Determinantal point processes

statistical modeling and inference

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Joint work

Determinantal point processes on $\mathbb{R}^d$:

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

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Determinantal point processes on $\mathbb{S}^d$ (in progress):

Collaborators: Emilio Porcu, University Federico Santa Maria, Valparaiso (Chile), Morten Nielsen and Ege Rubak, Dept. of Mathematical Sciences, Aalborg University.

Agenda

Definition, existence and basic properties

Stationary DPPs and approximations

Parametric models

Simulation

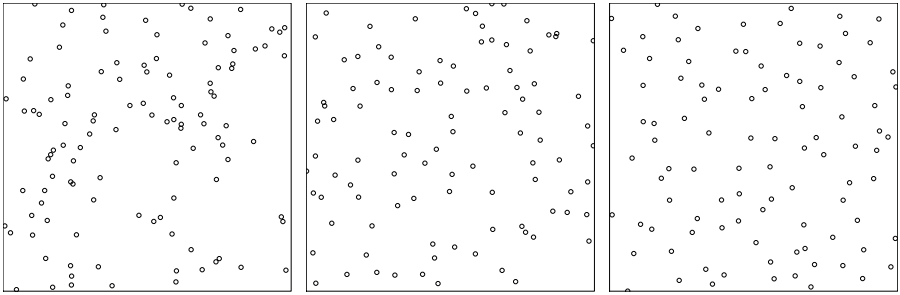
Stationary data example

Non-stationary data example

DPPs on the sphere (on going research project)

Concluding remarks

Introduction



Poisson DPP DPP with stronger inhibition

- Determinantal point processes (DPP) are inhibitive/regular/repulsive point processes.

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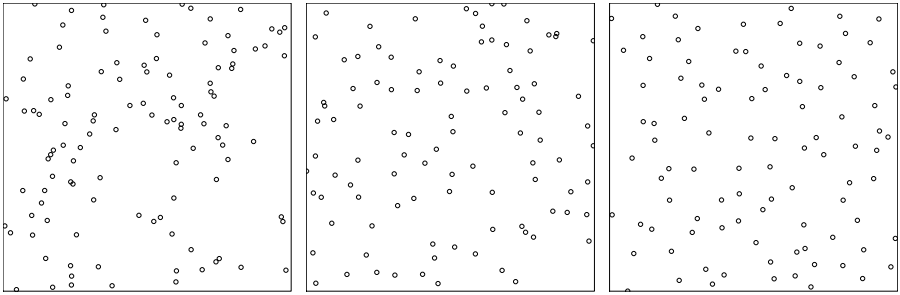

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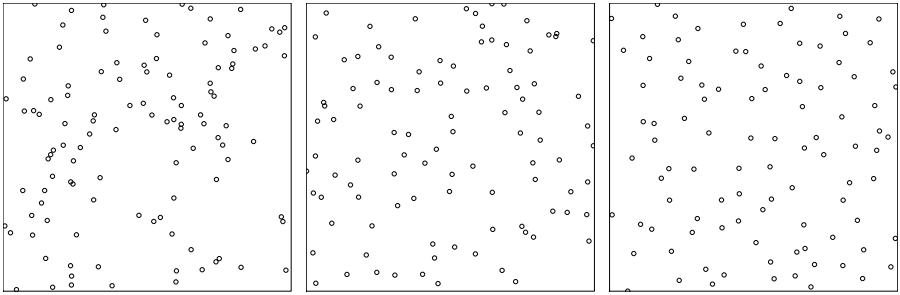

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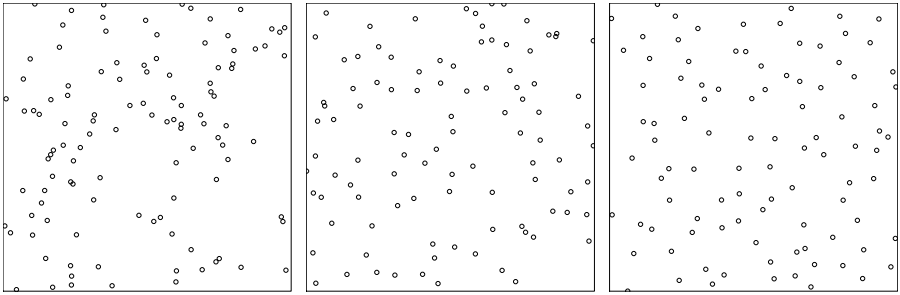

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- Introduced by O. Macchi in 1975 to model fermions in quantum mechanics.
- Several theoretical studies appeared in the 2000's.
- **Statistical models and inference have so far been largely unexplored.**

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

Example: *Strauss hard-core process*

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

where $S \subset \mathbb{R}^d$ is compact; $n = 0, 1, \ldots$; $0 \le r < R$, $\beta > 0$, $0 \le \gamma \le 1$ are parameters; the density is w.r.t. the unit rate Poisson process.

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- We have ignored edge effects: the restriction to $B \subset S$ ($B \neq S$) is not a Strauss hard-core process.
- On $\mathbb{R}^d$ a 'local specification' is needed and the issue of phase transition has to be clarified.

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

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

  - Intuitively,

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

Definition

Let C be a function $\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$.
X is a *determinantal point process* with *kernel* C, denoted $X \sim \mathrm{DPP}(C)$, if

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  E.g. $\det\{C(x_i, x_j\}_{i,j=1,\ldots,n} \geq 0$.

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Definition of a DPP

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For ease of exposition assume

(C1) C is a continuous (complex) covariance function.

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

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Theorem (Macchi, 1975)

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

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

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

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- Thus to calculate the density/likelihood we need the spectral representation.
- Conversely, 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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The algorithm starts by producing n points:

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NB: Since C is continuous,

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

Simulation (cont'd)

Effectively we pick out $n < \infty$ eigenfunctions with probability according to their eigenvalues and simulate the DPP with finite rank kernel

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This is a *projection kernel*, and the corresponding DPP can be simulated: The algorithm basically consists of taking a quite abstract procedure described by Hough et al. (2006) and translating it into implementable linear algebra.

Simulation (cont'd)

Effectively we pick out $n < \infty$ eigenfunctions with probability according to their eigenvalues and simulate the DPP with finite rank kernel

$$K(x,y) = \sum_{k:\, B_k=1} \phi_k^S(x)\overline{\phi_k^S(y)} = \sum_{i=1}^{n} \phi_{k_i}^S(x)\overline{\phi_{k_i}^S(y)}, \quad (x,y) \in S \times S.$$

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This leads to simulation of the first point, the second given the first point, the third given the first and second points,...

At each step we have been using rejection sampling...

Status

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Typically we don't know the spectral representation!

Stationary kernels

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

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$\rightarrow$ *This induces a restriction on the parameter space*:

That is, there is a trade-off between strong inhibiton and large intensity.

In practice, this restriction implies that if the intensity is large the range (effective support) of C_0 must be small.

Approximation

WLOG consider $S = [-1/2, 1/2]^d$.

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If $x - y \in S$ this 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 "most" interesting models

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

So we claim that $C_0(t) \approx 0$ for $t \notin S$: in practice, for any reasonable expected number of points, this is implied by the parameter restriction.

Modelling based on spectral densities

Idea: instead of modelling C_0, model λ_k^S and ϕ_k^S in

$$C_0(y-x) = \sum_{k=1}^{\infty} \lambda_k^S \phi_k^S(x) \overline{\phi_k^S(y)}.$$

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Following the previous approximation on the unit square:

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Main drawback:

- C_0 (and thus the moment properties) is given as an infinite sum $\rightarrow$ parameters may be harder to understand/interpret.

Intermezzo

This concludes the first part of the talk focusing on the probabilistic background and approximations for simulation and density expression.

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

Examples of parametric models

We will focus on the following parametric models, where $\rho > 0$ is the intensity, $\alpha > 0$ is a scale/range parameter, and $\nu > 0$ is a shape parameter:

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

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

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- *Power exponential spectral model*

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

  The parameter restriction is $\rho \leq \frac{\pi^{d/2}\Gamma(d/\nu+1)}{\Gamma(d/2)\alpha^d}$.

Parametric models in R (so far: contact Ege Rubak; later on: spatstat)

The parametric families 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)`
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Extract the kernel, spectral density, pair correlation function, K-function:

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

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)
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- Change the window (default is the unit square):
  ```
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  ```
- Several realizations:
  ```
  X <- simulate(model, nsim=4)
  ```
  ```

Illustration of simulation algorithm

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

Illustration of simulation algorithm

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

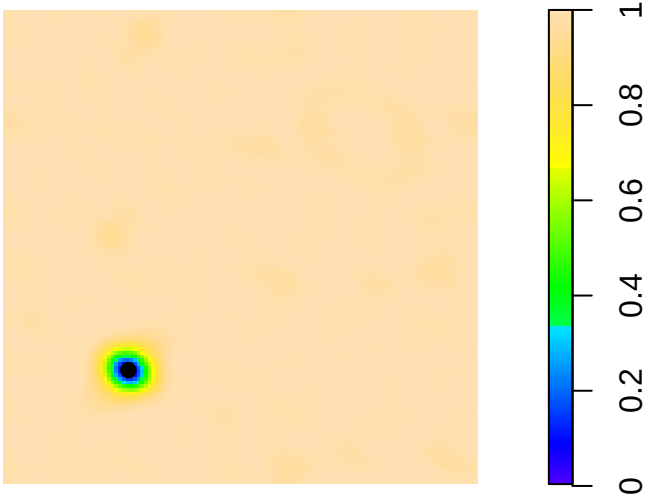

Illustration of simulation algorithm

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

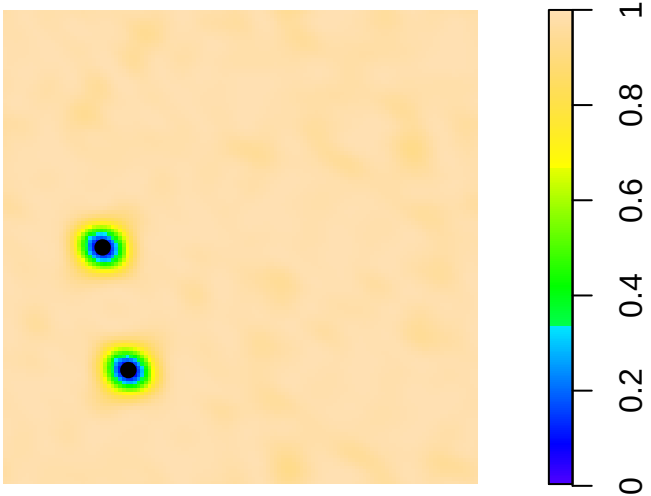

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Illustration of simulation algorithm

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

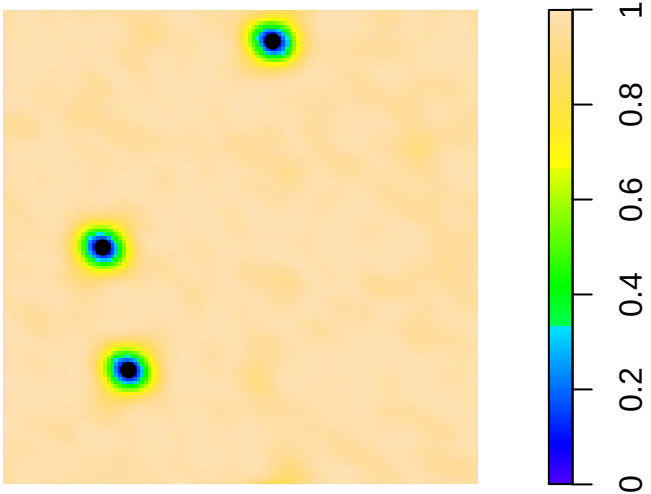

Illustration of simulation algorithm

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

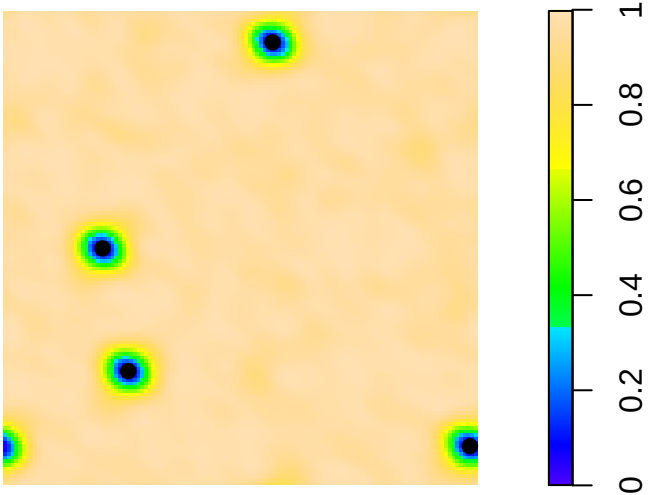

Illustration of simulation algorithm

...somewhere in the middle...

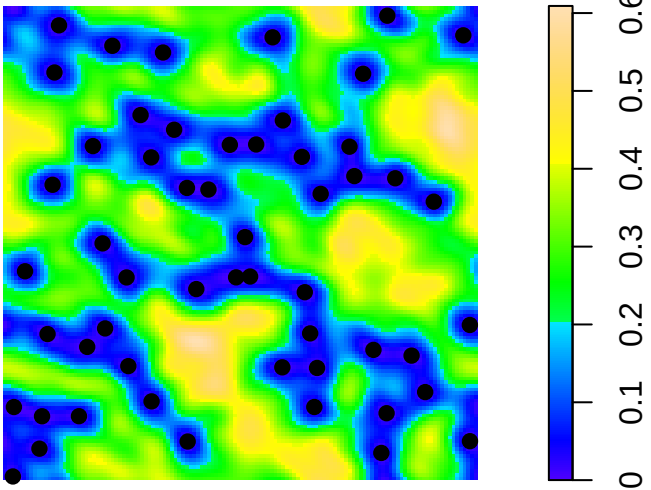

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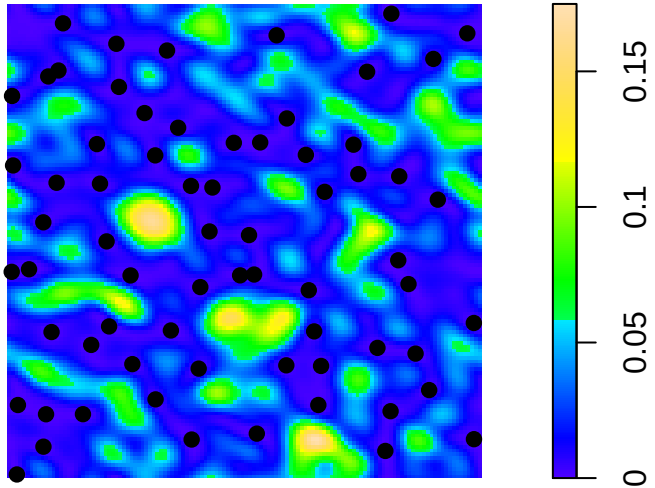
Illustration of simulation algorithm

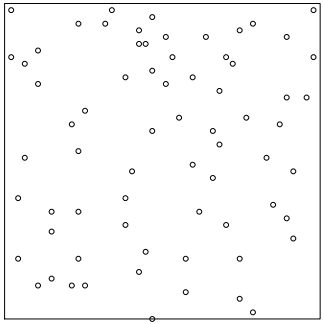
Final point is sampled w.r.t. the following density:



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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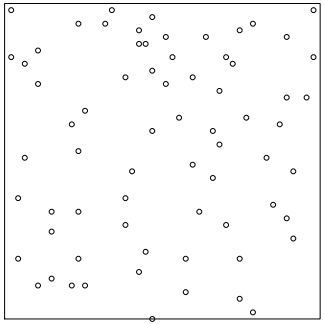

Following Illian et al. (2008): $\hat{r} = 0.83$, $\hat{R} = 3.5$.
Approximate likelihood method (Huang and Ogata (1999)): $\hat{\beta} = 0.12$ and $\hat{\gamma} = 0.76$.

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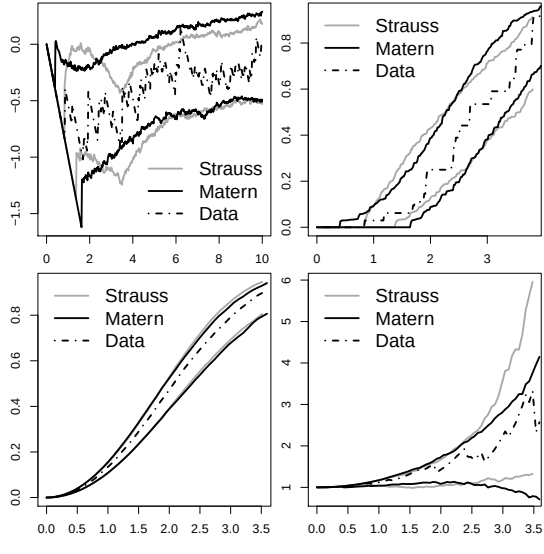
Simulation based likelihood-ratio test for the simpler Gaussian model vs the Whittle-Matérn model: $p = 3\%$.

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:

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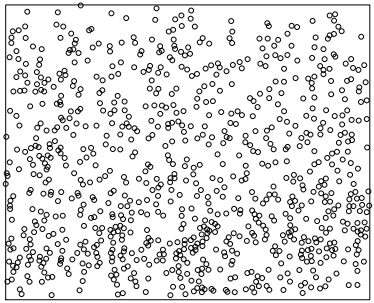
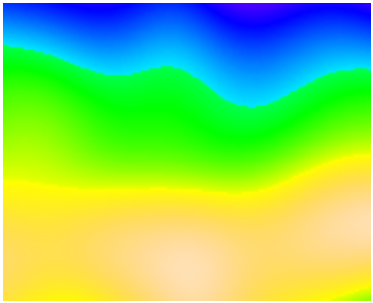
For the Strauss hard-core model

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

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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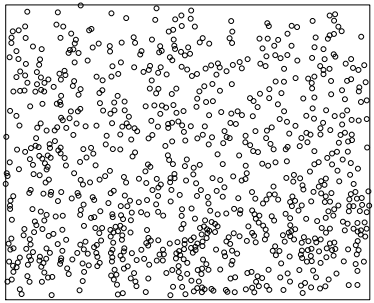

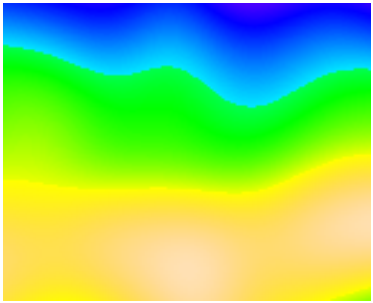

We use this unmarked point pattern to illustrate how an **inhomogenous DPP** can be fitted to a real dataset.

Modelling inhomogeneity

Assume *second-order intensity-reweighted stationarity* (Baddeley, Møller & Waagepetersen, 2000), i.e., the correlation function is translation invariant:

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

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- Fit a parametric model for R_0 via minimum contrast.
- The resulting DPP has kernel

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

Simulation of inhomogeneous model

NB: If a 'dominating DPP' with kernel $C^{\mathrm{dom}}(x, y)$ is thinned with retention probability $\pi(x)$, the resulting process is a new DPP with kernel

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Thus let $\hat{\rho}_{\max} = \sup_{x\in S}\{\hat{\rho}(x)\}$ and define a stationary DPP X^{dom} with kernel

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$$C^{\mathrm{dom}}(x,y) = C_0^{\mathrm{dom}}(x-y) = \hat{\rho}_{\max}\hat{R}_0(x-y).$$

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

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

DPPs on the sphere

- On the sphere the spherical harmonics constitute a set of basis functions (given in terms of associated Legendre polynomials).

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- Thus we only have to make a parametric model for the eigenvalues λ_k to have a DPP on the sphere.
- There are covariance functions on the sphere with known eigenvalues. One is the Inverse MultiQuadric covariance function.

DPPs on the sphere

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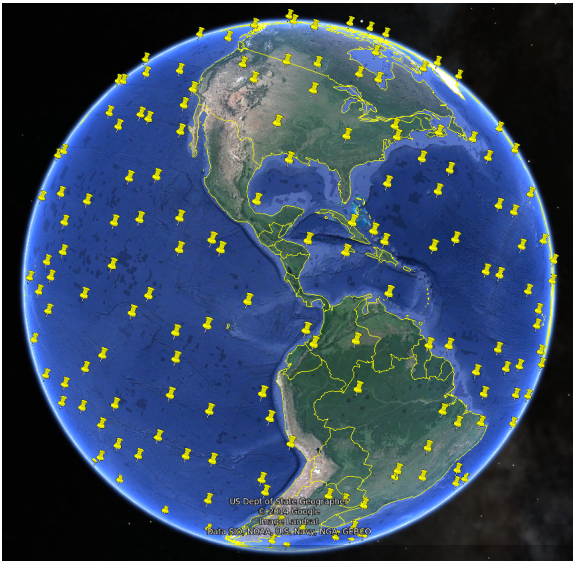
  `model <- detIMQ(rho=500,delta=0.998)`
- Simlulations rely on the previously developed code (with some modifications):
  `X <- simulate(model)`

A simulated DPP consisting of 441 points on planet Earth



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

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- Developing and implementing more models on the sphere.
- Implementing summary statistics on the sphere.

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Thank you for you attention!

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