Attractive coupling of determinantal point processes using nonsymmetric kernels

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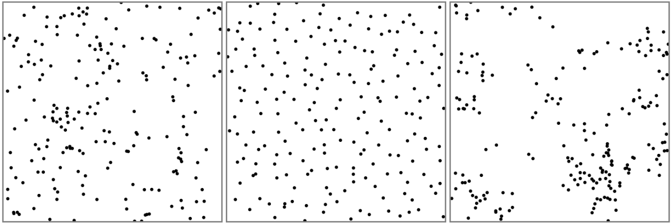
Outline

Determinantal point processes

- DPPs are a family of repulsive point processes.



- Introduced by O. Macchi in 1975 to model fermion systems in theory of quantum particles.
- Used for statistical purposes to model repulsive point data (e.g. trees, cells...)

Determinantal point processes

We write $[n] = \{1, \cdots, n\}$

Definition

Let K be an $n \times n$ matrix. We say that X is a determinantal point process with kernel K, written $X \sim DPP(K)$, if for all $S \subset [n]$,

$$\mathbb{P}(S \subset X) = \det(K_S) \quad \textit{where} \quad K_S = (K_{i,j})_{i,j \in S}$$

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- $\mathbb{P}(i \in X) = K_{i,i}$.
- $\mathbb{P}(\{i,j\} \subset X) - \mathbb{P}(i \in X)\mathbb{P}(j \in X) = \det \begin{pmatrix} K_{i,i} & K_{i,j} \\ K_{j,i} & K_{j,j} \end{pmatrix} - K_{i,i}K_{j,j}$.

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- $\mathbb{P}(\{i, j\} \subset X) - \mathbb{P}(i \in X)\mathbb{P}(j \in X) = -K_{i,j}K_{j,i}$.
- $\forall S \subset [n],\ X \cap S \sim DPP(K_S)$.

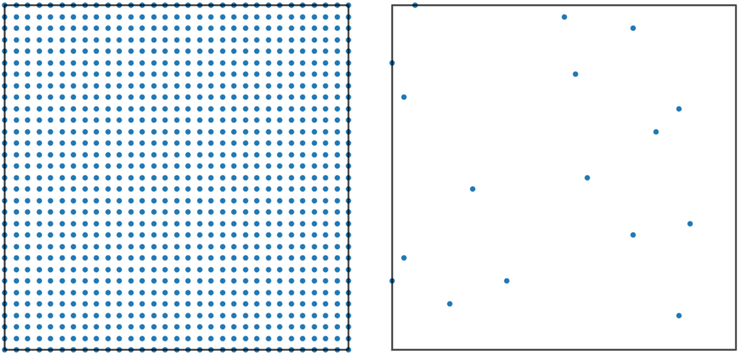
Proposition

If K is a symmetric matrix then the DPP with kernel K is well-defined if and only if the eigenvalues of K are in $[0, 1]$.

Example

Simulation of a DPP on $\{0, \frac{1}{30}, \cdots, 1\}^2$ with kernel

$$K(x, y) = 0.02e^{-\frac{\|y-x\|^2}{0.018}}.$$



Outline

1. Intro
   - Determinantal point processes
   - Motivation
   - A natural coupling
2. DPPs with nonsymmetric kernels
   - Known results
   - First examples of couplings
   - Characterization using the theory of P_0 matrices
3. Construction of positive coupling of DPPs
   - Simulation algorithm
   - Two different constructions
   - Numerical results
4. Conclusion

Two problems related to positive coupling of DPPs.

Proposition (Lyons (2002))

Let K_1, K_2 be two $n \times n$ symmetric positive semidefinite matrices such that

$$0 \preccurlyeq K_1 \preccurlyeq K_2 \preccurlyeq I_n$$

Then, the determinantal measure with kernel K_1 is stochastically dominated by the determinantal measure with kernel K_2.

By Strassen's theorem, there exists a coupling $(X, Y) \sim \mathbb{P}$ such that $X \sim DPP(K_1)$, $Y \sim DPP(K_2)$ and $\mathbb{P}(X \subset Y) = 1$.

Question: Is there a natural way of constructing such a coupling?

Two problems related to positive coupling of DPPs.

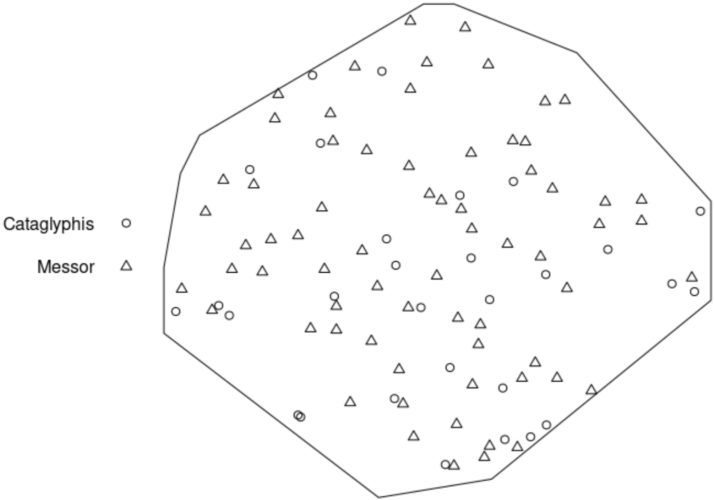


Figure: Nest locations of two species of ants at a site in northern Greece.

Outline

A natural coupling

Coupling of two point processes on $[n]$ $\Leftrightarrow$ Point process on $[2n]$

$$\begin{array}{ccc} [2n] & \leftrightarrow & [n]\times[n] \\ X & \leftrightarrow & (X_1, X_2) \end{array} \text{ where } \begin{cases} X_1 = X \cap [n]; \\ X_2 = \{i - n, i \in X \cap \{n+1, \cdots, 2n\}\}. \end{cases}$$

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Let $K_1, K_2 \in \mathcal{M}_n(\mathbb{R})$ and $(X_1, X_2) \sim DPP(\mathbb{K})$ where

$$\mathbb{K} = \begin{pmatrix} K_1 & * \\ * & K_2 \end{pmatrix} \in \mathcal{M}_{2n}(\mathbb{R}).$$

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- $X_1 \sim DPP(K_1)$ and $X_2 \sim DPP(K_2)$.
- $\mathbb{P}(i \in X_1, j \in X_2) - \mathbb{P}(i \in X_1)\mathbb{P}(j \in X_2) = -\mathbb{K}_{i,j+n}\mathbb{K}_{j+n,i}$

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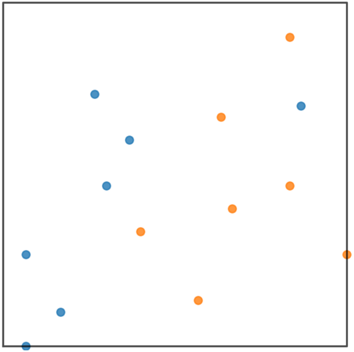
⚠ If $\mathbb{K}$ is symmetric then only negative cross-correlations are possible.

Example

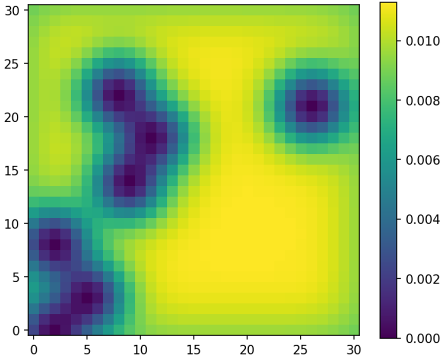
Simulation of a DPP on $(\{0, \frac{1}{30}, \cdots, 1\}^2)^2$ with kernel $\mathbb{K} = \begin{pmatrix} K & K \\ K & K \end{pmatrix}$

where

$$K(x, y) = 0.008e^{-\frac{\|y-x\|^2}{0.023}}$$



DPP coupling simulation



Inclusion probability for the orange DPP conditionally to the blue DPP

Proposed solution: Using nonsymmetric kernels!

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First major problem: The well-definedness of DPPs.

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First major problem: The well-definedness of DPPs.

Definition

We say that an $n \times n$ *matrix is a* ***DPP kernel*** *if the associated determinantal measure is a probability measure.*

Outline

Two methods of constructing DPPs with nonsymmetric kernels

Proposition

Let K be a DPP kernel and D be a diagonal matrix of same size. Then DKD^{-1} is also a DPP kernel and $DPP(K) \overset{d}{=} DPP(DKD^{-1})$

Proof.

Direct consequence of the fact that

$$\det((DKD^{-1})_S) = \frac{\prod_{i\in S} D_{i,i}}{\prod_{i\in S} D_{i,i}} \det(K_S)$$

□

Two methods of constructing DPPs with nonsymmetric kernels

Proposition (Borodin et al., 1999)

Let $X \sim DPP(K)$, $S \subset [n]$ and define the ***particle-hole transformation***

$$Y = (X \cap S^c) \cup (X^c \cap S).$$

Then Y is a DPP with kernel

$$\widetilde{K} = (I_n - D(\mathbb{1}_S))K + D(\mathbb{1}_S)(I_n - K)$$

where $D(\mathbb{1}_S)$ is a diagonal matrix with $D_{i,i} = \mathbb{1}_{i \in S}$.

Two methods of constructing DPPs with nonsymmetric kernels

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where $D(\mathbb{1}_S)$ is a diagonal matrix with $D_{i,i} = \mathbb{1}_{i \in S}$.

As a consequence we can write

$$\mathbb{P}(X = S^c) = \mathbb{P}([n] \subset Y) = \det(\widetilde{K})$$

Proposition (Generalized particle-hole involution)

Let $X \sim DPP(K)$. Let $p_1, \cdots, p_n \in [0,1]^n$ and $B_i \sim b(p_i)$ with $B_1, \cdots, B_n$ and X independent then define

$$Y = \{i \in [n] \text{ s.t. } i \in X \text{ and } B_i = 0 \text{ or } i \notin X \text{ and } B_i = 1\}$$

Then Y is a DPP with kernel

$$(I_n - D(p))K + D(p)(I_n - K)$$

where $D(p)$ is a diagonal matrix with $D_{i,i} = p_i$.

A few examples in the literature

- Schur measures on partitions (Okounkov (2000))
- One dependant process

Proposition (Borodin, A., Diaconis, P. and Fulman, J. (2009))

Let $X_1, \cdots, X_n \in \{0,1\}$ be a 1-dependant process ($X_i \perp\!\!\!\perp X_j$ if $|j-i| \geqslant 2$) and $X = \{i \text{ s.t. } X_i = 1\}$. Then X is a DPP with kernel of the form

$$K = \begin{pmatrix} * & \cdots & \cdots & * \\ -1 & \ddots & & \vdots \\ & \ddots & \ddots & * \\ 0 & & -1 & * \end{pmatrix}$$

Outline

Independent coupling

Proposition

Let $K \in \mathcal{M}_n(\mathbb{R})$ be a DPP kernel and define

$$\mathbb{K} = \begin{pmatrix} K & 0 \\ * & K \end{pmatrix}.$$

Then $\mathbb{K}$ is a DPP kernel.

If $(X_1, X_2) \sim DPP(\mathbb{K})$ then

- $X_1 \sim DPP(K)$;
- $X_2 \sim DPP(K)$;
- $X_1 \perp\!\!\!\perp X_2$.

Repulsive coupling

Proposition (Affandi et al. (2012))

Let $K \in \mathcal{M}_n(\mathbb{R})$ such that $2K$ is a DPP kernel and define

$$\mathbb{K} = \begin{pmatrix} K & K \\ K & K \end{pmatrix}.$$

Then $\mathbb{K}$ is a DPP kernel.

If $(X_1, X_2) \sim DPP(\mathbb{K})$ then

- $X_1 \sim DPP(K)$;
- $X_2 \sim DPP(K)$;
- $X_1 \cup X_2 \sim DPP(2K)$;
- $\mathbb{P}(X_1 \cap X_2 = \emptyset) = 1$.

Most attractive coupling

Proposition

Let $K \in \mathcal{M}_n(\mathbb{R})$ be a DPP kernel and define

$$\mathbb{K} = \begin{pmatrix} K & I_n - K \\ K & I_n - K \end{pmatrix}.$$

Then $\mathbb{K}$ is a DPP kernel.

If $(X_1, X_2) \sim DPP(\mathbb{K})$ then

- $X_1 \sim DPP(K)$;
- $X_2 \sim DPP(I_n - K)$;
- $\mathbb{P}(X_1 = X_2^c) = 1$.

Most attractive coupling

Proposition

Let $K \in \mathcal{M}_n(\mathbb{R})$ be a DPP kernel and define

$$\mathbb{K} = \begin{pmatrix} K & I_n - K \\ -K & K \end{pmatrix}.$$

Then $\mathbb{K}$ is a DPP kernel.

- $X_1 \sim DPP(K)$;
- $X_2 \sim DPP(K)$;
- $\mathbb{P}(X_1 = X_2) = 1$.

Outline

Link with P_0 matrices

Proposition

Let $X \sim DPP(K)$. If $I_n - K$ is invertible then for all $S \subset [n]$,

$$\mathbb{P}(X = S) = \frac{\det(L_S)}{\det(I_n + L)},$$

where $L = K(I_n - K)^{-1}$.

Link with P_0 matrices

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where $L = K(I_n - K)^{-1}$.

Since $\sum_{S \subset [n]} \det(L_S) = \det(I_n + L)$ is true for any matrix then the determinantal probability measure is well defined if and only if

$$\forall S \subset [n],\ \det(L_S) \geqslant 0 \quad \Leftrightarrow \quad L \text{ is a } P_0 \text{ matrix.}$$

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Theorem (Coxson (1993))

The problem of testing if a given matrix is P_0 is co-NP-complete.

Necessary and sufficient conditions

Proposition

Let L be an $n \times n$ matrix. Then L is a P_0 matrix if and only if one of the following assertions is satisfied:

1. $\forall p \in \{0,1\}^n,\ \det\left(D(p)I_n + (I_n - D(p))L\right) \geqslant 0$
2. $\forall p \in]0,1[^n,\ \det\left(D(p)I_n + (I_n - D(p))L\right) > 0$

Necessary and sufficient conditions

Proposition

Let K be an $n \times n$ matrix. Then K is a DPP kernel if and only if one of the following assertions is satisfied:

1. $\forall p \in \{0,1\}^n, \ \det\left(D(p)(I_n - K) + (I_n - D(p))K\right) \geqslant 0$
2. $\forall p \in]0,1[^n, \ \det\left(D(p)(I_n - K) + (I_n - D(p))K\right) > 0$

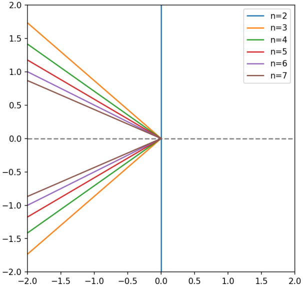
Necessary condition

Proposition

Let $\lambda \in \mathbb{C}^*$ *be an eigenvalue of a* P_0 *matrix* L *of size* $n \times n$ *then*

$$|\arg(\lambda)| \leqslant \pi - \frac{\pi}{n}.$$

In particular, if $\lambda \in \mathbb{R}$ *then* $\lambda \geqslant 0$.



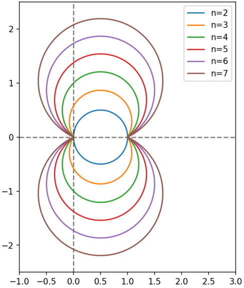
Necessary condition

Proposition

Let $\lambda \in \mathbb{C}$ be an eigenvalue of a DPP kernel K of size $n \times n$ then

$$\lambda \in \mathcal{B}_{\mathbb{C}}\left(\frac{1}{2} + \frac{1}{\tan\left(\frac{\pi}{n}\right)}i,\ \frac{1}{2\sin\left(\frac{\pi}{n}\right)}\right) \cup \mathcal{B}_{\mathbb{C}}\left(\frac{1}{2} - \frac{1}{\tan\left(\frac{\pi}{n}\right)}i,\ \frac{1}{2\sin\left(\frac{\pi}{n}\right)}\right).$$

In particular, if $\lambda \in \mathbb{R}$ then $\lambda \in [0,1]$.



Sufficient conditions

Proposition

Let L be an $n \times n$ matrix. If one of the following assertions is satisfied then L is a P_0 matrix.

1. *For all $i \in [n]$,*
$$L_{i,i} \geqslant 0 \text{ and } L_{i,i} > \sum_{j \neq i} |L_{i,j}|.$$
2. *$L + L^T$ is positive semi-definite.*

Sufficient conditions

Proposition

Let K be an $n \times n$ matrix. If one of the following assertions is satisfied then K is a DPP kernel.

1. *For all $i \in [n]$,*

$$K_{i,i} \in [0,1] \text{ and } \min(K_{i,i}, 1 - K_{i,i}) > \sum_{j \neq i} |K_{i,j}|.$$

2. $K := \frac{1}{2} I_n + M$ *where* $\|M\|_2 \leqslant \frac{1}{2}$.

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2. $K := \frac{1}{2} I_n + M$ *where* $\|M\|_2 \leqslant \frac{1}{2}$.

Remark: If $K = \frac{1}{2} I_n + M$ is symmetric then K is a DPP kernel if and only if $\|M\|_2 \leqslant \frac{1}{2}$. So, this condition includes all symmetric DPP kernels!

Sufficient conditions

Proposition

Let K be a DPP kernel and $\lambda \in [0,1]$ then $\lambda K + (1-\lambda)\frac{1}{2}I_n$ is a DPP kernel.

Sufficient conditions

Proposition

Let K be a DPP kernel and $\lambda \in [0, 1]$ then $\lambda K + (1 - \lambda)\frac{1}{2}I_n$ is a DPP kernel.

$\Rightarrow$ The set of DPP kernels is a star-convex set centered at $\frac{1}{2}I_n$ and containing the ball with center $\frac{1}{2}I_n$ and radius $\frac{1}{2}$ for the $\|.\|_2$ norm.

An additional result

Definition

Let $M \in \mathcal{M}_n(\mathbb{C})$ and $S \subset [n]$ such that M_S is invertible. With the right permutation of rows and columns we can write M as $\begin{pmatrix} M_S & M_{S,S^c} \\ M_{S^c,S} & M_{S^c} \end{pmatrix}$.

*We define the **principal pivot transform** of M relative to S as*

$$ppt(M,S) := \begin{pmatrix} M_S^{-1} & -M_S^{-1}M_{S,S^c} \\ M_{S^c,S}M_S^{-1} & M_{S^c} - M_{S^c,S}M_S^{-1}M_{S,S^c} \end{pmatrix}$$

Let $x, y \in \mathbb{R}^n$ written as $x = \begin{pmatrix} x_S \\ x_{S^c} \end{pmatrix}$ and $y = \begin{pmatrix} y_S \\ y_{S^c} \end{pmatrix}$. Then,

$$\begin{pmatrix} y_S \\ y_{S^c} \end{pmatrix} = M \begin{pmatrix} x_S \\ x_{S^c} \end{pmatrix} \Leftrightarrow \begin{pmatrix} x_S \\ y_{S^c} \end{pmatrix} = ppt(M,S) \begin{pmatrix} y_S \\ x_{S^c} \end{pmatrix}$$

Proposition

Let $X \sim DPP(K)$, $S \subset [n]$ *and define*

$$Y = (X \cap S^c) \cup (X^c \cap S) \sim DPP(\widetilde{K}).$$

Assume that $I_n - K$ *and* $I_n - \widetilde{K}$ *are invertible and define*

$$L := K(I_n - K)^{-1} \quad and \quad \widetilde{L} := \widetilde{K}(I_n - \widetilde{K})^{-1}.$$

Then $\widetilde{L} = ppt(L, S)$.

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Then $\widetilde{L} = ppt(L, S)$.

The Particle-Hole involution theorem is therefore closely linked to

Theorem (Tsatsomeros (2000))

Let $M \in \mathcal{M}_n(\mathbb{R})$ *be a* P_0 *matrix and* $S \subset [n]$ *such that* M_S *is invertible. Then,* $ppt(M, S)$ *is a* P_0 *matrix.*

Outline

Simulation algorithm

Define $K_{\bullet,i} := \begin{pmatrix} K_{1,i} \\ \vdots \\ K_{n,i} \end{pmatrix}$ and $K_{i,\bullet} := \begin{pmatrix} K_{i,1} & \cdots & K_{i,n} \end{pmatrix}$.

Proposition

If $X \sim DPP(K)$ then

$$X | i \notin X \sim DPP\left(K - \frac{1}{K_{i,i} - 1} K_{\bullet,i} K_{i,\bullet}\right)$$

$$X | i \in X \sim DPP\left(K - \frac{1}{K_{i,i}} K_{\bullet,i} K_{i,\bullet}\right)$$

Simulation algorithm

Algorithm 1: Poulson (2020)

Data: K, a DPP kernel of size $n \times n$.

$X = \emptyset$.

for $i = 1$ *to* n **do**

  $p_i = K_{i,i}$

  $B \sim b(p_i)$

  if $B = 1$ **then**

    $X = X \cup \{i\}$

    $K = K - \frac{1}{K_{i,i}} K_{\bullet,i} K_{i,\bullet}$

  else

    $K = K - \frac{1}{K_{i,i} - 1} K_{\bullet,i} K_{i,\bullet}$

return X

Outline

General construction

- Let K be a symmetric matrix with eigenvalues in $[0, 1]$.
- Let $(X_1, X_2) \sim DPP(\mathbb{K})$ with

$$\mathbb{K} = \begin{pmatrix} K & M \\ N & K \end{pmatrix}.$$

Since

$$\mathbb{P}(i \in X_1, j \in X_2) - \mathbb{P}(i \in X_1)\mathbb{P}(j \in X_2) = -M_{i,j}N_{j,i},$$

then in order to have positive cross correlations we thus need to have $M_{i,i}N_{i,i} \leqslant 0$ for all i.

Method 1: $N = -M$

Proposition

The kernel

$$\mathbb{K} = \begin{pmatrix} K & M \\ -M & K \end{pmatrix}$$

is a DPP kernel if and only if the symmetric matrix

$$\widetilde{\mathbb{K}} = \begin{pmatrix} K & M \\ M & I_n - K \end{pmatrix}$$

has eigenvalues in $[0, 1]$*. In particular,*

$$(X_1, X_2) \sim DPP(\mathbb{K}) \;\Leftrightarrow\; (X_1, X_2^c) \sim DPP(\widetilde{\mathbb{K}}).$$

Method 2: M and $-N$ are symmetric positive semidefinite and commute with K

There exist an orthogonal matrix P and $\lambda_1, \cdots, \lambda_n \in [0,1]$, $\mu_1, \cdots, \mu_n \in \mathbb{R}_+$ and $\nu_1, \cdots, \nu_n \in \mathbb{R}_-$ such that

$$K = PD(\lambda)P^T, \ M = PD(\mu)P^T \text{ and } N = PD(\nu)P^T$$

hence $\mathbb{K} = \frac{1}{2}I_{2n} + \mathbb{M}$ where

$$\mathbb{M} = \begin{pmatrix} P & 0 \\ 0 & P \end{pmatrix} \begin{pmatrix} D(\lambda - 1/2) & D(\mu) \\ D(\nu) & D(\lambda - 1/2) \end{pmatrix} \begin{pmatrix} P^T & 0 \\ 0 & P^T \end{pmatrix}$$

The $2n$ singular values squared of $\mathbb{M}$ corresponds to the eigenvalues of $\mathbb{M}\mathbb{M}^T$ and thus the 2 eigenvalues of the n matrices

$$\begin{pmatrix} (\lambda_i - 1/2)^2 + \mu_i^2 & (\mu_i + \nu_i)(\lambda_i - 1/2) \\ (\mu_i + \nu_i)(\lambda_i - 1/2) & (\lambda_i - 1/2)^2 + \nu_i^2 \end{pmatrix}$$

which are

$$(\lambda_i - 1/2)^2 + \frac{1}{2}\left(\mu_i^2 + \nu_i^2 \pm |\mu_i + \nu_i|\sqrt{4\left(\lambda_i - \frac{1}{2}\right)^2 + (\mu_i - \nu_i)^2}\right)$$

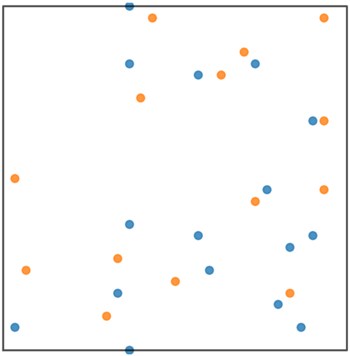
$\Rightarrow$ Taking μ_i and ν_i such that this expression is $\leqslant \frac{1}{4}$ yields a DPP kernel.

Outline

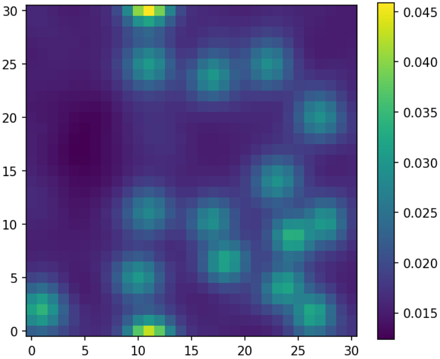
Example

DPP on $(\{0, \frac{1}{30}, \cdots, 1\}^2)^2$ with kernel $\mathbb{K} = \begin{pmatrix} K & M \\ N & K \end{pmatrix}$ where

$K(x,y) = 0.02e^{-\frac{\|y-x\|^2}{0.018}}$ and M, N generated by the second method.



DPP coupling simulation



Inclusion probability for the orange DPP conditionally to the blue DPP

Example

DPP on $(\{0, \frac{1}{30}, \cdots, 1\}^2)^2$ with kernel $\mathbb{K} = \begin{pmatrix} K & M \\ N & K \end{pmatrix}$ where

$K(x, y) = \frac{0.02}{\left(1+\left(\frac{\|y-x\|}{0.075}\right)^2\right)^{1.1}}$ and M, N generated by the second method.

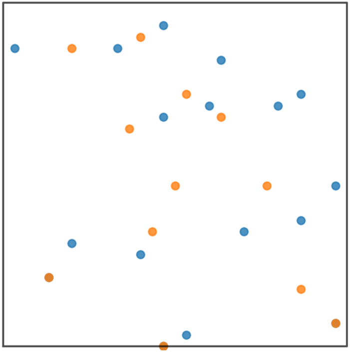
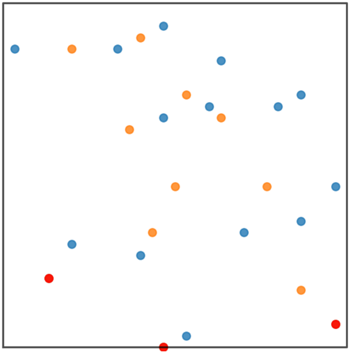


Figure: DPP coupling simulation

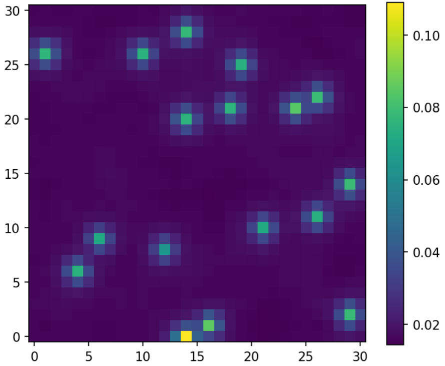
Example

DPP on $(\{0, \frac{1}{30}, \cdots, 1\}^2)^2$ with kernel $\mathbb{K} = \begin{pmatrix} K & M \\ N & K \end{pmatrix}$ where

$K(x, y) = \frac{0.02}{\left(1 + \left(\frac{\|y-x\|}{0.075}\right)^2\right)^{1.1}}$ and M, N generated by the second method.



DPP coupling simulation



Inclusion probability for the orange DPP conditionally to the blue DPP

Outline

- There is a natural way of constructing DPP couplings but it requires nonsymmetric kernels to get attraction.
- There is a lot in common between the theory of DPPs and the theory of P_0 matrices.
- An easy way to generate a DPP kernel is to take $K = \frac{1}{2} I_n + M$ with $\|M\|_2 \leqslant \frac{1}{2}$.
- We still need to find a way to control the strength of attraction in DPP couplings generated this way.

Thank you!

Proposition

Let $K_1, K_2 \in \mathcal{M}_n(\mathbb{R})$ be a DPP kernel and define

$$\mathbb{K} = \begin{pmatrix} K_1 & I_n - K_2 \\ -K_1 & K_2 \end{pmatrix}.$$

If $\mathbb{K}$ is a DPP kernel then if $(X_1, X_2) \sim DPP(\mathbb{K})$ then $X_1 \sim DPP(K_1)$, $X_2 \sim DPP(K_2)$ and $X_1 \subset X_2$ almost surely.

Simulations shows that it works in a lot of case when $0 \preccurlyeq K_1 \preccurlyeq K_2 \preccurlyeq I_n$ but not always.

Open problem: For which $K_1 \preccurlyeq K_2$ is $\mathbb{K}$ a DPP kernel?

Remark

If $K = \frac{1}{2}(I_n - M)$ *is a DPP kernel such that* $I_n - K$ *is invertible then* $L = (I_n - M)(I_n + M)^{-1}$ *is the* ***Cayley transform*** *of* M.