Stochastic Processes: Lecture 5

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Determinantal point processes

- ▶ A determinantal point process (DPP) on \mathbb{R}^D is determined by a kernel K(x, x').
- ► The joint intensities can be written

$$\det \left(\begin{array}{cc} K(x_i, x_i) & K(x_i, x_j) \\ K(x_i, x_j) & K(x_j, x_j) \end{array} \right)$$

▶ The kernel defines an integral operator \mathcal{K} acting on $L^2(\mathbb{R}^D)$ that is self-adjoint, positive semidefinite and trace class.

Joint intensities of a DPP

Definition 1

The joint intensities of a point process N are functions (if any exist) $\rho_k : (\mathbb{R}^D)^k \to [0,\infty)$ for $k \geq 1$, such that for any family of disjoint sets $D_1, \ldots, D_k \subset \mathbb{R}^D$,

$$E\left(\prod_{i=1}^k N(D_i)\right) = \int_{\prod D_i} \rho_k(x_1,\ldots,x_k) dx_1 \ldots dx_k.$$

Definition 2

A point process N on \mathbb{R}^D is said to be a DPP with kernel K if its joint intensities satisfy

$$\rho_k(x_1,\ldots,x_k) = \det\left(K(x_i,x_j)\right)_{1 \leq i,j \leq k}$$

for every $k \geq 1$ and $x_1, \ldots, x_k \in \mathbb{R}^D$.

Permanental point processes

Leibniz' formula for the determinant of a $k \times k$ matrix M is

$$\det(M) = \sum_{\sigma \in S_k} \left(\operatorname{sgn}(\sigma) \prod_{i=1}^k M_{i,\sigma(i)} \right) .$$

We denote the *permanent* of a $k \times k$ matrix M

$$\operatorname{per}(M) = \sum_{\sigma \in S_k} \prod_{i=1}^k M_{i,\sigma(i)}.$$

Definition 3

A point process N on \mathbb{R}^D is said to be a permanental point process with kernel K if its joint intensities satisfy

$$\rho_k(x_1,\ldots,x_k) = per(K(x_i,x_j))_{1 \le i,j \le k}$$

for every $k \geq 1$ and $x_1, \ldots, x_k \in \mathbb{R}^D$.

Poisson processes, DPPs and PPPs

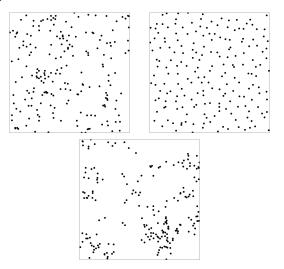


FIG 1. Samples of translation invariant point processes in the plane: Poisson (left), determinantal (center) and permanental for $K(z,w) = \frac{1}{\pi}e^{z\overline{w} - \frac{1}{2}(|z|^2 + |w|^2)}$. Determinantal processes exhibit repulsion, while permanental processes ethibit clumping.

DPP results

Lemma 1

Suppose $\{\phi_k\}_{k=1}^n$ is an orthonormal set in $L^2(\mathbb{R}^D)$. Then there exists a DPP with kernel

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

Theorem 1

Let K determine a self-adjoint integral operator K on $L^2(\mathbb{R}^D)$ that is locally trace-class. Then K defines a DPP on \mathbb{R}^D iff all the eigenvalues of K are in [0,1].

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DPP results

Theorem 2

Suppose N is a DPP with kernel K(x, y). Write

$$K(x,y) = \sum_{k=1}^{\infty} \lambda_k \phi_k(x) \overline{\phi}_k(y),$$

where ϕ_k are normalized eigenfunctions with eigenvalues $\lambda_k \in [0,1]$. Let $I_k \stackrel{\perp}{\sim} \mathsf{Bernoulli}(\lambda_k)$ and define K's random analogue

$$K_I(x,y) = \sum_{k=1}^{\infty} I_k \phi_k(x) \overline{\phi}_k(y).$$

Let N_i be a DPP with kernel K_i . Then

$$N \stackrel{d}{=} N_I$$
.

In particular, the total number of points in N follows the distribution of the sum of independent Bernoulli(λ_k) r.v.s.

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DPP example: non-intersecting random walks

Consider n independent simple symmetric walks on \mathbb{Z} started from $i_1 < \cdots < i_n$, all even. Let $P_{ij}(t)$ be the t-step transition probabilities. The probability the r.w.s are at $j_1 < \cdots < j_n$ at time t and have non-intersecting paths is

$$\det \left(egin{array}{ccc} P_{i_1j_1}(t) & \dots & P_{i_1j_n}(t) \ dots & \ddots & \ P_{i_nj_1}(t) & & P_{i_nj_n}(t) \end{array}
ight) \,.$$

If t is even and we condition the walks to return to i_1, \ldots, i_n at time t, then the positions at time t/2 follow a DPP with Hermitian kernel.

DPP example: Ginibre ensemble

Let Q be an $n \times n$ matrix with i.i.d. complex standard normal entries. The eigenvalues of Q form a DPP on $\mathbb C$ with the kernel

$$K_n(z,w) = \frac{1}{\pi} e^{-\frac{1}{2}(|z|^2 + |w|^2)} \sum_{k=0}^{n-1} \frac{(z\overline{w})^k}{k!}.$$

As $n \to \infty$, we have a DPP on $\mathbb C$ with kernel

$$K(z, w) = \frac{1}{\pi} e^{-\frac{1}{2}(|z|^2 + |w|^2)} \sum_{k=0}^{\infty} \frac{(z\overline{w})^k}{k!}$$
$$= \frac{1}{\pi} e^{-\frac{1}{2}(|z|^2 + |w|^2) + z\overline{w}}.$$

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Zero set of a Gaussian analytic function

The power series $f(z) = \sum_{n=0}^{\infty} a_n z^n$, where a_n are i.i.d. standard complex normals defines a random analytic function on the unit disk (a.s.). The zero set of f is a determinantal process in the disk with the Bergman kernel

$$K(z,w) = \frac{1}{\pi(1-z\overline{w})^2} = \frac{1}{\pi}\sum_{k=0}^{\infty}(k+1)(z\overline{w})^k$$
.

DPPs on discrete sets

Let \mathcal{Y} be a discrete set with n items. A point process N on \mathcal{Y} is a probability distribution on the power set $2^{\mathcal{Y}}$.

Definition 4

A point process N is a determinantal point process if for $Y \subseteq \mathcal{Y}$ randomly sampled according to N we have for every $S \subseteq \mathcal{Y}$

$$Pr(S \subseteq Y) = \det K_S$$

for some similarity matrix $K \in \mathbb{R}^{n \times n}$ that is symmetric and positive semidefinite.

Let S be a two-element set with elements i and j. Then

$$\Pr(S \subset Y) = K_{ii}K_{jj} - K_{ij}^2 = \Pr(i \subset Y)\Pr(j \subset Y) - K_{ij}^2.$$

Conditioning

DPPs are closed under conditioning:

$$\begin{aligned} \Pr(A \subseteq Y | B \subseteq Y) &= \Pr(A \cup B \subseteq Y) / \Pr(A \subseteq Y) \\ &= \frac{\det K_{A \cup B}}{\det K_A} \\ &= \frac{\det(K_A) \det(K_B - K_{BA} K_A^{-1} K_{AB})}{\det(K_A)} \\ &= \det(K_B - K_{BA} K_A^{-1} K_{AB}) \\ &= \det([K - K_{\mathcal{Y}A} K_A^{-1} K_{A\mathcal{Y}}]_B) \ . \end{aligned}$$

Restrictions on *K*

- ▶ Because marginal probabilities of any set $S \subseteq \mathcal{Y}$ must be in [0,1], all $\det(K_S) \ge 0$ and hence K must be positive semidefinite.
- ▶ Moreover, all eigenvalues of K must inhabit [0,1], i.e. $0 \le K \le 1$.
- ▶ Any K satisfying $0 \leq K \leq 1$ defines a DPP.

- ▶ L-ensembles provide a convenient way to avoid dealing with $K \leq 1$ constraints.
- ▶ An L-ensemble is defined using a symmetric matrix $L \succeq 0$ that defines the *atomic* probability of an event set S thus:

$$\Pr_L(S) = \Pr(S = Y) \propto \det(L_Y)$$

► Conveniently, the normalizing constant is known:

$$\sum_{S\subseteq\mathcal{Y}}\det\left(L_S
ight)=\det(L+I)\,.$$

Theorem 3 For any $S \subseteq \mathcal{Y}$

$$\sum_{\mathcal{S} \subseteq \mathcal{Y} \subseteq \mathcal{Y}} \det(\mathcal{L}_{\mathcal{Y}}) = \det(\mathcal{L} + \mathcal{I}_{\mathcal{S}^c})$$

Corollary 1

$$\sum_{Y\subset\mathcal{Y}}\det(L_Y)=\det(L+I)$$

Proof.

Let *S* from Theorem 3 equal the empty set.

Theorem 4

An L-ensemble is a DPP and its marginal kernel is

$$K = L(L+I)^{-1} = I - (L+I)^{-1}$$

Proof.

The marginal probability of a set S under the L-ensemble is

$$\begin{aligned} \mathsf{Pr}_L(S \subseteq Y) &= \frac{\sum_{S \subseteq Y \subseteq \mathcal{Y}} \det(L_Y)}{\sum_{Y \subseteq \mathcal{Y}} \det(L_Y)} = \frac{\det(L + I_{S^c})}{\det(L + I)} \\ &= \det\left((L + I_{S^c})(L + I)^{-1}\right) \\ &= \det\left(I_{S^c}(L + I)^{-1} + I - (L + I)^{-1}\right) \\ &= \det\left(I_{S^c}(L + I)^{-1} + (I_S + I_{S^c})\left(I - (L + I)^{-1}\right)\right) \\ &= \det(I_{S^c} + I_S K) = \begin{vmatrix} I_{|S^c| \times |S^c|} & 0 \\ K_{S,S^c} & K_S \end{vmatrix} = \det(I_{|S^c| \times |S^c|}) \det(K_S) \\ &= \det(K_S) \,. \end{aligned}$$

- ▶ Given a marginal kernel, we may construct an L-ensemble by setting $L = K(I K)^{-1}$.
- ▶ The inverse of I K might not exist, so DPPs are a larger class than L-ensembles.
- ▶ If $L = \sum_{k} \lambda_k v_k v_k^T$, then $K = \sum_{k} \frac{\lambda_k}{1 + \lambda_k} v_k v_k^T$.
- ▶ Linear kernel. Let X be an $n \times p$ design matrix (set of feature vectors). Taking $L = XX^T$, we have

$$\Pr_L(S) \propto \det(L_S) = Vol^2(\{x_i\}_{i \in S})$$

If p < n, the DPP will only have p points.

Working with DPPs

- ▶ Complements: if $Y \sim DPP(K)$, then $Y^c \sim DPP(I K)$
- ► Conditioning:

$$\Pr_{L}(Y = S_{in} \cup B | S_{in} \subseteq Y, S_{out} \cap Y = \emptyset) = \frac{\det(L_{S_{in} \cup B})}{\det(L_{S_{out}^c} + I_{S_{in}^c})}$$

► Marginalization:

$$\Pr(B \subseteq Y | S \subseteq Y) = \det\left(\left[I - \left[(L + I_{S^c})^{-1}\right]_{S^c}\right]_B\right)$$

▶ Scaling: if $K' = \gamma K$ for $\gamma \in [0,1]$, then for all $S \subseteq \mathcal{Y}$

$$\Pr_{K'}(S \subseteq Y) = \det(K'_S) = \gamma^{|S|}K_S$$
.

Elementary DPPs

- ► A DPP is elementary if every eigenvalue of *K* is 0 or 1.
- ▶ N^V denotes an elementary DPP with marginal kernel $K^V = \sum_{v \in V} vv^T$ if V is a set of orthonormal vectors.
- ► The expected total count for a DPP is

$$E(|Y|) = E(\sum_{i=1}^{n} 1\{i \in Y\}) = \sum_{i=1}^{n} \Pr(i \in Y) = \sum_{i=1}^{n} K_{ii} = \operatorname{tr}(K).$$

► For an elementary DPP this is

$$E(|Y|) = \operatorname{tr}(K^V) = \operatorname{tr}\left(\sum_{v \in V} vv^T\right) = \sum_{v \in V} v^T v = |V|.$$

▶ Furthermore, |Y| = |V| a.s. because $det(K_Y^V) = 0$ when |Y| > |V|.

DPPs as mixtures of elementary DPPs

Lemma 2 A DPP with kernel $L = \sum_{i=1}^{n} \lambda_i v_i v_i^T$ is a mixture of elementary DPPs:

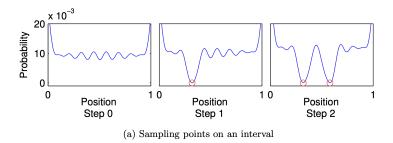
$$N_L = rac{1}{\det(L+I)} \sum_{J \subseteq \{1,2,\ldots,n\}} N^{V_J} \prod_{i \in J} \lambda_i$$

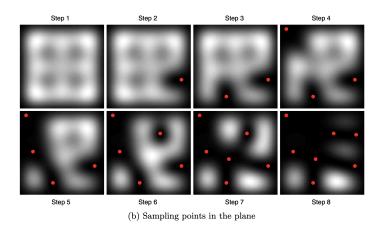
where
$$V_J = \{v_i\}_{i \in J}$$

Sampling DPPs

Algorithm 1 Sampling from a DPP

```
Input: eigendecomposition \{(\boldsymbol{v}_n, \lambda_n)\}_{n=1}^N of L J \leftarrow \emptyset for n=1,2,\ldots,N do J \leftarrow J \cup \{n\} with prob. \frac{\lambda_n}{\lambda_n+1} end for V \leftarrow \{\boldsymbol{v}_n\}_{n\in J} Y \leftarrow \emptyset while |V|>0 do Select i from \mathcal{Y} with \Pr(i)=\frac{1}{|V|}\sum_{\boldsymbol{v}\in V}(\boldsymbol{v}^{\top}\boldsymbol{e}_i)^2 Y \leftarrow Y \cup i V \leftarrow V_{\perp}, an orthonormal basis for the subspace of V orthogonal to \boldsymbol{e}_i end while Output: Y
```





Sampling DPPs

- ▶ Finding the eigendecomposition of *L* is $O(n^3)$.
- ▶ Sampling algorithm is $O(n|V|^3)$ for V the set of eigenvectors selected in phase 1 and each repeated Gram-Schmidt to compute V_{\perp} is $O(n|V|^2)$.

Dual representation

▶ Let B be the $D \times N$ matrix with columns $B_i = q_i \phi_i$ such that $L = B^T B$. Consider the $D \times D$ matrix

$$C = BB^T$$
.

- ▶ Here, *D* is the dimension of the diversity feature function ϕ .
- ▶ *D* is often fixed by design, whereas *N* may grow as more items are modeled.

Dual representation

Proposition 1

The non-zero eigenvalues of L and C are identical, and the corresponding eigenvectors are related by the matrix B. That is,

$$C = \sum_{d=1}^{D} \lambda_d \hat{\mathbf{v}}_d \hat{\mathbf{v}}_d^T$$

is an eigendecomposition of C if and only if

$$L = \sum_{d=1}^{D} \lambda_d \left(\frac{1}{\sqrt{\lambda_d}} B^T \hat{v}_d \right) \left(\frac{1}{\sqrt{\lambda_d}} B^T \hat{v}_d \right)^T$$

is an eigendecomposition of L.

Dual representation

Proof.

First, assume $\{\lambda_d, \hat{v}_d\}_{d=1}^D$ is an eigendecomposition of C. Then,

$$\sum_{d=1}^{D} \lambda_d \left(\frac{1}{\sqrt{\lambda_d}} B^T \hat{v}_d \right) \left(\frac{1}{\sqrt{\lambda_d}} B^T \hat{v}_d \right)^T = B^T \left(\sum_{d=1}^{D} \hat{v}_d \hat{v}_d^T \right) B = B^T B = L.$$

Furthermore, we have

$$\begin{split} ||\frac{1}{\sqrt{\lambda_d}}\boldsymbol{B}^T \hat{\boldsymbol{v}}_d||^2 &= \frac{1}{\lambda_d} (\boldsymbol{B}^T \hat{\boldsymbol{v}}_d)^T (\boldsymbol{B}^T \hat{\boldsymbol{v}}_d) = \frac{1}{\lambda_d} \hat{\boldsymbol{v}}_d^T \boldsymbol{C} \hat{\boldsymbol{v}}_d \\ &= \frac{1}{\lambda_d} \lambda_d \hat{\boldsymbol{v}}_d^T \hat{\boldsymbol{v}}_d = 1 \,, \end{split}$$

and

$$\begin{split} \left(\frac{1}{\sqrt{\lambda_d}}B^T\hat{v}_d\right)^T \left(\frac{1}{\sqrt{\lambda_{d'}}}B^T\hat{v}_{d'}\right) &= \frac{1}{\sqrt{\lambda_d\lambda_{d'}}}\hat{v}_d^T C\hat{v}_{d'} \\ &= \frac{\sqrt{\lambda_{d'}}}{\sqrt{\lambda_d}}\hat{v}_d^T\hat{v}_{d'} = 0 \,. \end{split}$$

A similar argument holds in the other direction when one accounts for the fact $L = B^T B$ and has rank at most D.

Dual representation and computing

► Normalization: the normalization constant is

$$\det(L+I) = \prod_{d=1}^{D} (\lambda_d + 1) = \det(C+I),$$

which only takes $O(D^3)$ time.

► Marginalization: get entries of K using C. First get the eigendecomposition $C = \sum_{d=1}^{D} \lambda_d \hat{v}_d \hat{v}_d^T$. Then

$$K_{ij} = \sum_{d=1}^{D} \frac{\lambda_d}{\lambda_d + 1} \left(\frac{1}{\sqrt{\lambda_d}} B_i^T \hat{v}_d \right)^T \left(\frac{1}{\sqrt{\lambda_d}} B_j^T \hat{v}_d \right).$$

One may therefore obtain the marginal probability of an event in time $O(D^2)$. For a k event, this becomes $O(D^2k^2+k^3)$. This beats the usual $O(n^3)$ to translate from L to K.

Dual representation and computing

In general, one may represent the orthonormal set V in \mathbb{R}^n using the set \hat{V} in \mathbb{R}^D with the mapping

$$V = \{B^T \hat{v} | \hat{v} \in \hat{V}\}.$$

One may implicitly obtain linear combinations of vectors in V by performing actions on their preimages: $v_1 + v_2 = B^T(\hat{v}_1 + \hat{v}_2)$. Moreover,

$$v_1^T v_2 = (B^T \hat{v}_1)^T (B^T \hat{v}_2) = \hat{v}_1^T C \hat{v}_2,$$

so we can compute dot products of elements in V in time $O(D^2)$. We can implicitly normalize the elements of V by updating

$$\hat{v} \longleftarrow \frac{\hat{v}}{\hat{v}^T C \hat{v}}.$$

Sampling DPPs

Algorithm 1 Sampling from a DPP

```
Input: eigendecomposition \{(\boldsymbol{v}_n, \lambda_n)\}_{n=1}^N of L J \leftarrow \emptyset for n=1,2,\ldots,N do J \leftarrow J \cup \{n\} with prob. \frac{\lambda_n}{\lambda_n+1} end for V \leftarrow \{\boldsymbol{v}_n\}_{n\in J} Y \leftarrow \emptyset while |V|>0 do Select i from \mathcal Y with \Pr(i)=\frac{1}{|V|}\sum_{\boldsymbol{v}\in V}(\boldsymbol{v}^{\top}\boldsymbol{e}_i)^2 Y \leftarrow Y \cup i V \leftarrow V_{\perp}, an orthonormal basis for the subspace of V orthogonal to \boldsymbol{e}_i end while Output: Y
```

Can we use the dual representation to speed up the sampling of i and Gram-Schmidt steps?

Dual representation and computing

The sampling step is handled thus:

$$Pr(i) = \frac{1}{|V|} \sum_{v \in V} (v^T e_i)^2 = \frac{1}{|\hat{V}|} \sum_{\hat{v} \in \hat{V}} ((B^T \hat{v})^T e_i)^2$$
$$= \frac{1}{|\hat{V}|} \sum_{\hat{v} \in \hat{V}} (B_i^T \hat{v})^2$$

The entire distribution may be computed in time $O(nD|\hat{V}|)$ instead of $O(n^3)$.

Sampling DPPs

Algorithm 3 Sampling from a DPP (dual representation)

```
Input: eigendecomposition \{(\hat{v}_n, \lambda_n)\}_{n=1}^N of C
  J \leftarrow \emptyset
  for n = 1, 2, ..., N do
        J \leftarrow J \cup \{n\} with prob. \frac{\lambda_n}{\lambda_n+1}
\begin{array}{l} \mathbf{end} \ \mathbf{for} \\ \hat{V} \leftarrow \left\{ \frac{\hat{\mathbf{v}}_n}{\sqrt{\hat{\mathbf{v}}_n^{\top} C \hat{\mathbf{v}}_n}} \right\}_{n \in J} \end{array}
  while |\hat{V}| > 0 do
        Select i from \mathcal{Y} with \Pr(i) = \frac{1}{|\hat{V}|} \sum_{\hat{v} \in \hat{V}} (\hat{v}^{\top} B_i)^2
        Y \leftarrow Y \sqcup i
         Let \hat{\boldsymbol{v}}_0 be a vector in \hat{V} with B_i^{\top} \hat{\boldsymbol{v}}_0 \neq 0
        \text{Update } \hat{V} \leftarrow \left\{ \boldsymbol{\hat{v}} - \frac{\boldsymbol{\hat{v}}^{\top}B_i}{\boldsymbol{\hat{v}}_0^{\top}B_i} \boldsymbol{\hat{v}}_0 \mid \boldsymbol{\hat{v}} \in \hat{V} - \left\{ \boldsymbol{\hat{v}}_0 \right\} \right\}
         Orthonormalize \hat{V} with respect to the dot product \langle \hat{\boldsymbol{v}}_1, \hat{\boldsymbol{v}}_2 \rangle = \hat{\boldsymbol{v}}_1^{\top} C \hat{\boldsymbol{v}}_2
  end while
  Output: Y
```

Quality-diversity representation

In addition to the Gram matrix representation $L = B^T B$, we can factor each column B_i as the product of a 'quality' term $q_i > 0$ and a normalized 'diversity feature' $\phi_i \in \mathbb{R}^D$. Thus,

$$L_{ij} = q_i \phi_i^T \phi_j q_j.$$

If q_i communicates the 'goodness' of item i, then

$$S_{ij} = \frac{L_{ij}}{\sqrt{L_{ii}L_{jj}}}.$$

This representation allows one to independently model quality and diversity using the model

$$\mathsf{Pr}_L(Y) \propto \left(\prod_{i \in Y} q_i^2\right) \mathsf{det}(\mathcal{S}_Y)$$

Conditional DPPs

► A conditional DPP takes the form of an L-ensemble

$$\Pr_L(Y|X) \propto \det(L_Y(X))$$
.

- L is a positive semi-definite kernel matrix.
- ▶ The normalizing constant takes the form det(L(X) + I).
- Using the quality-diversity decomposition, we have

$$L_{ij}(X) = q_i(X)\phi_i(X)^T\phi_j(X)q_j(X)$$

for $q_i > 0$, $\phi_i \in \mathbb{R}^D$ and $||\phi_i|| = 1$.

Supervised learning

We observe $\{Y_t, X_t\}_{t=1}^T$ and assume individual Y_t s generated independently with probabilities

$$\Pr(Y|X,\theta) = \frac{\det(L_Y(X,\theta))}{\det(L(X,\theta)+I)}$$
.

Then the log-likelihood takes the form

$$\begin{split} \ell(\theta) &= \log \left(\prod_{t=1}^{T} \Pr(Y_t | X_t, \theta) \right) \\ &= \sum_{t=1}^{T} \left(\log \det \left(L_{Y_t} \left(X_t, \theta \right) \right) - \log \det \left(L \left(X_t, \theta \right) + I \right) \right). \end{split}$$

Supervised learning

Suppose one keeps the feature functions $\phi_i(X)$ fixed but models the quality scores with the log-linear model

$$q_i(X,\theta) = e^{f_i(X)^T\theta}$$
.

Then the probability of a single sample can be written

$$\Pr(Y|X,\theta) = \frac{\det S_Y \prod_{i \in Y} e^{f_i(X)^T \theta}}{\sum_{Y' \subseteq \mathcal{Y}} \det S_{Y'} \prod_{i \in Y'} e^{f_i(X)^T \theta}}.$$

The resulting log-likelihood is convex in θ :

$$\ell(\theta) \propto \theta^T \sum_{i \in Y} f_i(X) - \log \sum_{Y' \subseteq \mathcal{Y}} \exp \left(\theta^T \sum_{i \in Y'} f_i(X) \right) \det S_{Y'}(X).$$

k-DPPs

- ▶ A k-DPP on a discrete set $\mathcal{Y} = \{1, 2, ..., N\}$ is a distribution over all sets $Y \subseteq \mathcal{Y}$ with cardinality k.
- ► A k-DPP is obtained by conditioning a standard DPP on the event that the set *Y* has cardinality *k*.
- ► The k-DPP N_L^k has probabilities

$$P_L^k(Y) = \frac{\det(L_Y)}{\sum_{|Y'|=k} \det(L_{Y'})}$$