Statistical aspects of determinantal point processes

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Joint work with
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Determinantal point processes (DPP) form a class of repulsive point processes.

They were introduced in their general form by O. Macchi in 1975 to model fermions (i.e. particles 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.

The statistical aspects have so far been largely unexplored.
Examples

- Poisson
- DPP
- DPP with stronger repulsion
Do DPP’s constitute a *tractable* and *flexible* class of models for *repulsive* point processes?

**Answer:** YES.

- DPP's can be easily simulated.
- There are closed form expressions for the moments.
- There is a 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. the Strauss process).
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2. Definition, existence and basic properties

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4. Parametric models

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Notation

- We view a spatial point process $X$ on $\mathbb{R}^d$ as a random locally finite subset of $\mathbb{R}^d$. 
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For any borel set $B \subseteq \mathbb{R}^d$, $X_B = X \cap B$. 

Intuitively, $\rho(n)(x_1, \ldots, x_n) \, dx_1 \cdots dx_n$ is the probability that for each $i = 1, \ldots, n$, $X$ has a point in a region around $x_i$ of volume $dx_i$. In particular $\rho = \rho(1)$ is the intensity function.
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- For any borel set $B \subseteq \mathbb{R}^d$, $X_B = X \cap B$.
- For any integer $n > 0$, denote $\rho^{(n)}$ the $n$'th order product density function of $X$.
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Definition of a determinantal point process

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

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

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

For existence, conditions on the kernel $C$ are mandatory, e.g. $C$ must satisfy: for all $x_1, \ldots, x_n$, $\det[C](x_1, \ldots, x_n) \geq 0$. 
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**Definition**

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

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First properties

- From the definition, if $C$ is continuous,

\[ \rho^{(n)}(x_1, \ldots, x_n) \approx 0 \quad \text{whenever} \quad x_i \approx x_j \quad \text{for some} \ i \neq j, \]

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■ The intensity of $X$ is $\rho(x) = C(x, x)$.

■ The pair correlation function is

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

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- Thus $g \leq 1$ (i.e. repulsiveness).

- If $X \sim \text{DPP}(C)$, then $X_B \sim \text{DPP}_B(C_B)$

- Any smooth transformation or independent thinning of a DPP is still a DPP with explicit given kernel.

- There exists at most one DPP$(C)$. 
In all that follows we assume

(C1) \( C \) is a continuous complex covariance function.
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 \( \int_S \phi_k^S(x) \overline{\phi_l^S(x)} \, dx = 1 \{ k = l \} \).
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**Theorem (Macchi, 1975; Hough et al., 2009; our paper)**

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

\[
\lambda_k^S \leq 1 \text{ for all compact } S \subset \mathbb{R}^d \text{ and all } k.
\]
Density on a compact set $S$

Let $X_S \sim \text{DPP}_S(C_S)$ with $S \subset \mathbb{R}^d$ compact.

Recall that $C_S(x, y) = \sum_{k=1}^{\infty} \lambda_k^S \phi_k^S(x)\phi_k^S(y)$. 

\[ D = -\sum_{k=1}^{\infty} \log(1 - \lambda_k^S) \]

\[ \tilde{C}_{S} : S \times S \to \mathbb{C} \]
Density on a compact set $S$

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Recall that $C_S(x, y) = \sum_{k=1}^{\infty} \lambda^S_k \phi^S_k(x) \phi^S_k(y)$.

**Theorem (Macchi, 1975)**

Assuming $\lambda^S_k < 1$, for all $k$, then $X_S$ is absolutely continuous with respect to the homogeneous Poisson process on $S$ with unit intensity, and has density

$$f(\{x_1, \ldots, x_n\}) = \exp(|S| - D) \det[\tilde{C}](x_1, \ldots, x_n),$$

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

$$\tilde{C}(x, y) = \sum_{k=1}^{\infty} \frac{\lambda^S_k}{1 - \lambda^S_k} \phi^S_k(x) \phi^S_k(y).$$
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We want to simulate $X_S$.

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

**Theorem (Hough et al., 2006)**

For $k \in \mathbb{N}$, let $B_k$ be independent Bernoulli r.v.'s with means $\lambda_k^S$. 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 $\text{DPP}_S(C_S) \overset{d}{=} \text{DPP}_S(K)$. 
So simulating $X_S$ is equivalent to simulate $\text{DPP}_S(K)$ with

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Let $M = \max\{k \geq 0; B_k \neq 0\}$.

Note that $M$ is a.s. finite, since $\sum \lambda^S_k = \int_S C(x, x) \, dx < \infty$. 
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3. simulate the point process $DPP_S(K)$ given $B_1, \ldots, B_M$ and $M = m$. 

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In step 3, the kernel $K$ becomes a projection kernel, and w.l.o.g.

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

where $n = \#\{1 \leq k \leq M : B_k = 1\}$. 
Simulation of determinantal projection processes

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

$$K(x, y) = \sum_{k=1}^{n} \phi_k^S(x)\overline{\phi_k^S(y)} = \mathbf{v}(y) \ast \mathbf{v}(x)$$
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The point process $\text{DPP}_S(K)$ has a.s. $n$ points $(X_1, \ldots, X_n)$ that can be simulated by the following Gram-Schmidt procedure:
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The point process $\text{DPP}_S(K)$ has a.s. $n$ points $(X_1, \ldots, X_n)$ that can be simulated by the following Gram-Schmidt procedure:

- Sample $X_n$ from the distribution with density $p_n(x) = \|\mathbf{v}(x)\|^2/n$.
- Set $e_1 = \mathbf{v}(X_n)/\|\mathbf{v}(X_n)\|$.
- For $i = (n-1)$ to 1 do
  - Sample $X_i$ from the distribution (given $X_{i+1}, \ldots, X_n$):
    $$p_i(x) = \frac{1}{i} \left[ \|\mathbf{v}(x)\|^2 - \sum_{j=1}^{n-i} |e_j^* \mathbf{v}(x)|^2 \right], \quad x \in S$$
  - Set $w_i = \mathbf{v}(X_i) - \sum_{j=1}^{n-i} (e_j^* \mathbf{v}(X_i)) e_j$, $e_{n-i+1} = w_i/\|w_i\|$
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**Theorem**

$\{X_1, \ldots, X_n\}$ generated as above has distribution $\text{DPP}_S(K)$. 

Illustration of simulation algorithm

Example: Let $S = [-1/2, 1/2]^2$ and

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

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

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

and $X_S \sim \text{DPP}_S(K)$ is homogeneous and has a.s. $n$ points.
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**Step 1.** The first point is sampled uniformly on $S$
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etc.
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etc.
Illustration of simulation algorithm

e etc.
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etc.
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Stationary models

We focus on a 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

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Stationary models

We focus on a kernel $C$ of the form

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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

$$\varphi \leq 1.$$*

To construct parametric families of DPP:
Consider parametric families of $C_0$ and rescale so that $\varphi \leq 1.$

→ This will induce a bound 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 $\alpha$ is given by

$$C_0(x) = \rho \frac{2}{\pi} \left( \arccos\left(\frac{\|x\|}{\alpha}\right) - \frac{\|x\|}{\alpha} \sqrt{1 - \left(\frac{\|x\|}{\alpha}\right)^2} \right) \mathbf{1}_{\|x\| < \alpha}.$$

DPP($C_0$) exists iff $\varphi \leq 1 \Leftrightarrow \rho \alpha^2 \leq 4/\pi$.

⇒ Tradeoff between the intensity $\rho$ and the range of repulsion $\alpha$. 
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  \( \Rightarrow \) Tradeoff between the intensity \( \rho \) and the range of repulsion \( \alpha \).

- 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:

- **In blue**: $C_0$ is the **circular** covariance function.
- **In red**: $C_0$ is Whittle-Matérn, for different values of $\nu$.
- **In green**: $C_0$ is generalized Cauchy, for different values of $\nu$.

The parameter $\alpha$ is chosen such that the range of corr. $\approx 1$. 

![Diagram showing pair correlation functions for different models.](image-url)
Spectral approach

- Specify a parametric class of integrable functions \( \varphi_\theta : \mathbb{R}^d \rightarrow [0, 1] \) (spectral densities).
- This is all we need for having a well-defined DDP.
- Is convenient for simulation and for (approximate) density calculations as seen later.
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- This is all we need for having a well-defined DDP.
- Is convenient for simulation and for (approximate) density calculations as seen later.
- Example: *power exponential spectral model*:

$$
\varphi_{\rho,\nu,\alpha}(x) = \rho \frac{\Gamma(d/2 + 1)\nu\alpha^d}{d\pi^{d/2}\Gamma(d/\nu)} \exp \left( -\|\alpha x\|^{\nu} \right)
$$

with

$$
\rho > 0, \quad \nu > 0, \quad 0 < \alpha < \alpha_{\text{max}}(\rho, \nu) := \left( \frac{2\pi^{d/2}\Gamma(d/\nu + 1)}{\rho\Gamma(d/2)} \right)^{1/d}.
$$
Power exponential spectral model: (isotropic) spectral densities and pair correlation functions
Approximation of stationary models

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

- 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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- **Consider the unit box** $S = [-\frac{1}{2}, \frac{1}{2}]^d$ and the Fourier expansion

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

The Fourier coefficients are

\[
c_k = \int_S C_0(u) e^{-2\pi i k \cdot u} \, du \approx \int_{\mathbb{R}^d} C_0(u) e^{-2\pi i k \cdot u} \, du = \varphi(k)
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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 $\text{DPP}(C_0)$ on $S$ is then $\text{DPP}_S(C_{\text{app},0})$ with

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

where $\varphi$ is the Fourier transform of $C_0$. 

Approximation of stationary models

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

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where $\varphi$ 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 $S$. 
1 Introduction

2 Definition, existence and basic properties

3 Simulation

4 Parametric models

5 Inference
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 and second moments are easily deduced:

- The intensity is $\rho$.
- The pair correlation function is

$$g(x, y) = g_0(\|x - y\|) = 1 - R^2_\alpha(\|x - y\|).$$

- Ripley’s $K$-function is easily expressible in terms of $R_\alpha$: if $d = 2$,

$$K_\alpha(r) := 2\pi \int_0^r tg_0(t) \, dt = \pi r^2 - 2\pi \int_0^r t|R_\alpha(t)|^2 \, dt.$$
Parameter estimation can be conducted as follows.

1. Estimate $\rho$ by $\#\{\text{obs. points}\}/\text{area of obs. window}$.
2. Estimate $\alpha$
   - either by **minimum contrast** estimator (MCE):
     \[
     \hat{\alpha} = \arg\min_{\alpha} \int_{0}^{r_{\text{max}}} \left| \sqrt{\hat{K}(r)} - \sqrt{K_{\alpha}(r)} \right|^2 \, dr
     \]
   - or by **maximum likelihood** estimator: given $\hat{\rho}$, the likelihood is deduced from the kernel approximation.
Two model examples

- Exponential model with $\rho = 200$ and $\alpha = 0.014$:
  \[ C_0(x) = \rho \exp(-\|x\|/\alpha). \]

- 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 $\alpha$ from 200 realisations

Gaussian model

Exponential model
Example: 134 Norwegian pine trees observed in a $56 \times 38$ m region

Møller and Waagpetersen (2004): a five parameter multiscale process is fitted using elaborate MCMC MLE methods.

Here we fit a more parsimonious DPP models.
First,

- Whittle-Matérn model;
- Cauchy model;
- Gaussian model: the best fit, but plots of summary statistics indicate a lack of fit.
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- Whittle-Matérn model;
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- Gaussian model: the best fit, but plots of summary statistics indicate a lack of fit.

Second,

- power exponential spectral model: provides a much better fit, with

\[ \hat{\nu} = 10, \quad \hat{\alpha} = 6.36 \approx \alpha_{\text{max}} = 6.77 \]

i.e. close to the “most repulsive possible stationary DPP”.
Clockwise from top left: $L(r) - r$; $G(r)$; $F(r)$; $J(r)$. Simulated 2.5% and 97.5% envelopes are based on 4000 realizations of the fitted Gaussian model resp. power exponential spectral model.
Conclusions

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- DPP’s possess the following appealing properties:
  - Easily simulated.
  - Closed form expressions for the moments.
  - Closed form expression for the density of a DPP on any bounded set.
  - Inference is feasible, including likelihood inference.
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  ■ Closed form expression for the density of a DPP on any bounded set.
  ■ Inference is feasible, including likelihood inference.

⇒ Promising alternative to repulsive Gibbs point processes.


