Statistics for determinantal point process models and its usefulness

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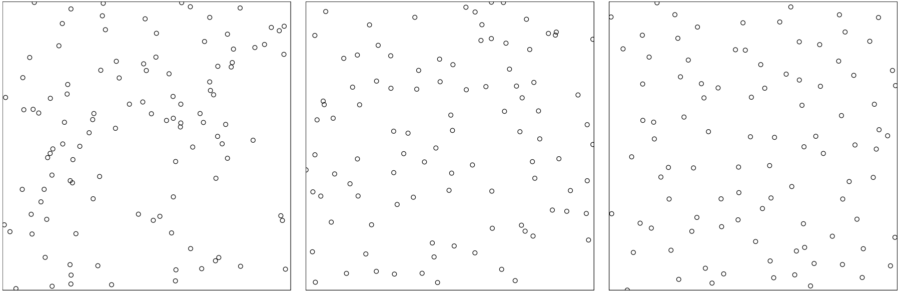
Jesper Møller
jm@math.aau.dk

Department of Mathematical Sciences
Aalborg University
Denmark

AALBORG UNIVERSITY
DENMARK

Introduction



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- DPPs are inhibitive/regular/repulsive point processes.
- Introduced by O. Macchi in 1975 to model fermions in quantum mechanics.
- Several theoretical studies appeared in the 2000's.

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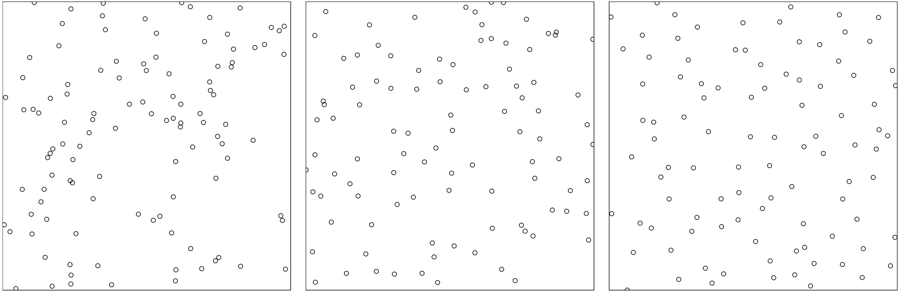

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- DPPs are inhibitive/regular/repulsive point processes.
- Introduced by O. Macchi in 1975 to model fermions in quantum mechanics.
- Several theoretical studies appeared in the 2000's.
- **Until recently statistical models and inference had been largely unexplored.**

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Main questions re. DPPs

How do we make statistical inference (parameter estimation; simulation based procedures used e.g. for model checking)?

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- Focus on DPPs defined on $\mathbb{R}^d$;
- something about DPPs defined on other spaces ($\mathbb{S}^d$).

Gibbs point processes — the usual class of point processes used for modelling inhibition

Example: A *Strauss hard-core process* on a compact set $S \subset \mathbb{R}^d$ has density

$$f(\{x_1,\ldots,x_n\}) = \frac{1}{c(r,R,\beta,\gamma)} \beta^n \gamma^{\sum_{i<j} \mathbf{1}_{\{\|x_i-x_j\| \le R\}}} \prod_{i<j} \mathbf{1}_{\{\|x_i-x_j\|>r\}}, \qquad \{x_1,\ldots,x_n\} \subset S,$$

w.r.t. the unit rate Poisson process, where $n = 0, 1, \ldots$, and $0 < r < R$ and $\beta, \gamma > 0$ are parameters.

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- On $\mathbb{R}^d$ a 'local specification' is needed and the issue of phase transition has to be clarified.

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Notation

- X : simple point process on $\mathbb{R}^d$, with Lebesgue measure as reference measure (or any locally compact Polish space equipped with a Radon measure).

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- For any integer $n > 0$, denote $\rho^{(n)}$ the n'th *order joint intensity* of X:

$$\mathrm{E}\left[X(B_1)\cdots X(B_n)\right] = \int_{B_1}\cdots\int_{B_n}\rho^{(n)}(x_1,\ldots,x_n)\,\mathrm{d}x_1\cdots\mathrm{d}x_n$$

  for any disjoint Borel sets $B_1,\ldots,B_n \subseteq \mathbb{R}^d$.

  - Intuitively,

$$\rho^{(n)}(x_1,\ldots,x_n)\,\mathrm{d}x_1\cdots\mathrm{d}x_n$$

    is the probability that for each $i = 1,\ldots,n$,
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  - $\rho^{(n)}(x_1,\ldots,x_n) = 0$ if $x_i = x_j$ for some $i \neq j$.

Definition of a DPP

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Definition

Let C be a function $\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$, called the *kernel*.
$X \sim \mathrm{DPP}(C)$ if

$$\rho^{(n)}(x_1, \ldots, x_n) = \det\{C(x_i, x_j)\}_{i,j=1,\ldots,n}, \quad n = 1, 2, \ldots$$

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For ease of exposition, assume

(C1) $\quad C$ is a continuous (complex) covariance function.

Jesper Møller

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Basic properties (if $X \sim DPP(C)$ exists)

- *Intensity*: $\rho(x) = C(x, x)$.

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

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- Given C, there *exists at most one* $\mathrm{DPP}(C)$.

Jesper Møller

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Aalborg University
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Existence

For any compact set $S \subset \mathbb{R}^d$, there is 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 $\{\phi_k^S\}$ is a set of orthonormal basis functions for $L^2(S)$, i.e.,

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Theorem (Macchi, 1975)

Under (C1), existence of $\mathrm{DPP}(C)$ *is equivalent to*

$$\textit{spectrum}(C) \leq 1$$

meaning that

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

Jesper Møller

Dept. of Mathematical Sciences
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Density on a compact set S

Theorem (Macchi, 1975)

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Let $X \sim DPP(C)$ and $S \subset \mathbb{R}^d$ be compact. If $\lambda_k^S < 1\ \forall k$, then $X_S \ll Poisson(S, 1)$, with density

$$f_S(\{x_1, \ldots, x_n\}) = \exp(|S| - D) \det\{\tilde{C}(x_i, x_j)\}_{i,j=1,\ldots,n},$$

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

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

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- Thus to calculate the density/likelihood we need the spectral representation.

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- Thus to calculate the density/likelihood we need the spectral representation.
- Conversely, using f_S, existence of X_S is ensured by that

$$\lambda_k^S = \frac{\tilde{\lambda}_k^S}{1 + \tilde{\lambda}_k^S} < 1.$$

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Theorem (Hough, Krishnapur, Peres & Viràg (2006))

Let $B_1, B_2, \ldots$ be independent Bernoulli variables with means $\lambda_1^S, \lambda_2^S, \ldots$, and

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

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We start by producing n points:

$$n \sim \sum_{k=1}^{\infty} B_k, \quad \mathrm{E}[n] = \sum_{k=1}^{\infty} \lambda_k^S, \quad \mathrm{Var}[n] = \sum_{k=1}^{\infty} \lambda_k^S (1 - \lambda_k^S),$$

where since C is continuous,

$$\sum_{k=1}^{\infty} \lambda_k^S = \int_S C(x,x)\,\mathrm{d}x < \infty.$$

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Simulation (cont'd)

Next, if e.g. $B_1 = \ldots = B_n = 1$ and $B_k = 0$ for $k > n$, we simulate the DPP with finite rank kernel

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Dept. of Mathematical Sciences
Aalborg University
Denmark

Simulation (cont'd)

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$$p(x_k \,|\, x_1, \ldots, x_{k-1}) = \frac{\rho(x_k \,|\, x_1, \ldots, x_{k-1})}{n-k+1}, \qquad x_k \in S,$$

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At each step we use rejection sampling...

Status

- We let a DPP on $\mathbb{R}^d$ be specified through a continuous (complex) covariance function $C : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$.

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
Denmark

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Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
Denmark

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- C determines the moment properties of the DPP.
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  - there is an existence condition;
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  - have no problem with boundary effects.

But we need to know the spectral representation — typically we don't!

Stationary kernels

Consider a stationary kernel,

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

with Fourier transform (spectral density) $\varphi := \mathcal{F}(C_0)$:

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

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Theorem (Lavancier, Møller & Rubak, 2015)

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

$$DPP(C_0) \text{ exists} \quad \Leftrightarrow \quad \varphi \le 1.$$

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
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$\rightarrow$ *This induces a restriction*:

There will be a trade-off between intensity and the degree of repulsiveness:

If the intensity is large, the "effective support" of $C_0 = \mathcal{F}^{-1}(\varphi)$ must be small (i.e. small range of correlation/interaction, as detailed later).

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
Denmark

Approximation

For simplicity and specificity, consider $S = [-1/2, 1/2]^d$.

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
Denmark

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

Turns out to work well in practice!

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
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Turns out to work well in practice!

For $x - y \in S$, it is effectively the Fourier expansion

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

since for "interesting models" (for any reasonable expected number of points) the existence condition $\varphi \leq 1$ implies $C_0(t) \approx 0$ for $t \notin S$ and

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

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Modelling based on spectral densities

Idea: Start by modelling $0 \leq \varphi \leq 1$ s.t. $C_0 := \mathcal{F}^{-1}(\varphi) \in L^2(\mathbb{R}^d)$.

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Modelling based on spectral densities

Idea: Start by modelling $0 \leq \varphi \leq 1$ s.t. $C_0 := \mathcal{F}^{-1}(\varphi) \in L^2(\mathbb{R}^d)$.

Then $DPP(C_0)$ is well-defined and using the approximation based on the Fourier basis, X_S can easily be simulated and the density/likelihood can be evaluated exactly (up to series truncation).

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Then $DPP(C_0)$ is well-defined and using the approximation based on the Fourier basis, X_S can easily be simulated and the density/likelihood can be evaluated exactly (up to series truncation).

Main drawback:

- In general the parameters in $C_0 = \mathcal{F}^{-1}(\varphi)$ (and thus in $\rho^{(n)}$) may be hard to understand/interpret.

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
Denmark

Intermezzo

This concludes the first part of the talk focusing on

- the probabilistic background,
- approximations for simulation and density expression.

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
Denmark

Intermezzo

This concludes the first part of the talk focusing on

- the probabilistic background,
- approximations for simulation and density expression.

Now we start doing statistics, so if you got lost or fell asleep you get a fresh start!

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Dept. of Mathematical Sciences
Aalborg University
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Examples of parametric models

Focus on the following parametric models
($\rho > 0$ intensity; $\alpha > 0$ scale/range; $\nu > 0$ shape):

Jesper Møller

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Aalborg University
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Examples of parametric models

Focus on the following parametric models
($\rho > 0$ intensity; $\alpha > 0$ scale/range; $\nu > 0$ shape):

- *Whittle-Matérn model*, which includes the exponential model ($\nu = 1/2$) and the Gaussian model ($\nu = \infty$):

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

  Parameter restriction:

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

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- *Power exponential spectral model*:

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

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Parametric models in R (available via the spatstat package)

Parametric models are specified in R via the determinantal family functions (of class `detfamily`): `detGauss`, `detMatern`, `detPowerExp`.
E.g:

- `model <- detGauss(rho=100, alpha=0.05, d=2)`
- `model <- detMatern(rho=100, alpha=0.03, nu=0.5, d=2)`
- `model <- detPowerExp(rho=100, alpha=0.17, nu=2, d=2)`

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Extract the kernel, spectral density, pair correlation function, K-function:

- `detkernel(model)`
- `detspecden(model)`
- `pcfmodel(model)`
- `Kmodel(model)`

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Simulation in R

Simply use the generic function `simulate` (then R automatically calls the function `simulate.detmodel`):

- ```
  model <- detGauss(rho=100, alpha=0.05, d=2)
  X <- simulate(model)
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- Change the window (default is the unit square):
  ```
  W <- owin(poly=list(x=c(-1,0,1),y=c(0,1,0)))
  X <- simulate(model, W=W)
  ```
  ```

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  ```
  W <- owin(poly=list(x=c(-1,0,1),y=c(0,1,0)))
  X <- simulate(model, W=W)
  ```
- Several realizations:
  ```
  X <- simulate(model, nsim=4)
  ```
  ```

Illustration of simulation algorithm

Step 1. The first point is sampled uniformly on S (stationary case).

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Illustration of simulation algorithm

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

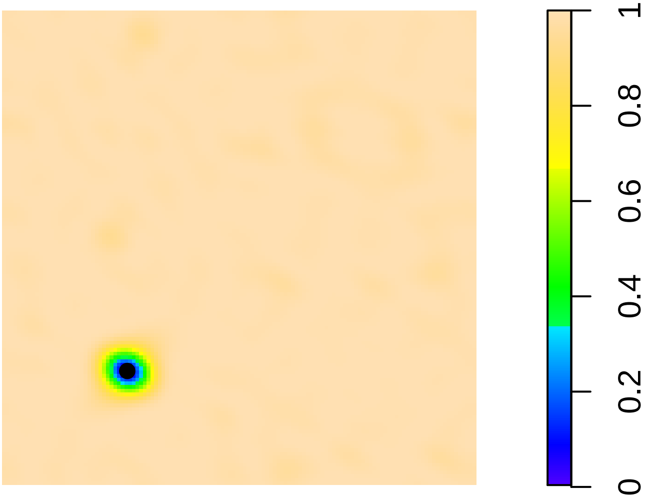

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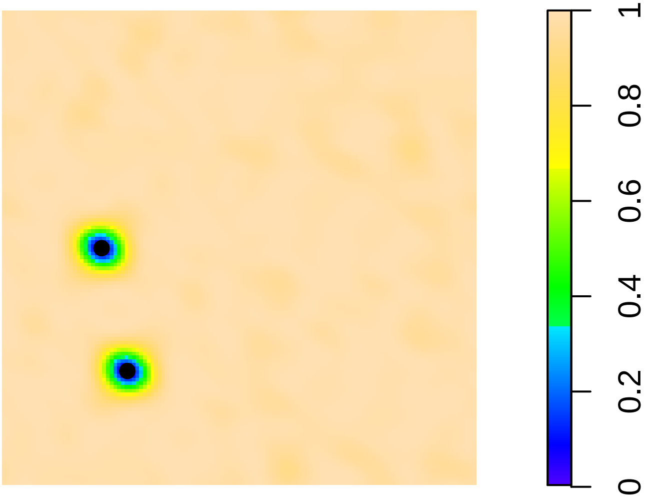
Illustration of simulation algorithm

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



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Step 4. The fourth point is sampled w.r.t. the following density:

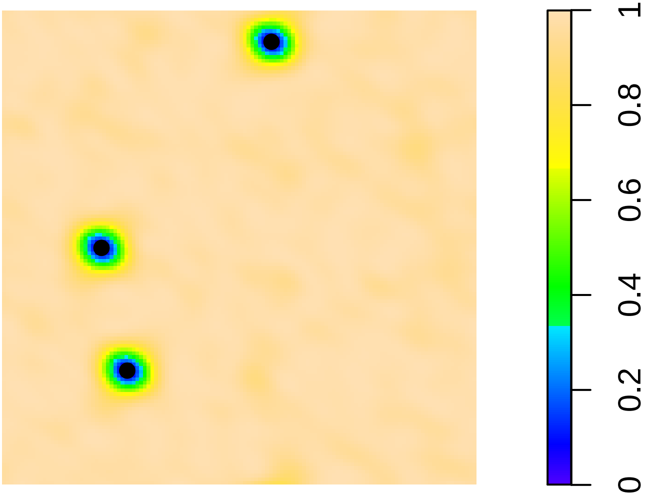

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Illustration of simulation algorithm

Step 5. The sixth point is sampled w.r.t. the following density:

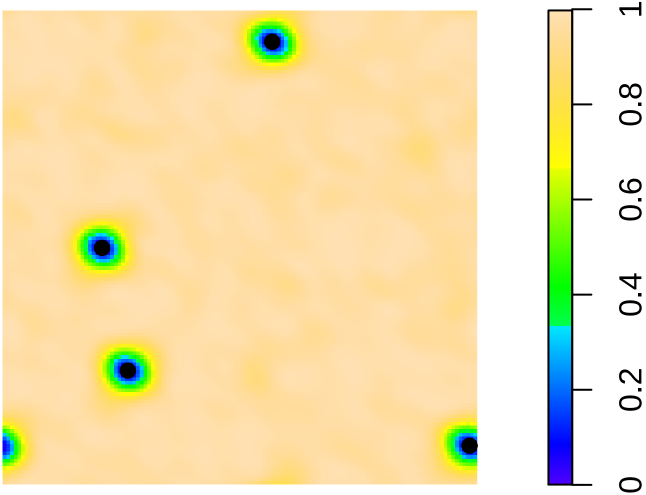

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Illustration of simulation algorithm

...somewhere in the middle...

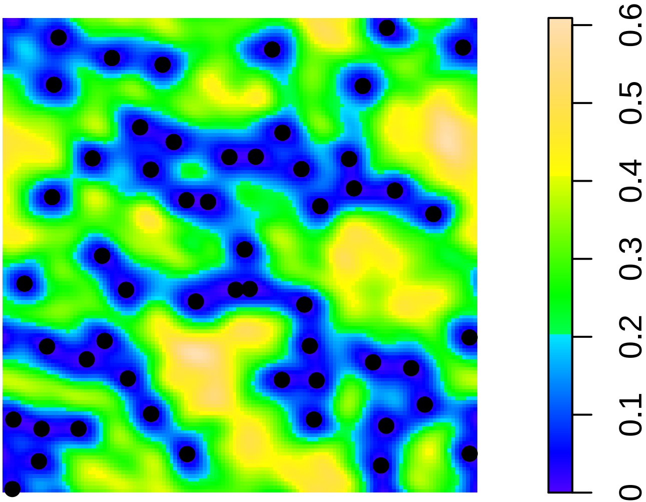

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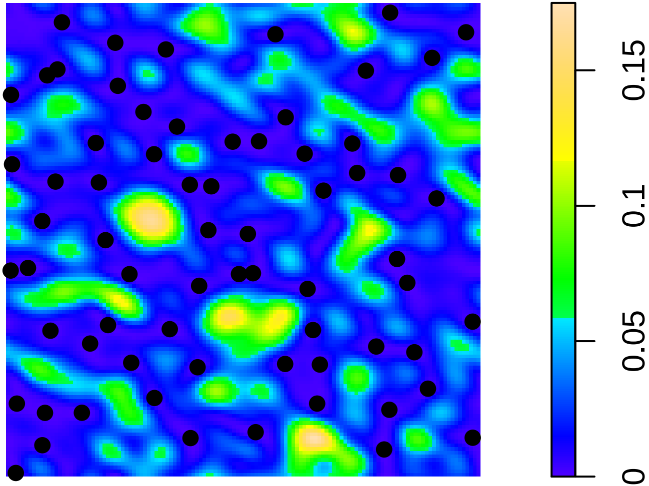
Illustration of simulation algorithm

Final point is sampled w.r.t. the following density:



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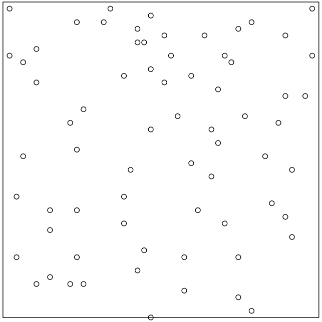
Spanish towns dataset

Ripley (1988): Strauss hard-core model with 4 parameters:

r=hard-core, R=range of interaction, β=abundance, γ=interaction.



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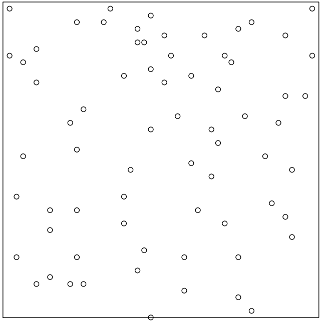

Following Illian, Penttinen, Stoyan & Stoyan (2008): $\hat{r} = 0.83$, $\hat{R} = 3.5$.
Approximate likelihood method (Huang and Ogata, 1999): $\hat{\beta} = 0.12$ and $\hat{\gamma} = 0.76$.

Alternative DPP models

Gaussian, Whittle-Matérn, and power exponential spectral models fitted using the function `dppm`:

- Default estimation method is "partial likelihood" where we use $\hat{\rho} = n/|W| = 0.043$ and MLEs for the rest:

```
fit <- dppm(X, detGauss())
```

- Full likelihood:

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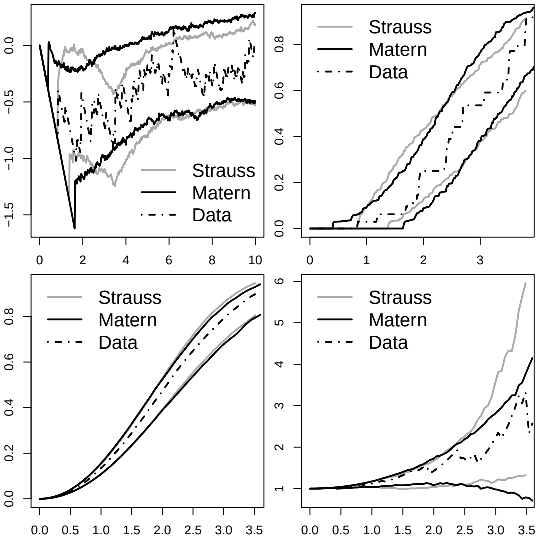
Highest likelihood: fitted Whittle-Matérn model.

Simulation based likelihood-ratio test for the simpler Gaussian model vs the Whittle-Matérn model: $p = 3\%$.

Clockwise from top left: Non-parametric estimate of $L(r) - r$, $G(r)$, $J(r)$, $F(r)$, and simulation based 2.5% and 97.5% pointwise quantiles (based on 400 realizations).



Conclusion of data analysis

Whittle-Matérn model:

- has **less parameters**
- (arguably) provides a better fit
- has a canonical way of estimating parameters (**likelihood**)
- direct **access to the moments** (intensity, pair correlation function, ...)

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For the Strauss hard-core model

- parameter estimation relies to a certain extend on “ad-hoc” methods
- the density and moments can only be obtained by MCMC simulation.

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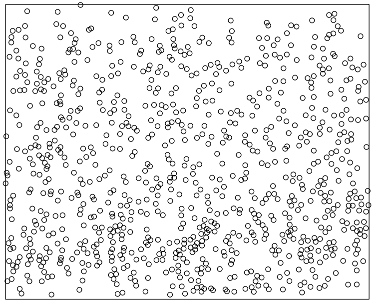
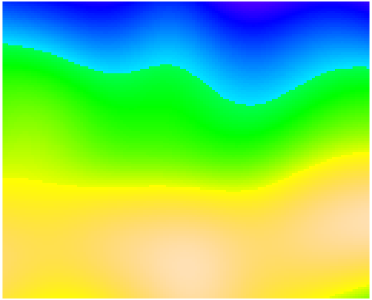
Mucous membrane dataset

Consists of the most abundant type of cell in a bivariate point pattern analysed in Møller and Waagepetersen (2004).





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Aalborg University
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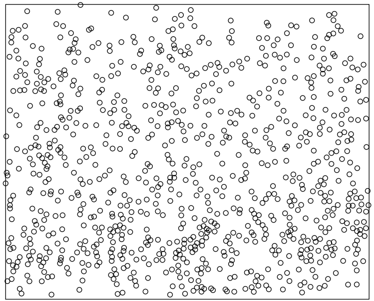

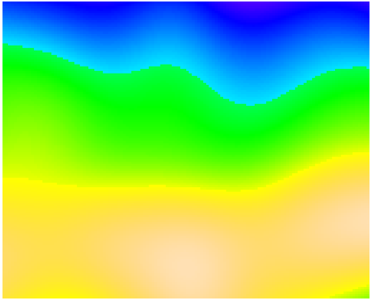

We use this to illustrate how an **inhomogenous DPP** can be fitted to a real dataset.

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
Denmark

Modelling inhomogeneity

Assume the correlation function is translation invariant:

$$R(x,y) = \frac{C(x,y)}{\sqrt{C(x,x)C(y,y)}} = \frac{C(x,y)}{\sqrt{\rho(x)\rho(y)}} = R_0(x-y).$$

Jesper Møller

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Aalborg University
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This implies

$$g(x,y) = g_0(x-y) = 1 - |R_0(x-y)|^2$$

(*second-order intensity-reweighted stationarity*; Baddeley, Møller & Waagepetersen, 2000).

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- 2. Use this when estimating g_0 (by kernel methods).

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
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- 3. Fit a parametric model for g_0 via a minimum contrast method.

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- 3. Fit a parametric model for g_0 via a minimum contrast method.
- 4. The estimated kernel of the DPP is

$$\hat{C}(x,y) = \sqrt{\hat{\rho}(x)}\hat{R}_0(x-y)\sqrt{\hat{\rho}(y)}.$$

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Simulation of the inhomogeneous DPP

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Then our fitted model is simulated by thinning $\tilde{X}$ with retention probability $\pi(x) = \hat{\rho}(x)/\hat{\rho}_{\max}$, since

$$C(x,y) = \sqrt{\frac{\hat{\rho}(x)}{\hat{\rho}_{\max}}}\tilde{C}(x,y)\sqrt{\frac{\hat{\rho}(y)}{\hat{\rho}_{\max}}} = \sqrt{\hat{\rho}(x)}\hat{R}_0(x-y)\sqrt{\hat{\rho}(y)} = \hat{C}(x,y).$$

Plots (omitted) of empirical summaries compared to simulations show a satisfactory fit.

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Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
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- Thus, to obtain a parametric model for a DPP on the sphere, we only have to make a parametric model for the eigenvalues λ_k.

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
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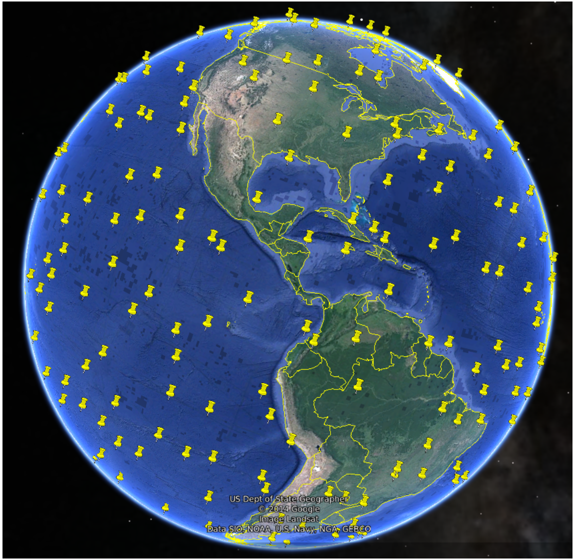
A simulated DPP consisting of 441 points on planet Earth



A new coupling result

Consider $X \sim \text{DPP}(C)$, defined on a locally compact Polish space Ω (e.g. $\mathbb{R}^d$ or $\mathbb{S}^d$), and satisfying certain weak conditions (C is a complex covariance function of locally trace class and with spectrum ≤ 1).

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$$X^u \sim \text{DPP}(C^u), \qquad C^u(x,y) = C(x,y) - \frac{C(x,u)C(u,y)}{C(u,u)}.$$

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Theorem (Møller and O'Reilly, 2018 – Extension of Goldman, 2010)

There exists a coupling of X and X^u such that almost surely

$$X^u \subseteq X \qquad \text{and} \qquad \kappa^u := X \setminus X^u \text{ consists of at most one point}$$

and κ^u has intensity function

$$\rho_{\kappa^u}(x) = \rho_X(x) - \rho_{X^u}(x) = C(x,x) - C^u(x,x) = \frac{|C(x,u)|^2}{C(u,u)}.$$

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Quantifying repulsiveness

A *global measure of repulsiveness*:

$$p_u := \mathrm{P}\left(\kappa^u \neq \emptyset\right) = \int \frac{|C(x,u)|^2}{C(u,u)}\,\mathrm{d}x.$$

- In line with Lavancier, Møller & Rubak (2014, 2015).

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- Trade-off between intensity and pcf:

$$p_u = \int \rho(v)(1 - g(u,v))\,\mathrm{d}v.$$

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Conditioned on $\kappa^u \neq \emptyset$, the point in κ^u has density

$$f_u(x) = \frac{|C(x,u)|^2}{\|C(\cdot,u)\|_2^2}, \qquad x \in \Omega.$$

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Example 1: Ginibre DPP

The standard Ginibre point process is a stationary and isotropic DPP on $\mathbb{C} \equiv \mathbb{R}^2$ with kernel

$$C(x, y) = \frac{1}{\pi} \exp\left(x\overline{y} - \frac{|x|^2 + |y|^2}{2}\right), \qquad x, y \in \mathbb{C}.$$

NB: This kernel is not stationary!

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We have

$$\rho_{\kappa^u}(x) = \frac{|C(x, u)|^2}{C(u, u)} = \frac{1}{\pi} \exp(-|x - u|^2) \sim \mathrm{N}_{\mathbb{C}}(u, 1),$$

so $p_u = 1$ (i.e. most repulsive) and if Z_u is the point in κ^u, then

$$Z_u \sim \mathrm{N}_{\mathbb{C}}(u, 1).$$

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Example 2: Most repulsive DPPs with a stationary kernel

Fact: a DPP with a stationary kernel satisfying (C1)-(C2) is *most repulsive* iff φ is an indicator function with $\int \varphi = \rho$ (Lavancier, Møller & Rubak, 2014, 2015).

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Natural candidate:

$$\varphi(x) \propto \mathbf{1}_{\{\|x\| \leq r\}}.$$

Then C_0 is a sinc function if $d = 1$ and a jinc-like function

$$C_0(x) = \frac{J_1(2\|x\|)}{\pi\|x\|} \qquad \text{if } d = 2.$$

Jesper Møller

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K-functions of Ginibre and jinc-like DPPs ($\rho = 1/\pi$)

For a stationary point process: $K(r) = \int_{\|u\| \le r} g(u) \, \mathrm{d}u$, $\rho K(r) = \mathrm{E}\left[X^0(b(0,r))\right]$.

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$L(r) - r = 0$ if Poisson, $L(r) - r \leq 1 \rightarrow$ repulsiveness.

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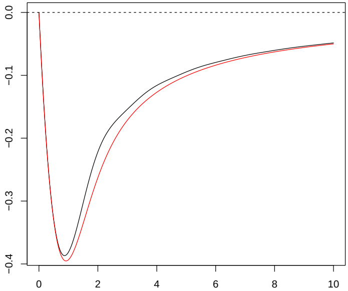
Red: $L(r) - r$ for Ginibre DPP. Black: $L(r) - r$ for jinc-like DPP.



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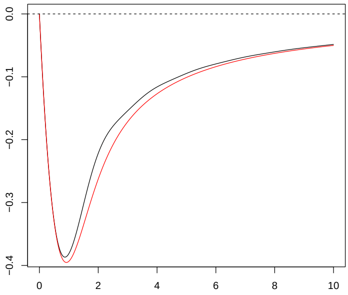
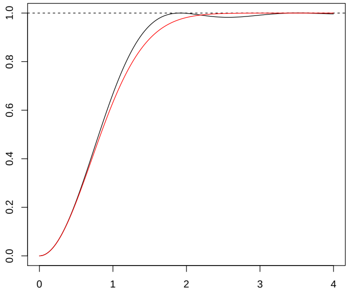


So is Ginibre DPP more repulsive?

Pcfs $g_0(r) = g(u, v)$ $(r = \|u - v\|)$ of Ginibre and jinc-like DPPs



No: the two DPPs are equally repulsive according to the global repulsiveness criteria (that averages at all scales through the integral over the whole space).

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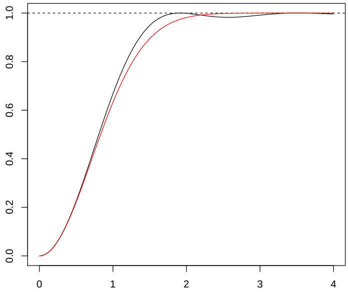

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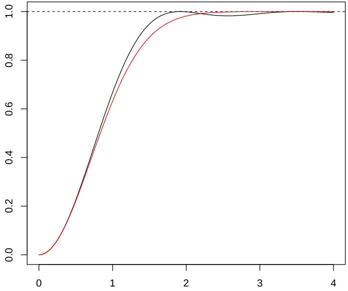

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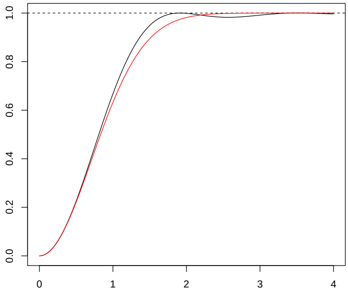

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• At medium scales: Ginibre DPP more repulsive.

• At large scales: jinc-like DPP more repulsive (the distribution of Z_0 is heavy tailed, cf. Møller and O'Reilly, 2018).

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Conclusion

DPP's possess **appealing properties**:

Jesper Møller

Dept. of Mathematical Sciences
Aalborg University
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$\Rightarrow$ **Promising alternative to Gibbs point processes**.

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Joint work on DPPs

F. Lavancier, J. Møller and E. Rubak (2015). Determinantal point process models and statistical inference. *Journal of Royal Statistical Society: Series B (Statistical Methodology)*, 77, 853-877.

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Thank you for your attention!

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