Determinantal point processes
statistical modeling and inference

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Agenda

Definition, existence and basic properties

Stationary DPPs and approximations

Parametric models

Simulation

Data example

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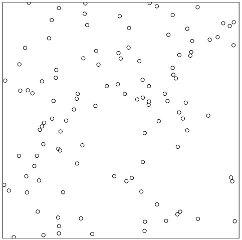
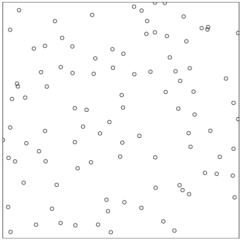
Introduction

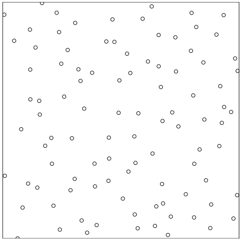
- Determinantal point processes (DPP) are inhibitive (or regular, or repulsive) point processes.
- Introduced by O. Macchi in 1975 to model fermions in quantum mechanics.
- Several theoretical studies appeared in the 2000's.
- Statistical modeling came along in the 2010's and onward.



Poisson



DPP



DPP with stronger inhibition

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Notation

- For any integer $n > 0$, denote $\rho^{(n)}$ 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 $\mathrm{d}x_i$.

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

- 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 $C(x_i, x_j)$.

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

Definition of a DPP

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 its product density functions satisfy

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

For existence, conditions on the kernel C are mandatory

- C must e.g. satisfy: $\det[C](x_1, \dots, x_n) \geq 0$ for all $x_1, \dots, x_n$.
- Henceforth we assume

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

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

- The intensity of X is $\rho(x) = C(x, x)$.
- The pair correlation function is

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

  where R is the correlation function corresponding to C.
- Thus $g \leq 1$ (i.e. inhibition) since C is Hermitian by (C1).
- If $X \sim \mathrm{DPP}(C)$, then $X_B \sim \mathrm{DPP}_B(C_B)$
- Any smooth transformation or independent thinning of a DPP is still a DPP with an explicitly given kernel.

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Existence

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 $\{\phi_k\}$ is a set of orthonormal basis functions on S, i.e.,

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

Theorem (Macchi, 1975)

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

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

Simulation

Let $X \sim \mathrm{DPP}(C)$. We want to simulate X_S for $S \subset \mathbb{R}^d$ compact.

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 $\mathrm{DPP}(C_S) \stackrel{d}{=} \mathrm{DPP}(K)$.

Note that almost surely there is a finite number of ones in the Bernoulli sequence B_k since $\sum \lambda_k^S = \int_S C(x,x)\,\mathrm{d}x < \infty$.

Simulation (cont'd)

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

$$K(x, y) = \sum_{k'=1}^{n} \phi_{k'}^S(x)\overline{\phi_{k'}^S(y)}, \quad (x, y) \in S \times S.$$

This is a *projection kernel*, and the corresponding DPP can be simulated using rejection sampling.

The algorithm always produces n points. Thus,

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

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Stationary kernels

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

Its Fourier transform (or spectral density) is:

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

Theorem

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

$$\varphi \leq 1.$$

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

In practice, this restriction implies that if the intensity is large the range (effective support) of C_0 must be small. I.e. there is a trade-off between strong inhibiton and large intensity.

Approximation

Without loss of generality we consider $S = [-1/2, 1/2]^d$. To approximate X_S we consider $X^{\text{app}} \sim DPP_S(C_{\mathrm{app}})$ where

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

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:

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

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

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

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Parametric models in R

The parametric families are specified in R via the determinantal family functions: `dppGauss`, `dppMatern`, `dppPowerExp`. E.g:

- `model <- dppGauss(lambda=100, alpha=0.05, d=2)`
- `model <- dppMatern(lambda=100, alpha=0.03, nu=0.5, d=2)`
- `model <- dppPowerExp(lambda=100, alpha=0.17, nu=2, d=2)`

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

- `dppkernel(model)`
- `dppspecden(model)`
- `pcfmodel(model)`
- `Kmodel(model)`

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Illustration of simulation algorithm

Step 1. The first point is sampled uniformly on S.

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Illustration of simulation algorithm

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

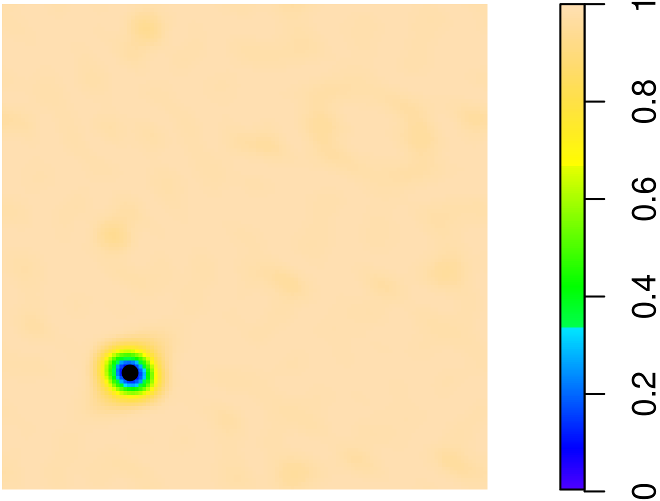

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Illustration of simulation algorithm

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

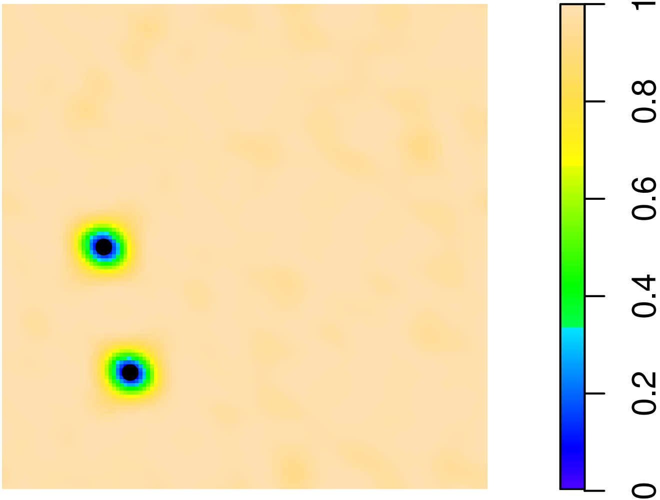

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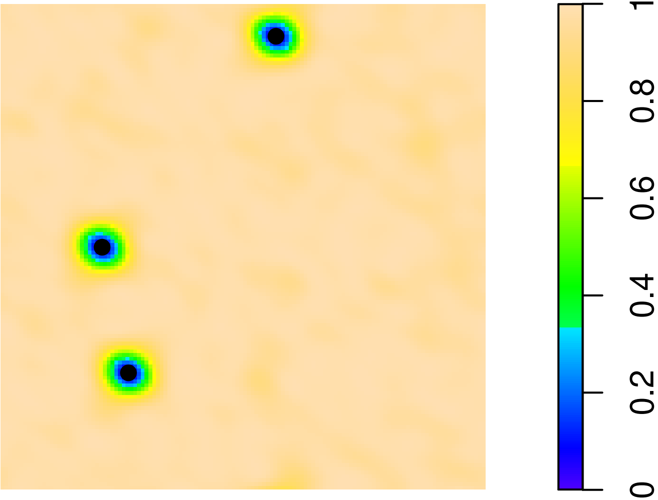
Illustration of simulation algorithm

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



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

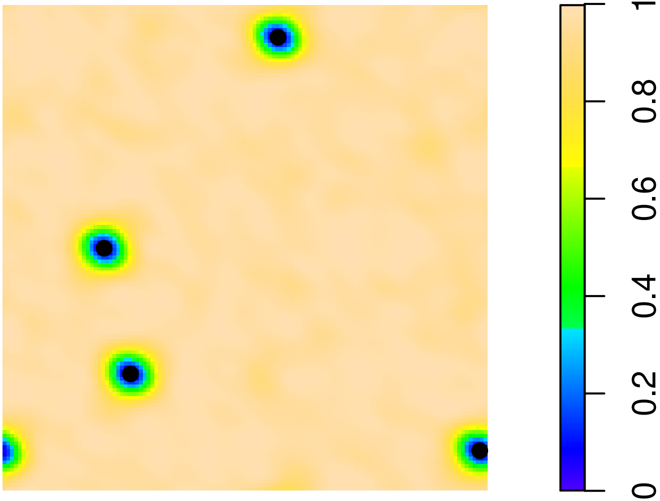

Illustration of simulation algorithm

...somewhere in the middle...

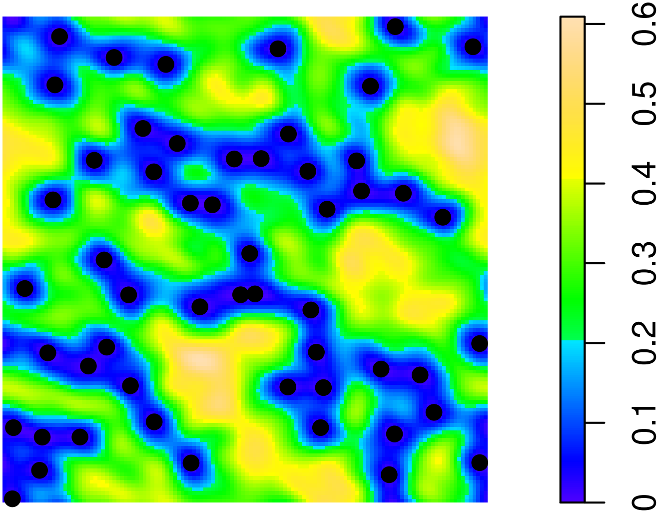

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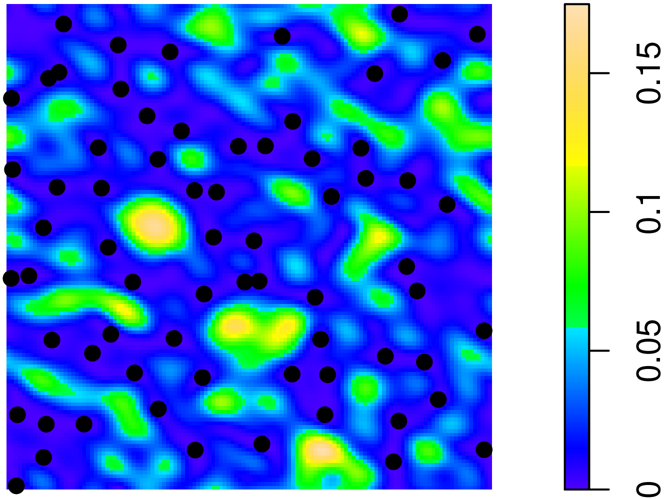
Illustration of simulation algorithm

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



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Simulation in R

Simply use the generic function `simulate`:

- ```
  model <- dppGauss(lambda=100, alpha=0.05, d=2)
  X <- simulate(model)
  ```
- 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)
  ```
- Several realizations:
  ```
  X <- simulate(model, nsim=4)
  ```

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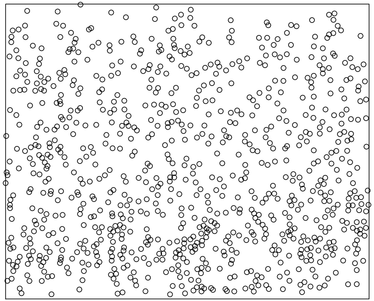
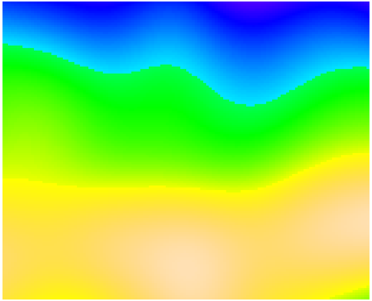
  ```

Mucous membrane dataset

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





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

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Modelling inhomogeneity

Assume *correlation stationarity* (second-order intensity-reweighted stationarity) i.e. the correlation function is translation invariant:

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

such that $R(x,x) = 1$.

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- Use the fitted intensity to estimate the inhomogeneous g- og K-function.

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- Fit a parametric model to ρ depending on relevant covariates (second coordinate axis in our case).
- Use the fitted intensity to estimate the inhomogeneous g- og K-function.
- Fit a parametric model for R_0 via minimum contrast.

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- Fit a parametric model to ρ depending on relevant covariates (second coordinate axis in our case).
- Use the fitted intensity to estimate the inhomogeneous g- og K-function.
- Fit a parametric model for R_0 via minimum contrast.
- The resulting DPP has

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

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