Statistical aspects of determinantal point processes

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Introduction

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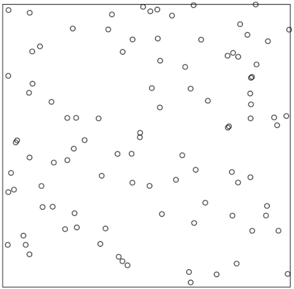
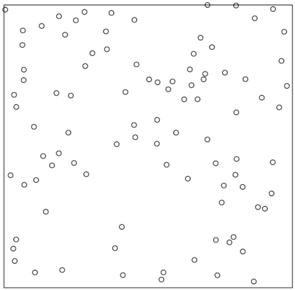
- They were introduced in their general form by O. Macchi in 1975 to model fermions (i.e. particules with repulsion) in quantum mechanics.
- Particular cases include the law of the eigenvalues of certain random matrices (Gaussian Unitary Ensemble, Ginibre Ensemble,...)
- Most theoretical studies have been published in the 2000's.

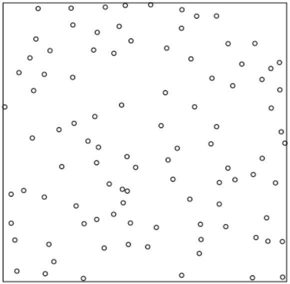
Examples



Poisson



DPP



DPP with
stronger repulsion

Statistical motivations

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Furthermore DPP possess the following appealing properties :

- They can be easily simulated
- There are closed form expressions for the moments
- There are closed form expression for the density of a DPP on any bounded set
- Inference is feasible, including likelihood inference.

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

Notation

- We consider a spatial point process X on $\mathbb{R}^d$, i.e. we can view X as a random locally finite subset of $\mathbb{R}^d$.
- For any borel set $B \subseteq \mathbb{R}^d$, $X_B = X \cap B$.
- For any integer $n > 0$, we let $\rho^{(n)}$ denote the n'th order product density function of X.
  Intuitively,
  $$\rho^{(n)}(x_1, \ldots, x_n) \, \mathrm{d}x_1 \cdots \mathrm{d}x_n$$
  is the probability that for each $i = 1, \ldots, n$, X has a point in a region around x_i of volume $\mathrm{d}x_i$.
  In particular $\rho = \rho^{(1)}$ is the intensity function.

Definition of a determinantal point process

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

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

Definition

X is a *determinantal point process* with *kernel* C, denoted $X \sim \mathrm{DPP}(C)$, 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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- The pair correlation function is

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

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- If $X \sim \mathrm{DPP}(C)$, then $X_B \sim \mathrm{DPP}(C_B)$
- Any smooth transformation or independent thinning of a DPP is still a DPP with explicit given kernel.
- Given a kernel C, there exists at most one $\mathrm{DPP}(C)$.

Existence

In all that follows we assume

(C1) C is a continuous complex covariance function.

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 $\int_S \phi_k^S(x)\overline{\phi_l^S(x)}\,\mathrm{d}x = \mathbf{1}_{\{k=l\}}$.

Theorem (Macchi (1975))

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

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

Density on a compact set S

Let $X \sim \text{DPP}(C)$ and $S \subset \mathbb{R}^d$ be any compact set.
Recall that $C_S(x,y) = \sum_{k=1}^{\infty} \lambda_k^S \phi_k^S(x)\overline{\phi_k^S(y)}$.

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 $\tilde{C} : S \times S \to \mathbb{C}$ is given by

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

Let $X \sim \mathrm{DPP}(C)$.

We want to simulate X_S for $S \subset \mathbb{R}^d$ compact.

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

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Theorem (Hough et al. (2006))

For $k \in \mathbb{N}$, let B_k be independent Bernoulli r.v. with mean 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 $DPP(C_S) \stackrel{d}{=} DPP(K)$.

Simulating X_S is equivalent to simulate DPP(K) with

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

Let $M = \max\{k \geq 0; B_k \neq 0\}$.
Note that M is a.s. finite since $\sum \lambda_k^S < \infty$.

1. simulate M (by the inversion method)

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In the last step, the kernel K (given $B_1,\ldots,B_M$) becomes a *projection kernel*, which can be written, w.l.g :

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

where $n=card\{1\leq k\leq M; B_k=1\}$.

Simulation of determinantal projection processes

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

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

The point process DPP(K) has a.s. n points $(X_1, \dots, X_n)$ that can be simulated by the following Gram-Schmidt procedure :

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sample X_n from the distribution with density $p_n(x) = \|\boldsymbol{v}(x)\|^2/n$.
set $\boldsymbol{e}_1 = \boldsymbol{v}(X_n)/\|\boldsymbol{v}(X_n)\|$.
for $i = (n-1)$ to 1 **do**
  sample X_i from the distribution (given $X_{i+1}, \dots, X_n$) :

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

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

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Theorem

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

Illustration of simulation algorithm

Example : Consider the unit box $S = [-1/2, 1/2]^2$ and :

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

for a set of indices $k_1, \dots, k_n$ in $\mathbb{Z}^2$.
So the projection kernel writes

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

$X_S \sim \mathrm{DPP}(K)$ is homogeneous and has a.s. n points on S.

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Step 1. The first point is sampled uniformly on S

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

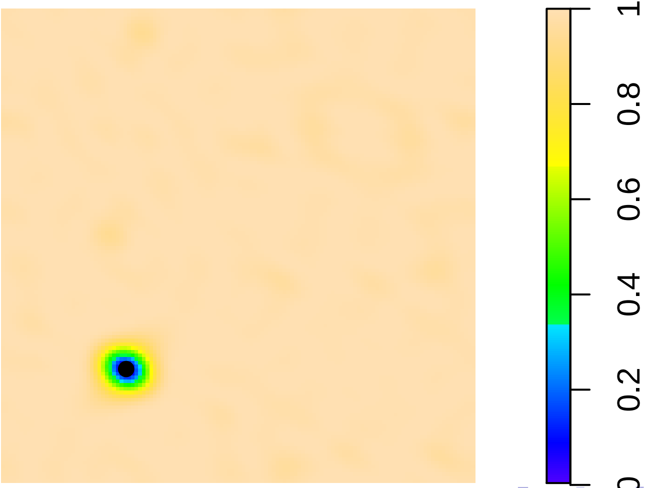
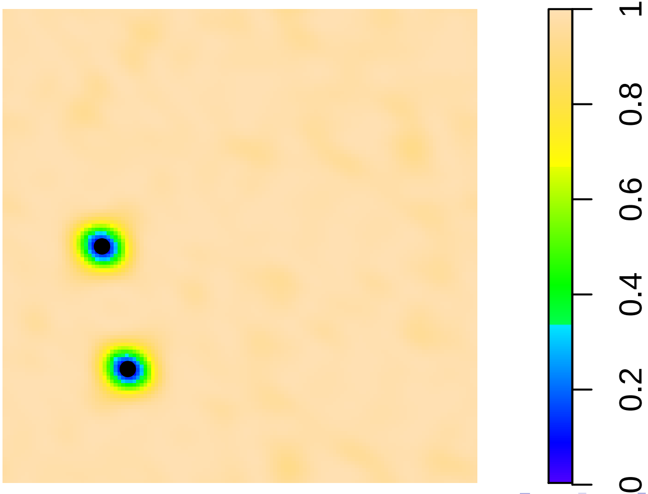


Illustration of simulation algorithm

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



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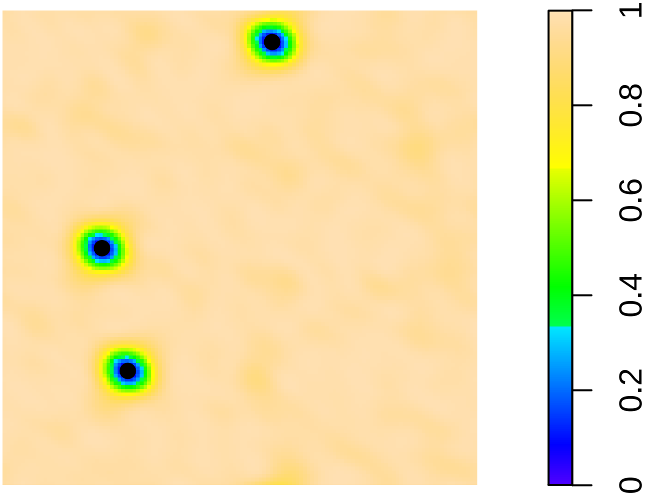

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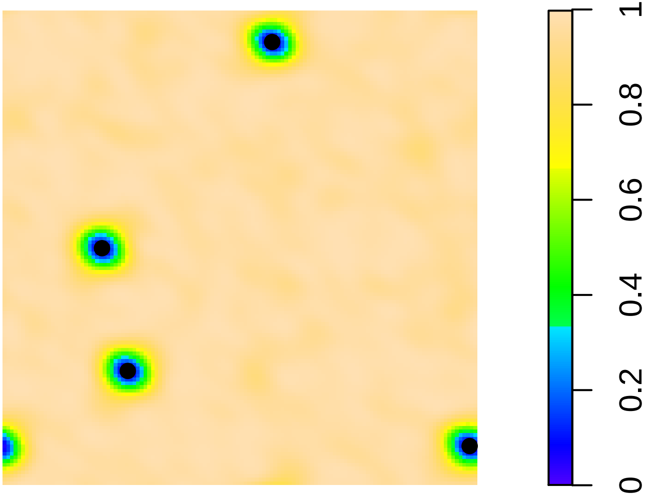

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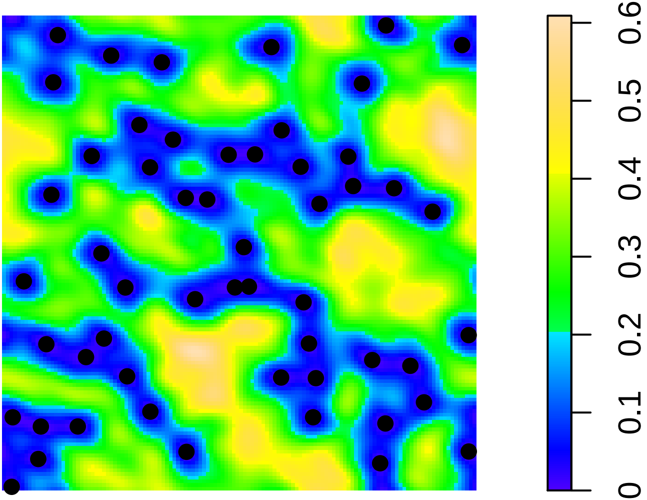

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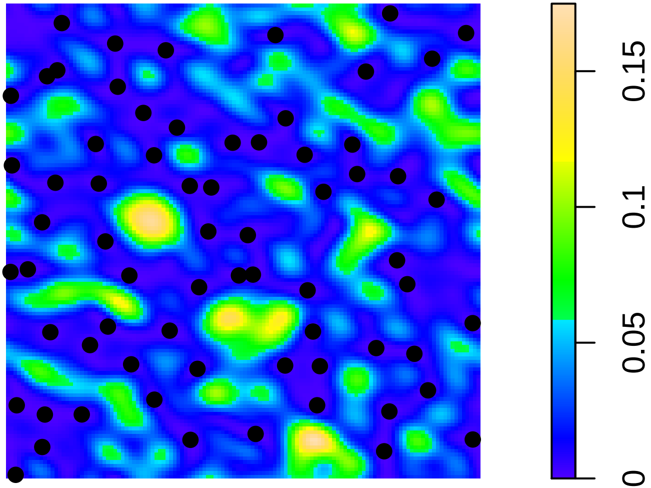

Stationary models

We focus on 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

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

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To construct parametric families of DPP :
Consider parametric families of C_0 and rescale so that $\varphi \leq 1$.
$\rightarrow$ This will induce restriction 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 $\varphi \leq 1 \Leftrightarrow \rho\alpha^2 \leq 4/\pi$.

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- Whittle-Matérn (includes Exponential and Gaussian) :

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

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

- 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 $\rho \leq \frac{\Gamma(\nu+d/2)}{\Gamma(\nu)(\sqrt{\pi}\alpha)^d}$

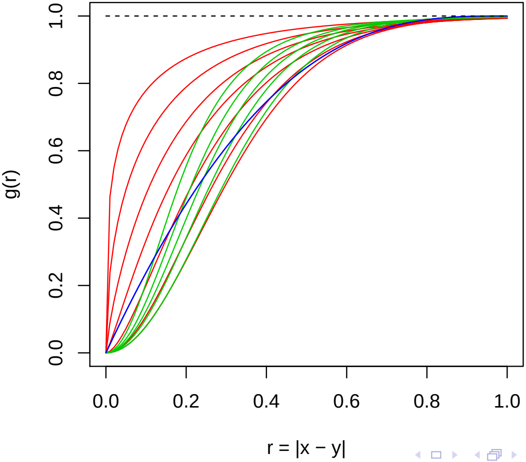
Pair correlation functions of DPP(C_0) for previous models :

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 ≈ 1.



Approximation of stationary models

Consider a parametric stationary kernel C_0 and $X \sim \mathrm{DPP}(C_0)$.
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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$\longrightarrow$ This is in general not know.
Consider w.l.g the unit box $S = [-\frac{1}{2}, \frac{1}{2}]^d$ and the Fourier expansion :

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

The Fourier coefficients are

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

which is a good approximation if $C_0(u) \approx 0$ for $|u| > \frac{1}{2}$.
Example : For the circular covariance, this is true whenever $\rho > 5$

Approximation of stationary models

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

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

where φ is the Fourier transform of C_0.

This approximation allows us

- to simulate DPP(C_0) on S
- to compute the (approximated) density of DPP(C_0) on S

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 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 as,

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

Inference

The estimation can be conducted as follows

1. Estimate ρ by the mean number of points.
2. Estimate α
   - either by **minimum contrast** estimator (MCE) :

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

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

Two model examples

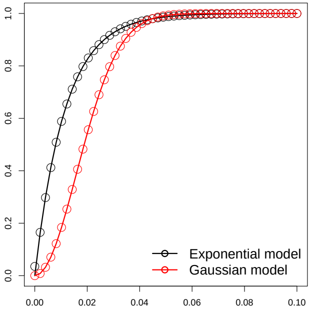
In the following we will consider two different model examples :

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

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

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

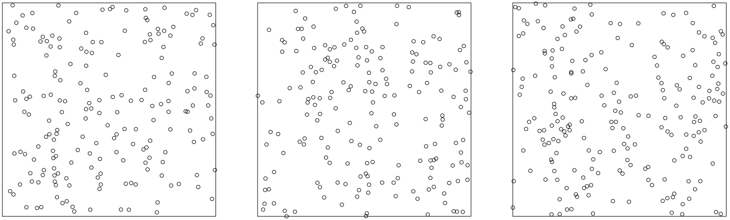
$$C_0(x) = \rho \exp(-\|x/\alpha\|^2)$$



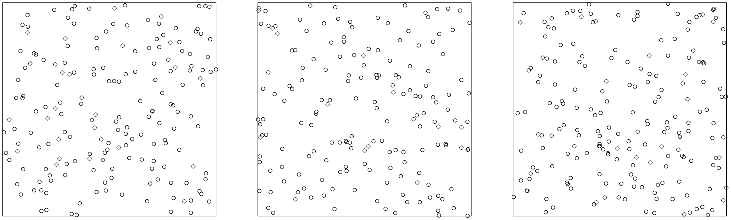
– Solid lines : theoretical pair correlation function

∘ Circles : pair correlation from the approximated kernel

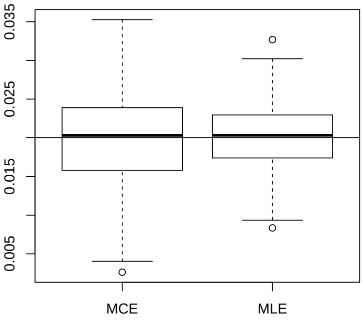
Samples from the Gaussian model on $[0,1]^2$:



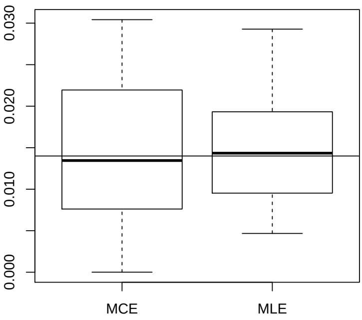
Samples from the Exponential model on $[0,1]^2$:



Estimation of α from 200 realisations



Gaussian model



Exponential model

Conclusion

DPP provides some flexible parametric models of repulsive point processes.

Furthermore DPP possess the following appealing properties :

- They can be easily simulated
- There are closed form expressions for the moments of a DPP
- There are closed form expression for the density of a DPP on any bounded set
- Inference is feasible, including likelihood inference.

$\Rightarrow$ Promising alternative to repulsive Gibbs point processes.

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