Kernel reconstruction of DPPs

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September 13, 2018

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Setting and basic definitions

Setting

Let $\mathcal{Y}$ be a finite set, which we call the *ground set* and $N := |\mathcal{Y}|$ its cardinality. We call the elements of $\mathcal{Y}$ *items* and assume for the sake of easy notation $\mathcal{Y} = \{1, \ldots, N\}$ unless specified differently.

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Point process

A *point process* on $\mathcal{Y}$ is a random subset of $\mathcal{Y}$, i.e. a random variable with values in the powerset $2^{\mathcal{Y}}$. We identify this random variable with its law $\mathbb{P}$ and thus refer to probability measures $\mathbb{P}$ on $2^{\mathcal{Y}}$ as point processes. Further, $\mathbf{Y}$ will always denote a random subset distributed according to $\mathbb{P}$.

Definition of DPP and repulsive structure

Determinantal point process

We call $\mathbb{P}$ a *determinantal point process*, or in short a *DPP*, if we have

$$\mathbb{P}(A \subseteq \mathbf{Y}) = \det(K_A) \quad \text{for all } A \subseteq \mathcal{Y} \tag{1}$$

where K is a symmetric matrix indexed by the elements in $\mathcal{Y}$ and K_A denotes the submatrix $(K_{ij})_{ij \in A}$ of K indexed by the elements of A. We call K the *marginal kernel* of the DPP. If the marginal kernel K is diagonal, we call $\mathbb{P}$ a *Poisson point process*.

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Choosing $A = \{i\}$ and $A = \{i, j\}$ for $i, j \in \mathcal{Y}$ in (1) yields

$$\begin{aligned} \mathbb{P}(i \in \mathbf{Y}) &= K_{ii} \quad \text{and} \\ \mathbb{P}(i, j \in \mathbf{Y}) &= K_{ii}K_{jj} - K_{ij}^2 = \mathbb{P}(i \in \mathbf{Y}) \cdot \mathbb{P}(j \in \mathbf{Y}) - K_{ij}^2. \end{aligned} \tag{2}$$

Properties of the marginal kernel and existence

Positivity

The marginal kernel is always positive semi-definite. Further the complement of a DPP is also a DPP with marginal kernel $I - K$ and hence $0 \leq K \leq I$.

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The marginal kernel is always positive semi-definite. Further the complement of a DPP is also a DPP with marginal kernel $I - K$ and hence $0 \le K \le I$.

Theorem (Existence of DPPs)

Let K be a symmetric $N \times N$ matrix. Then K is the marginal kernel of a DPP if and only if $0 \le K \le I$.

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Main idea

Setting

Let $\mathcal{Y}$ be a finite set of cardinality N and let $K \in \mathbb{R}^{N\times N}_{\text{sym}}$ satisfy $0 \le K \le I$. Let further $\mathbf{Y}_1, \mathbf{Y}_2, \dots$ be independent and distributed according to a DPP with marginal kernel K. The goal is to estimate the kernel K based on the observations $(\mathbf{Y}_n)_{n\in\mathbb{N}}$.

Main idea

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Consider now the empirical measures

$$\hat{\mathbb{P}}_n := \frac{1}{n}\sum_{i=1}^{n} \delta_{\mathbf{Y}_i}$$

and assume that they are determinantal with marginal kernel $\hat{K}_n$. Then $\hat{K}_n$ would be a natural estimate for K since by the SLLN we have

$$\hat{\mathbb{P}}_n \xrightarrow{n\to\infty} \mathbb{P}.$$

The principal minor assignment problem

The principal minor assignment problem (PMAP)

Let $K \in \mathbb{R}^{N\times N}$ be a symmetric matrix. We want to investigate whether K is uniquely specified by its principal minors

$$\Delta_S := \det(K_S) \quad \text{where } S \subseteq \{1, \ldots, N\}$$

and if so how it can be reconstructed from those.

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Determinantal equivalence

Two symmetric matrices $A, B \in \mathbb{R}^{N\times N}$ are called *determinantally equivalent* if they have the same principal minors and we write $A \sim B$.

Reconstruction for 3×3 matrix

The diagonal and absolut values of the off diagonal can be obtained by

$$K_{ii} = \Delta_{\{i\}} \quad \text{and}$$
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In order to reconstruct the signs we need to consider the determinant

$$\Delta_{\{1,2,3\}} = K_{11} K_{22} K_{33} + 2K_{12} K_{13} K_{23} - K_{11} K_{23}^2 - K_{22} K_{13}^2 - K_{33} K_{12}^2.$$

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Any assignment of the signs that satisfies this, i.e. such that

$$K_{12}K_{13}K_{23} = \frac{1}{2}\left(\Delta_{\{1,2,3\}} + K_{11}K_{23}^2 + K_{22}K_{13}^2 + K_{33}K_{12}^2 - K_{11}K_{22}K_{33}\right)$$

yields a matrix K with the prediscribed principles minors.

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Let $G = (V, E)$ be a finite graph. We will need the following notions:

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(v) *Connected graph:* A graph where every two vertices $v, w \in V$ there is a path from v to w.

(vi) *Cycle:* A *cycle* C is a connected subgraph such that every vertex has even degree in C.

Graph theoretical preliminaries II

(*vii*) *Cycle space:* Identify a cycle C with $x = x(C) \in \mathbb{F}_2^E$ such that

$$x_e := \begin{cases} 1 & \text{if } e \in C \\ 0 & \text{if } e \notin C. \end{cases}$$

The *cycle space* $\mathcal{C}$ is the span of $\{x(C) \mid C \text{ is a cycle}\}$ in $\mathbb{F}_2^E$.

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(*xi*) *Pairings:* A *pairing* P of $S \subseteq V$ is a subset of edges of $G(S)$ such that two different edges of P are disjoint. Vertices contained in the edges of P are denoted by $V(P)$, the set of all pairings by $\mathcal{P}(S)$.

Graph theoretical preliminaries III

Proposition (Existence of SMCBs)

There always exists a basis $\{x(C_1), \ldots, x(C_k)\}$ *of the cycle space where* $C_1, \ldots, C_k$ *are chordless simple cycles.*

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We proceed in the two following steps:

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We proceed in the two following steps:

- (i) Decompose a cycle into disjoint simple cycles.
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Those two steps show that the set of simple chordless cycles generates the cycle space. □

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The adjacency graph and sign function

The adjacency graph

The adjacency graph $G_K = (V_K, E_K)$ associated with K consists of the vertex set $\{1, \dots, N\}$ and $\{i, j\}$ form an edge if and only if $K_{ij} \neq 0$. Further, we introduce the *weights*

$$w_{ij} := w(\{i, j\}) := \operatorname{sgn}(K_{ij})$$

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The sign function

We define the *sign* $\operatorname{sgn}(C)$ of a cycle $C = (S, E)$ to be

$$\operatorname{sgn}(C) := \prod_{e \in E} w_e \quad \text{or equivalently} \quad \operatorname{sgn}(x(C)) := \prod_{e \in E} w_e^{x(C)_e}.$$

Note that this is a group homomorphism from the cycle space $\mathcal{C}$ to $\{\pm 1\}$ and therefore it is uniquely determined by its values on a generator, for example on a shortest maximal cycle basis.

Principal minors of simple chordless cycles

Proposition (Principal minors of simple chordless cycles)

Let $C = (S, E(S))$ be a simple and chordless cycle. Then the principal minor of K with respect to S is given by

$$\Delta_S = \sum_{P \in \mathcal{P}(S)} (-1)^{|P|} \cdot \prod_{\{i,j\} \in P} K_{ij}^2 \cdot \prod_{i \notin V(P)} K_{ii} + 2 \cdot (-1)^{|S|+1} \cdot \prod_{\{i,j\} \in E(S)} K_{ij}. \quad (3)$$

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Proof.

The idea is to express the determinant in terms of permutations and to note that all contributions vanish apart from the pairings and the two shifts along the cycle in either direction. □

An equivalent formulation of this is

$$\operatorname{sgn}(E(S)) = \operatorname{sgn}\left(\Delta_S - \sum_{P \in \mathcal{P}(S)} (-1)^{|P|} \cdot \prod_{\{i,j\} \in P} K_{ij}^2 \cdot \prod_{i \notin V(P)} K_{ii}\right) \cdot (-1)^{|S|+1}.$$

Sign determines principal minors

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The knowledge of all principal minors up to size two and the sign function

$$\mathrm{sgn}\colon \mathcal{C} \to \{\pm 1\}$$

completely determines all principal minors of K. In particular, it suffices to reconstruct the sign function.

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Proof.

Write the determinant using permutations

$$\sum_{\sigma \in S_k} \prod_{i \in S} \mathrm{sgn}(K_{i\sigma(i)}).$$

Express the permutation as the product of disjoint cycles which can be associated with a cycle for which the sign is known. □

Solution of the Principal minor assignment problem

Theorem (Solution of the PMAP)

Let $K \in \mathbb{R}^{N \times N}$ be a symmetric matrix and l be the sparsity of its adjacency graph. Then the principal minors up to size l uniquely determine all principal minors of K and therefore the matrix K up to determinantal equivalence.

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Proof.

(i) Principle minors of simple chordless cycles determine the sign of a this cycle.

(ii) Since there is a SMCB, the principal minors determine the signs of those cycles which determines the sign function on the cycle space.

□

Reconstruction of the matrix

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$$K_{ii} := \Delta_{\{i\}} \quad \text{and } K_{ij}^2 := K_{ii}K_{jj} - \Delta_{\{i,j\}}.$$

(ii) We saw that the sign function is uniquely specified by its values on a SMCB. Hence it remains to choose the signs w_{ij} such that

$$(-1)^{|S_k|+1} \cdot \mathrm{sgn}(H_k) = \mathrm{sgn}(C_k) = \prod_{e \in E} w_e^{x(e)}$$

where $C_k = (S_k, E(S_k))$ is a SMCB.

Reconstruction of the matrix II

(iii) Transform this into a linear equation via $\{\pm 1\} \cong \mathbb{Z}_2$ to get

$$(Ax)_k = b_k$$

where the rows of A consist of $x(C_k)^T$.

Reconstruction of the matrix II

(*iii*) Transform this into a linear equation via $\{\pm 1\} \cong \mathbb{Z}_2$ to get

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where the rows of A consist of $x(C_k)^T$.

(*iv*) Any solution of this linear equation (and at least one exists!) satisfies the desired properties for the signs.

(*v*) This solution can in practice be obtained by Gauss elimination.

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Fix $\alpha > 0$ and assume from now on that

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(*ii*) Estimate the adjacency graph $\hat{G} = (\hat{E}, \hat{V})$ such that $\hat{E}$ consists of all sets $\{i, j\}$ such that $\hat{B}_{ij} \geq \frac{1}{2}\alpha^2$.

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(iv) If $\hat{A}\hat{x} = \hat{b}$ possesses a solution, then set $\hat{w}_{ij}$ to be the preimage under the isomorphism of $\hat{x}_{ij}$, otherwise set $\hat{w}_{ij}$ arbitrary.

Pseudometric and consistency

Pseudometric on the marginal kernels

Define the distance between two marginal kernels $A, B \in \mathbb{R}^{N\times N}$ through

$$d(A, B) := \inf_{C\sim A} \|B - C\|_\infty .$$

Pseudometric and consistency

Pseudometric on the marginal kernels

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Theorem (Consistency)

Let K be the marginal kernel of a DPP that satisfies the previous assumption. Then we have for any $\varepsilon > 0$

$$\mathbb{P}\left(d(\hat{K}, K) \leq \varepsilon\right) \to 1 \quad \textit{for } n \to \infty.$$

Proof of the consistency result

Proof.

(i) Using the SLLN we get

$$\hat{K}_{ii} \to K_{ii} \quad \text{and } \hat{K}_{ij}^2 \to K_{ij}^2 \quad \text{almost surely.}$$

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(*iii*) Additionally we have $\hat{b} = b$ with probability tending to one. In this case $\hat{A}\hat{x} = \hat{b}$ has a solution which we identify with $\hat{w}$.

(*iv*) Obviously $\tilde{K}_{ij} := \hat{w}_{ij} \left| K_{ij} \right|$ is determinantally equivalent to K. Thus we have

$$d(\hat{K}, K) \leq \left\| \hat{K} - \tilde{K} \right\| < \varepsilon$$

with probability tending to one.

□