} \|x/\alpha\|^\nu K_\nu(\|x/\alpha\|), \quad x \in \mathbb{R}^d.$$

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- Generalized Cauchy

$$C_0(x) = \frac{\rho}{(1 + \|x/\alpha\|^2)^{\nu+d/2}}, \quad x \in \mathbb{R}^d.$$

DPP(C_0) exists iff $\rho \leq \frac{\Gamma(\nu+d/2)}{\Gamma(\nu)(\sqrt{\pi}\alpha)^d}$.

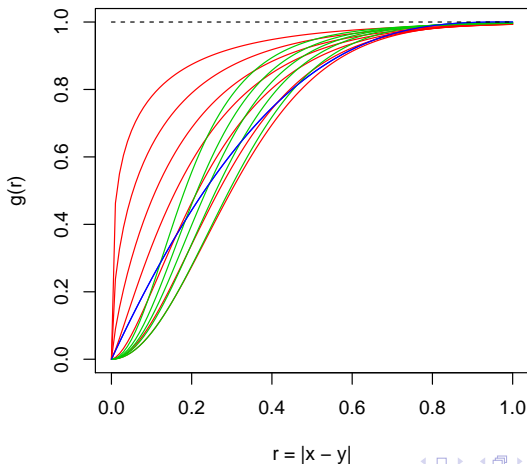
Pair correlation functions of $\text{DPP}(C_0)$ for previous models :

In blue : C_0 is the **circular** covariance function.

In red : C_0 is **Whittle-Matérn**, for different values of ν

In green : C_0 is generalized **Cauchy**, for different values of ν

The parameter α is chosen such that the range of corr. ≈ 1 .



Spectral approach

- Specify a parametric class of integrable functions $\varphi_\theta : \mathbb{R}^d \rightarrow [0, 1]$ (spectral densities).
- This is all we need for having a well-defined DDP.
- Is convenient for simulation and for (approximate) density calculations as seen later.

Spectral approach

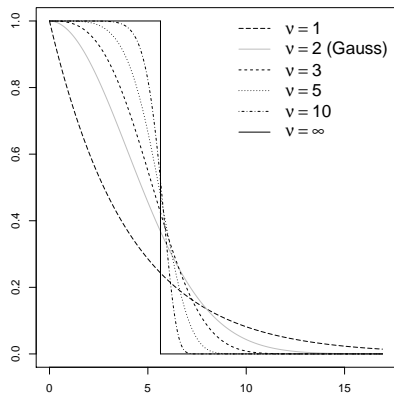
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- This is all we need for having a well-defined DDP.
- Is convenient for simulation and for (approximate) density calculations as seen later.
- Example: *power exponential spectral model*:

$$\varphi_{\rho, \nu, \alpha}(x) = \rho \frac{\Gamma(d/2 + 1) \nu \alpha^d}{d \pi^{d/2} \Gamma(d/\nu)} \exp(-\|\alpha x\|^\nu)$$

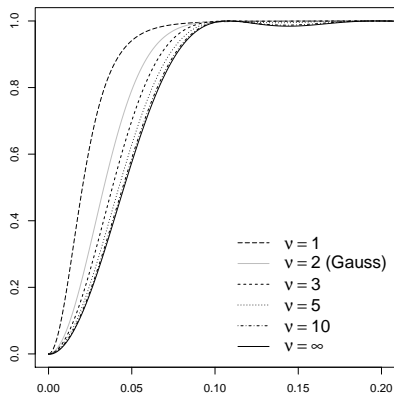
with

$$\rho > 0, \quad \nu > 0, \quad 0 < \alpha < \alpha_{\max}(\rho, \nu) := \left(\frac{2\pi^{d/2} \Gamma(d/\nu + 1)}{\rho \Gamma(d/2)} \right)^{1/d}.$$

Power exponential spectral model: (isotropic) spectral densities and pair correlation functions



Spectral densities



Pair correlation functions

Approximation of stationary models

Consider a stationary kernel C_0 and $X \sim \text{DPP}(C_0)$.

- The simulation and the density of X_S requires the expansion

$$C_S(x, y) = C_0(y - x) = \sum_{k=1}^{\infty} \lambda_k^S \phi_k^S(x) \overline{\phi_k^S(y)}, \quad (x, y) \in S \times S,$$

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- Consider the unit box $S = [-\frac{1}{2}, \frac{1}{2}]^d$ and the Fourier expansion

$$C_0(y - x) = \sum_{k \in \mathbb{Z}^d} c_k e^{2\pi i k \cdot (y-x)}, \quad y - x \in S.$$

The Fourier coefficients are

$$c_k = \int_S C_0(u) e^{-2\pi i k \cdot u} du \approx \int_{\mathbb{R}^d} C_0(u) e^{-2\pi i k \cdot u} du = \varphi(k)$$

which is a good approximation if $C_0(u) \approx 0$ for $|u| > \frac{1}{2}$.

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- Example: For the circular covariance, this is true whenever $\rho > 5$.

Approximation of stationary models

The approximation of $\text{DPP}(C_0)$ on S is then $\text{DPP}_S(C_{\text{app},0})$ with

$$C_{\text{app},0}(x - y) = \sum_{k \in \mathbb{Z}^d} \varphi(k) e^{2\pi i(x-y) \cdot k}, \quad x, y \in S,$$

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This approximation allows us

- to simulate $\text{DPP}(C_0)$ on S ;
- to compute the (approximated) density of $\text{DPP}(C_0)$ on S .

- 1 Introduction
- 2 Definition, existence and basic properties
- 3 Simulation
- 4 Parametric models
- 5 Inference**

Consider a stationary and isotropic parametric DPP(C), i.e.

$$C(x, y) = C_0(x - y) = \rho R_\alpha(\|x - y\|),$$

with $R_\alpha(0) = 1$.

The first and second moments are easily deduced:

- The intensity is ρ .
- The pair correlation function is

$$g(x, y) = g_0(\|x - y\|) = 1 - R_\alpha^2(\|x - y\|).$$

- Ripley's K -function is easily expressible in terms of R_α : if $d = 2$,

$$K_\alpha(r) := 2\pi \int_0^r t g_0(t) dt = \pi r^2 - 2\pi \int_0^r t |R_\alpha(t)|^2 dt.$$

Inference

Parameter estimation can be conducted as follows.

- 1 Estimate ρ by $\#\{\text{obs. points}\}/\text{area of obs. window}$.
- 2 Estimate α
 - either by **minimum contrast** estimator (MCE):

$$\hat{\alpha} = \operatorname{argmin}_{\alpha} \int_0^{r_{\max}} \left| \sqrt{\widehat{K}(r)} - \sqrt{K_{\alpha}(r)} \right|^2 dr$$

- or by **maximum likelihood** estimator: given $\hat{\rho}$, the likelihood is deduced from the kernel approximation.

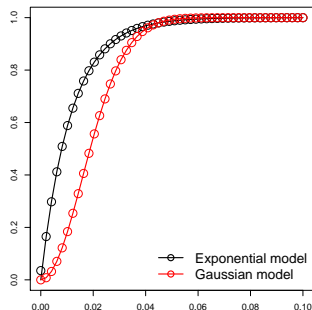
Two model examples

- Exponential model with $\rho = 200$ and $\alpha = 0.014$:

$$C_0(x) = \rho \exp(-\|x\|/\alpha).$$

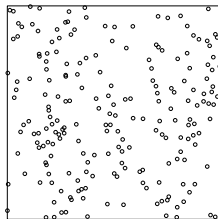
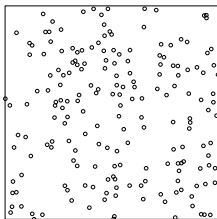
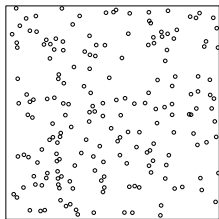
- Gaussian model with $\rho = 200$ and $\alpha = 0.02$:

$$C_0(x) = \rho \exp(-\|x/\alpha\|^2).$$

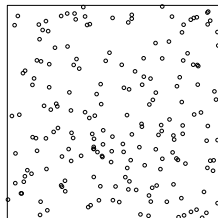
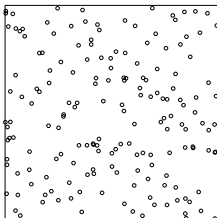
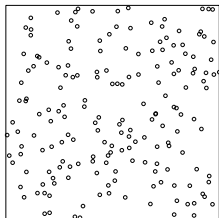


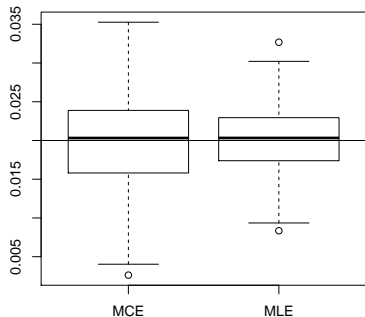
- Solid lines: theoretical pair correlation function
- Circles: pair correlation from the approximated kernel

Samples from the Gaussian model on $[0, 1]^2$:

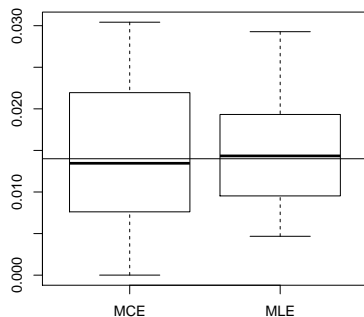


Samples from the exponential model on $[0, 1]^2$:



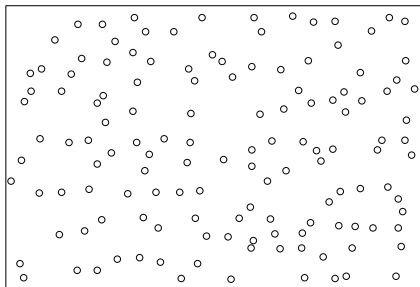
Estimation of α from 200 realisations

Gaussian model



Exponential model

Example: 134 Norwegian pine trees observed in a 56×38 m region



Møller and Waagpetersen (2004): a five parameter multiscale process is fitted using elaborate MCMC MLE methods.

Here we fit a more parsimonious DPP models.

First,

- Whittle-Matérn model;
- Cauchy model;
- Gaussian model: the best fit, but plots of summary statistics indicate a lack of fit.

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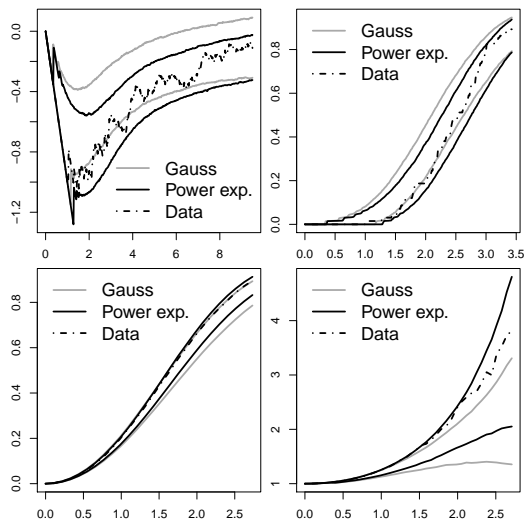
- Whittle-Matérn model;
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- Gaussian model: the best fit, but plots of summary statistics indicate a lack of fit.

Second,

- power exponential spectral model: provides a much better fit, with

$$\hat{\nu} = 10, \quad \hat{\alpha} = 6.36 \approx \alpha_{\max} = 6.77$$

i.e. close to the “most repulsive possible stationary DPP”.



Clockwise from top

left: $L(r) - r$; $G(r)$; $F(r)$; $J(r)$. Simulated 2.5% and 97.5% envelopes are based on 4000 realizations of the fitted Gaussian model resp. power exponential spectral model.

Conclusions

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- ⇒ Promising alternative to repulsive Gibbs point processes.

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