Determinantal point process models and statistical inference

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GDR GeoSto

In short

- DPPs are general models for random processes with **negative dependencies**.
- Their general definition has been introduced by O. Macchi in 1975 to model fermions (i.e. particles in repulsion)
- DPPs arise in many examples of Probability theory (much before 1975)
- They have been used for statistical purposes more recently (for about 5 years).

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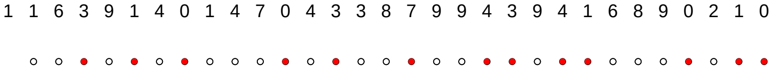

This is a DPP!

With $N = 100$.

From the "descent subsequence"

From an independent sampling

Example 2: the Ginibre DPP

Let M be an $n \times n$ matrix with iid complex Gaussian entries.
Then the n eigenvalues of M are

- "mainly" concentrated in the complex disk with radius $\sqrt{n}$
- distributed as a DPP on the complex plane

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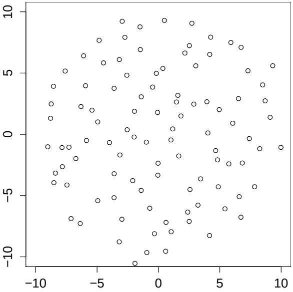
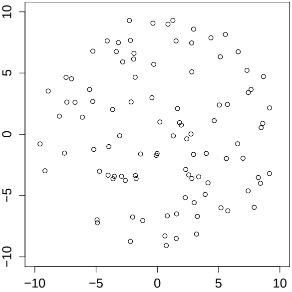
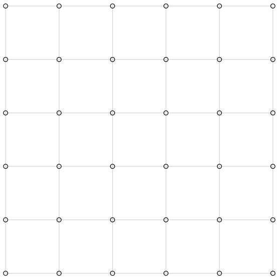
Left : Ginibre DPP ($n = 100$). Right : 100 iid points in the disk.





Example 3: spanning tree

Aim : sample edges (with negative dependence) from a graph



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Random spanning tree

"tree" = any 2 vertices are connected by exactly one path
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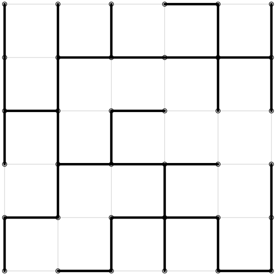
"random" = uniform over all possible spanning trees



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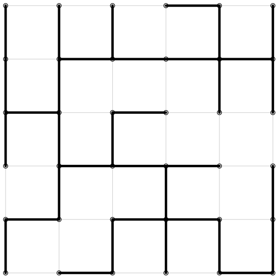
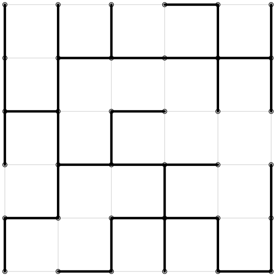
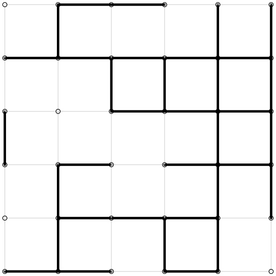


The repartition of the edges on the graph is a DPP!

Left: spanning tree. Right: independent sampling of the edges





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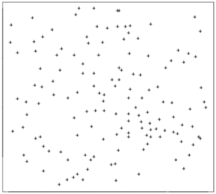
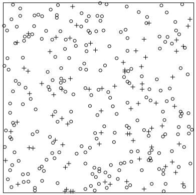
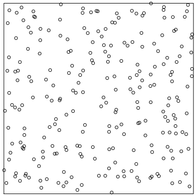
- In surveys or random designs : negative dependencies in the sampling may reduce the variance of an estimate (ex : Monte Carlo approximation of the integral of a smooth function)
- Some real-data naturally involve negative dependencies:



Cellular Network



Kidney cells (hamster)



Oak and Beech trees

Gibbs point processes vs DPPs (on $\mathbb{R}^d$)

Gibbs point processes: The usual class when modelling repulsiveness on $\mathbb{R}^d$ (e.g. Strauss model).

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In general:

- moments are not expressible in closed form;
- likelihoods involve intractable normalizing constants;
- elaborate McMC methods are needed for simulations and approximate likelihood inference;
- for infinite Gibbs point processes defined on $\mathbb{R}^d$, 'things' become rather complicated (existence and uniqueness)

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(c) the density of the DPP restricted to any compact set is expressible on closed form;

(d) the DPP on any compact set can easily be simulated;

(e) parametric models are available, and inference can be done by MLEs or using the moments.

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where $K_A = [K_{ij}]_{i,j \in A}$.

Interpretation: for $i, j \in \{1, \ldots, N\}$,

$K_{ii} = P(i \in X)$

$K_{ij} \approx$ measure of similarity between i and j. If K is symmetric

$$P(i, j \in X) = \begin{vmatrix} K_{ii} & K_{ij} \\ K_{ji} & K_{jj} \end{vmatrix} = P(i \in X)P(j \in X) - K_{ij}^2$$

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- For any borel set $B \subseteq \mathbb{R}^d$, $X_B = X \cap B$.
- For $n > 0$, $\rho^{(n)}$ is 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 $i = 1, \ldots, n$,
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  In particular $\rho = \rho^{(1)}$ is the *intensity function*.

Definition of a DPP on $\mathbb{R}^d$

Let C be a function from $\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$.
Denote $[C](x_1, \ldots, x_n)$ the $n \times n$ matrix with entries $C(x_i, x_j)$.

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

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

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Basic example : The Poisson point process with intensity $\rho(x)$ is the special case where $C(x, x) = \rho(x)$ and $C(x, y) = 0$ if $x \neq y$.

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- 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 $\text{DPP}(C)$.

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

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

If $\lambda_k^S < 1 \ \forall k$, then $X_S \ll Poisson(S,1)$, with 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

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

Simulation

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

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

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2. Given $M = m$, generate $B_1, \dots, B_{m-1}$
3. simulate $\mathrm{DPP}(K)$ given $B_1, \dots, B_M$ and $M = m$. The kernel K becomes w.l.o.g.

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

and $\mathrm{DPP}(K)$ is a *determinantal projection process*.

Simulation of a determinantal projection process:

$$K(x,y)=\sum_{k=1}^{n}\phi_k^S(x)\overline{\phi_k^S(y)}=\boldsymbol{v}(y)^*\boldsymbol{v}(x),\quad \boldsymbol{v}(x)=(\phi_1^S(x),\dots,\phi_n^S(x))^T.$$

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

---

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

Summary

Therefore, given a kernel C :

- condition for existence of DPP(C) are known*
- all moments of DPP(C) are explicitly known
- the density of DPP(C) on any compact set is known*
- DPP(C) can be easily and quickly simulated on any compact set*

* if the spectral representation of C_S is known on any S (see later for an approximation).

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

Theorem

Under (C1), if $C_0 \in L^2(\mathbb{R}^d)$, then existence of 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 $\varphi \leq 1$.

$\rightarrow$ *This will induce restriction on the parameter space.*

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

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- 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

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

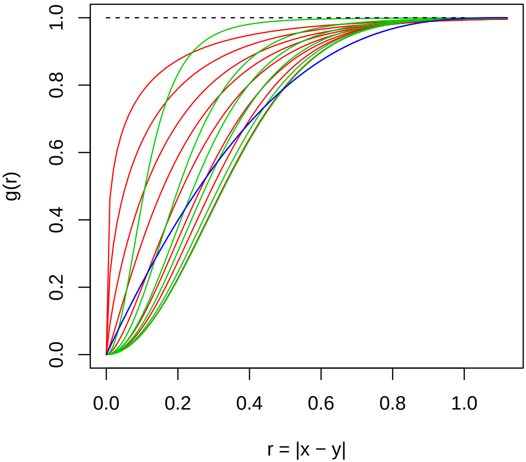
  DPP(C_0) exists iff $\rho \leq \frac{\Gamma(\nu+d/2)}{\Gamma(\nu)(\sqrt{\pi}\alpha)^d}$

Pair correlation functions of DPP(C_0) for previous models when $\rho = 1$ and $\alpha = \alpha_{max}(\nu)$:

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



- Are the previous parametric families "rich enough"?

- How repulsive a stationary DPP can be?

  - Less repulsive DPP = Poisson Point Process.

  - What is the most repulsive DPP?

- We introduce criteria of repulsiveness based on the pair correlation function g.

How repulsive a stationary DPP can be?

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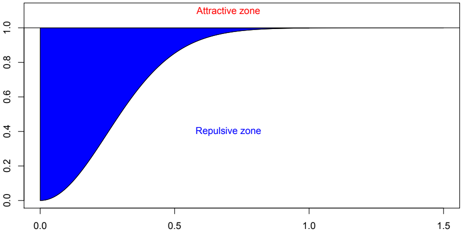
Criteria of repulsiveness based on the pair correlation function.



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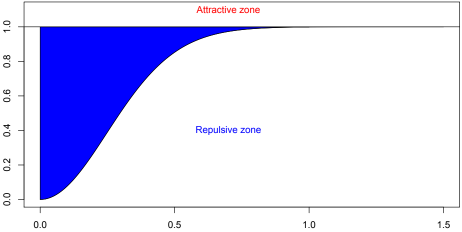

Let X and Y be two DPPs with the same intensity ρ and pcf g_X, g_Y.

Definition

- X is *globally more repulsive* than Y if "g_X has a larger blue zone", i.e. $\int(1 - g_X) \geq \int(1 - g_Y)$.

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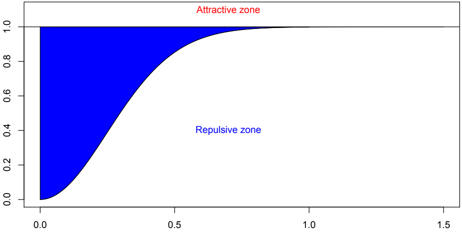

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- X is *locally more repulsive* than Y if "g_X is more flat near 0", i.e. $g_X(0) = g_Y(0) = 0$, $\nabla g_X(0) = \nabla g_Y(0) = 0$ and $\Delta g_X(0) \leq \Delta g_Y(0)$.

Note that for a hardcore point process: $g(0) = \nabla g(0) = \Delta g(0) = 0$.

Let J_ν be the Bessel function of the first kind with order ν.

Proposition

There exists a unique DPP that is both the most globally and the most locally repulsive DPP with intensity ρ. Its kernel in dimension $d = 2$ is given by:

$$C_0(x) = \sqrt{\rho}\frac{J_1(2\sqrt{\pi\rho}||x||)}{\sqrt{\pi}||x||} \quad \text{and} \quad \varphi(x) = \mathbf{1}_{||x||^2 \leq \rho\pi^{-1}}$$

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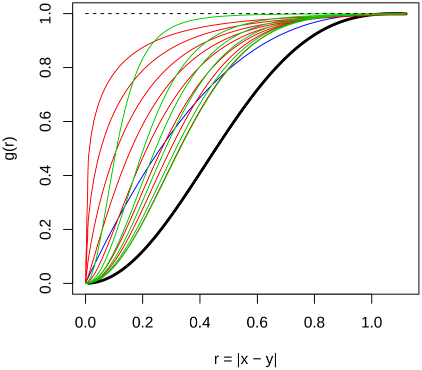
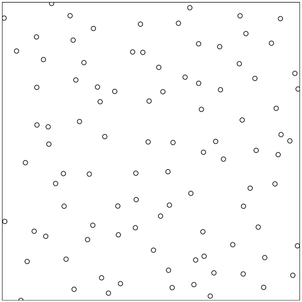




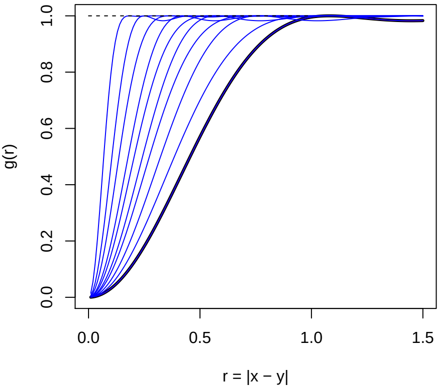
New parametric families of kernels

New parametric families of kernels

- Laguerre-Gauss family, for $n \in \mathbb{N}$ and $0 < \alpha \leq \alpha_{max}(d, \rho, n)$

$$C_0(x) \propto L_{n-1}^{\frac{d}{2}}\left(\frac{1}{n}\left\|\frac{x}{\alpha}\right\|^2\right) e^{-\frac{1}{n}\|\frac{x}{\alpha}\|^2} \quad \varphi(x) \propto e^{-n(\pi\alpha\|x\|)^2} \sum_{k=0}^{n-1} \frac{(\pi\sqrt{n}\|\alpha x\|)^{2k}}{k!}$$

$\longrightarrow$ covers all possible degrees of repulsiveness.

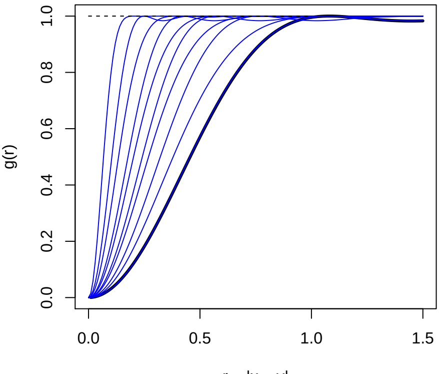


- Generalized-Sinc family, for $\sigma \geq 0$, $0 < \alpha \leq \alpha_{max}(d, \rho, \sigma)$

$$C_0(x) \propto \frac{J_{\frac{\sigma+d}{2}}\left(2\|\frac{x}{\alpha}\|\sqrt{\frac{\sigma+d}{2}}\right)}{\left(2\|\frac{x}{\alpha}\|\sqrt{\frac{\sigma+d}{2}}\right)^{\frac{\sigma+d}{2}}} \qquad \varphi(x) \propto \left(1 - \frac{2(\pi\|\alpha x\|)^2}{\sigma + d}\right)_+^{\frac{\sigma}{2}}$$

$\longrightarrow$ covers all possible degrees of repulsiveness.

$\longrightarrow$ φ is compactly supported.



Approximation of stationary DPP's models

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

- The simulation and the density of X_S requires the expansion

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

but in general λ_k^S and ϕ_k^S are not expressible on closed form.

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

Approximation of stationary models

So, DPP(C_0) on S can be approximated by DPP($C_{\mathrm{app},0}$) with

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

where φ is the Fourier transform of C_0.

This **kernel approximation** allows us

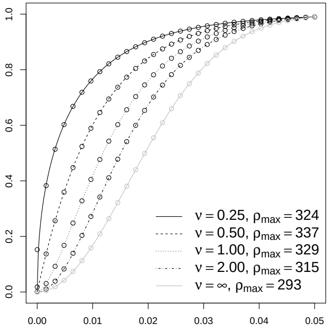
- to simulate DPP(C_0) on S, by simulating DPP($C_{\mathrm{app},0}$)
- to compute the (approximated) density of DPP(C_0) on S.

Turns out to be a very good approximation in most cases.

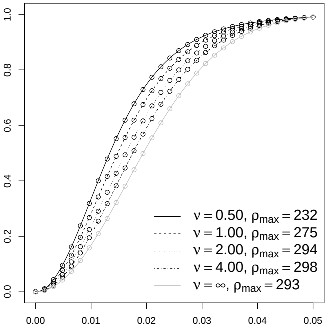
Exemples of approximations

– Solid lines : theoretical pair correlation function

∘ Circles : pair correlation from the approximated kernel



Whittle-Matérn



Generalized Cauchy

Consider a stationary and isotropic parametric DPP(C_0), with

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

where $R_\theta(0) = 1$ and θ is some parameter.

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For this model:

- $\rho =$ intensity.
- Pair correlation function:

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

Parameter estimation

In

$$C_0(x-y) = \rho R_\theta(\|x-y\|)$$

we can estimate (ρ, θ)

- by MLE using the kernel approximation for the likelihood
- or using the moments, for instance :

$$\hat{\rho} = \#\{\text{obs. points}\}/[\text{area of obs. window}]$$

$$\hat{\theta} = \text{argmin}_\theta \int_{r_{\min}}^{r_{\max}} \left| \sqrt{\widehat{g}(r)} - \sqrt{g_\theta(r)} \right|^2 \mathrm{d}r$$

Conclusion

• DPPs provide **flexible** (parametric) models of repulsive point processes and possess **appealing properties**:

- Easily and rather quickly simulated
- Closed form expressions for all moments.
- Closed form expression for the density on any bounded set.
- Parametric models are available
- Inference is feasible, including likelihood inference.
- More: Laplace transform, mixing properties, concentration inequalities, asymptotic inference,...

• Parametric models, inference methods and so on are available in R in the package `spatstat`.

Conclusion

Some open questions :

- Can we simulate DPP(C) without the spectral representation of C?
- Theoretical properties for the MLE?
- Theory for inference in the non-homogeneous case
- Semi or non-parametric inference
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THANK YOU