# Stochastic Processes: Lecture 5 

Andrew J. Holbrook

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## Determinantal point processes

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

$$
\operatorname{det}\left(\begin{array}{ll}
K\left(x_{i}, x_{i}\right) & K\left(x_{i}, x_{j}\right) \\
K\left(x_{i}, x_{j}\right) & K\left(x_{j}, x_{j}\right)
\end{array}\right)
$$

- The kernel defines an integral operator $\mathcal{K}$ acting on $L^{2}\left(\mathbb{R}^{D}\right)$ 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) $\rho_{k}:\left(\mathbb{R}^{D}\right)^{k} \rightarrow[0, \infty)$ for $k \geq 1$, such that for any family of disjoint sets $D_{1}, \ldots, D_{k} \subset \mathbb{R}^{D}$,

$$
E\left(\prod_{i=1}^{k} N\left(D_{i}\right)\right)=\int_{\prod_{D_{i}}} \rho_{k}\left(x_{1}, \ldots, x_{k}\right) d x_{1} \ldots d x_{k}
$$

Definition 2
A point process $N$ on $\mathbb{R}^{D}$ is said to be a DPP with kernel $K$ if its joint intensities satisfy

$$
\rho_{k}\left(x_{1}, \ldots, x_{k}\right)=\operatorname{det}\left(K\left(x_{i}, x_{j}\right)\right)_{1 \leq i, j \leq k}
$$

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

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

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

$$
\rho_{k}\left(x_{1}, \ldots, x_{k}\right)=\operatorname{per}\left(K\left(x_{i}, x_{j}\right)\right)_{1 \leq i, j \leq k}
$$

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 $K(z, w)=\frac{1}{\pi} e^{z \bar{w}-\frac{1}{2}\left(|z|^{2}+|w|^{2}\right)}$. Determinantal processes exhibit repulsion, while permanental processes exhibit clumping.

## DPP results

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

$$
K(x, y)=\sum_{k=1}^{n} \phi_{k}(x) \bar{\phi}_{k}(y)
$$

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

## DPP results

Theorem 2
Suppose $N$ is a DPP with kernel $K(x, y)$. Write

$$
K(x, y)=\sum_{k=1}^{\infty} \lambda_{k} \phi_{k}(x) \bar{\phi}_{k}(y),
$$

where $\phi_{k}$ are normalized eigenfunctions with eigenvalues $\lambda_{k} \in[0,1]$. Let $I_{k} \stackrel{\perp}{\sim} \operatorname{Bernoulli}\left(\lambda_{k}\right)$ and define $K$ 's random analogue

$$
K_{l}(x, y)=\sum_{k=1}^{\infty} I_{k} \phi_{k}(x) \bar{\phi}_{k}(y)
$$

Let $N_{l}$ be a DPP with kernel $K_{i}$. Then

$$
N \stackrel{d}{=} N_{l} .
$$

In particular, the total number of points in $N$ follows the distribution of the sum of independent Bernoulli $\left(\lambda_{k}\right)$ r.v.s.

## 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 $P_{i j}(t)$ 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

$$
\operatorname{det}\left(\begin{array}{ccc}
P_{i_{1} j_{1}}(t) & \ldots & P_{i_{1} j_{n}}(t) \\
\vdots & \ddots & \\
P_{i_{n} j_{1}}(t) & & P_{i_{n} j_{n}}(t)
\end{array}\right)
$$

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

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

As $n \rightarrow \infty$, we have a DPP on $\mathbb{C}$ with kernel

$$
\begin{aligned}
K(z, w) & =\frac{1}{\pi} e^{-\frac{1}{2}\left(|z|^{2}+|w|^{2}\right)} \sum_{k=0}^{\infty} \frac{(z \bar{w})^{k}}{k!} \\
& =\frac{1}{\pi} e^{-\frac{1}{2}\left(|z|^{2}+|w|^{2}\right)+z \bar{w}}
\end{aligned}
$$

## 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

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

## 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 $S \subseteq \mathcal{Y}$

$$
\operatorname{Pr}(S \subseteq Y)=\operatorname{det} K_{S}
$$

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

$$
\operatorname{Pr}(S \subset Y)=K_{i i} K_{j j}-K_{i j}^{2}=\operatorname{Pr}(i \subset Y) \operatorname{Pr}(j \subset Y)-K_{i j}^{2}
$$

## Conditioning

DPPs are closed under conditioning:

$$
\begin{aligned}
\operatorname{Pr}(A \subseteq Y \mid B \subseteq Y) & =\operatorname{Pr}(A \cup B \subseteq Y) / \operatorname{Pr}(A \subseteq Y) \\
& =\frac{\operatorname{det} K_{A \cup B}}{\operatorname{det} K_{A}} \\
& =\frac{\operatorname{det}\left(K_{A}\right) \operatorname{det}\left(K_{B}-K_{B A} K_{A}^{-1} K_{A B}\right)}{\operatorname{det}\left(K_{A}\right)} \\
& =\operatorname{det}\left(K_{B}-K_{B A} K_{A}^{-1} K_{A B}\right) \\
& =\operatorname{det}\left(\left[K-K_{\mathcal{Y}_{A}} K_{A}^{-1} K_{A \mathcal{Y}}\right]_{B}\right) .
\end{aligned}
$$

## Restrictions on $K$

- Because marginal probabilities of any set $S \subseteq \mathcal{Y}$ must be in $[0,1]$, all $\operatorname{det}\left(K_{S}\right) \geq 0$ and hence $K$ must be positive semidefinite.
- Moreover, all eigenvalues of $K$ must inhabit [0, 1], i.e. $0 \preceq K \preceq 1$.
- Any $K$ satisfying $0 \preceq K \preceq 1$ defines a DPP.


## L-ensembles

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

$$
\operatorname{Pr}_{L}(S)=\operatorname{Pr}(S=Y) \propto \operatorname{det}\left(L_{Y}\right)
$$

- Conveniently, the normalizing constant is known:

$$
\sum_{S \subseteq \mathcal{Y}} \operatorname{det}\left(L_{S}\right)=\operatorname{det}(L+I)
$$

## L-ensembles

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

$$
\sum_{S \subseteq Y \subseteq \mathcal{Y}} \operatorname{det}\left(L_{Y}\right)=\operatorname{det}\left(L+I_{s c}\right)
$$

Corollary 1

$$
\sum_{Y \subseteq \mathcal{Y}} \operatorname{det}\left(L_{Y}\right)=\operatorname{det}(L+I)
$$

Proof.
Let $S$ from Theorem 3 equal the empty set.

## L-ensembles

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

$$
\begin{aligned}
\operatorname{Pr}_{L}(S \subseteq Y) & =\frac{\sum_{S \subseteq Y \subseteq \mathcal{Y}} \operatorname{det}\left(L_{Y}\right)}{\sum_{Y \subseteq \mathcal{Y}} \operatorname{det}\left(L_{Y}\right)}=\frac{\operatorname{det}\left(L+I_{s c}\right)}{\operatorname{det}(L+I)} \\
& =\operatorname{det}\left(\left(L+I_{S c}\right)(L+I)^{-1}\right) \\
& =\operatorname{det}\left(I_{S_{c}}(L+I)^{-1}+I-(L+I)^{-1}\right) \\
& =\operatorname{det}\left(I_{s c}(L+I)^{-1}+\left(I_{S}+I_{s c}\right)\left(I-(L+I)^{-1}\right)\right) \\
& =\operatorname{det}\left(I_{S_{c}}+I_{S} K\right)=\left|\begin{array}{cc}
I_{S c}\left|\times\left|S^{c}\right|\right. & 0 \\
K_{S, s^{c}} & K_{S}
\end{array}\right|=\operatorname{det}\left(I_{\left|S^{c}\right| \times\left|S^{c}\right|}\right) \operatorname{det}\left(K_{S}\right) \\
& =\operatorname{det}\left(K_{S}\right) .
\end{aligned}
$$

## L-ensembles

- 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 $L=X X^{T}$, we have

$$
\operatorname{Pr}_{L}(S) \propto \operatorname{det}\left(L_{S}\right)=\operatorname{Vol}^{2}\left(\left\{x_{i}\right\}_{i \in S}\right)
$$

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

## Working with DPPs

- Complements: if $Y \sim \operatorname{DPP}(K)$, then $Y^{c} \sim \operatorname{DPP}(I-K)$
- Conditioning:

$$
\operatorname{Pr}_{L}\left(Y=S_{i n} \cup B \mid S_{i n} \subseteq Y, S_{o u t} \cap Y=\emptyset\right)=\frac{\operatorname{det}\left(L_{S_{\text {in }} \cup B}\right)}{\operatorname{det}\left(L_{S_{\text {out }}^{c}}+I_{S_{\text {in }}^{c}}\right)}
$$

- Marginalization:

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

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

$$
\operatorname{Pr}_{K^{\prime}}(S \subseteq Y)=\operatorname{det}\left(K_{S}^{\prime}\right)=\gamma^{|S|} K_{S}
$$

## Elementary DPPs

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

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

- For an elementary DPP this is

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

- Furthermore, $|Y|=|V|$ a.s. because $\operatorname{det}\left(K_{Y}^{V}\right)=0$ when $|Y|>|V|$.


## DPPs as mixtures of elementary DPPs

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

$$
\operatorname{Pr}_{L}=\frac{1}{\operatorname{det}(L+I)} \sum_{J \subseteq\{1,2, \ldots, n\}} \operatorname{Pr}^{V_{J}} \prod_{i \in J} \lambda_{i}
$$

where $V_{J}=\left\{v_{i}\right\}_{i \in J}$

## Sampling DPPs

```
Algorithm 1 Sampling from a DPP
    Input: eigendecomposition \(\left\{\left(\boldsymbol{v}_{n}, \lambda_{n}\right)\right\}_{n=1}^{N}\) 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
    \(V \leftarrow\left\{\boldsymbol{v}_{n}\right\}_{n \in J}\)
    \(Y \leftarrow \emptyset\)
    while \(|V|>0\) do
        Select \(i\) from \(\mathcal{Y}\) with \(\operatorname{Pr}(i)=\frac{1}{|V|} \sum_{\boldsymbol{v} \in V}\left(\boldsymbol{v}^{\top} \boldsymbol{e}_{i}\right)^{2}\)
        \(Y \leftarrow Y \cup i\)
        \(V \leftarrow V_{\perp}\), an orthonormal basis for the subspace of \(V\) orthogonal to \(\boldsymbol{e}_{i}\)
    end while
    Output: \(Y\)
```


## Sampling DPPs



## Sampling DPPs



## Sampling DPPs

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


## 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

$$
C=B B^{T} .
$$

- Here, $D$ is the dimension of the diversity feature function $\phi$.
- $D$ 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,

$$
C=\sum_{d=1}^{D} \lambda_{d} \hat{v}_{d} \hat{v}_{d}^{T}
$$

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 $\left\{\lambda_{d}, \hat{v}_{d}\right\}_{d=1}^{D}$ 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

$$
\begin{aligned}
\left\|\frac{1}{\sqrt{\lambda_{d}}} B^{T} \hat{v}_{d}\right\|^{2} & =\frac{1}{\lambda_{d}}\left(B^{T} \hat{v}_{d}\right)^{T}\left(B^{T} \hat{v}_{d}\right)=\frac{1}{\lambda_{d}} \hat{v}_{d}^{T} C \hat{v}_{d} \\
& =\frac{1}{\lambda_{d}} \lambda_{d} \hat{v}_{d}^{T} \hat{v}_{d}=1
\end{aligned}
$$

and

$$
\begin{aligned}
\left(\frac{1}{\sqrt{\lambda_{d}}} B^{T} \hat{v}_{d}\right)^{T}\left(\frac{1}{\sqrt{\lambda_{d^{\prime}}}} B^{T} \hat{v}_{d^{\prime}}\right) & =\frac{1}{\sqrt{\lambda_{d} \lambda_{d^{\prime}}}} \hat{v}_{d}^{T} C \hat{v}_{d^{\prime}} \\
& =\frac{\sqrt{\lambda_{d^{\prime}}}}{\sqrt{\lambda_{d}}} \hat{v}_{d}^{T} \hat{v}_{d^{\prime}}=0
\end{aligned}
$$

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

$$
\operatorname{det}(L+I)=\prod_{d=1}^{D}\left(\lambda_{d}+1\right)=\operatorname{det}(C+I)
$$

which only takes $O\left(D^{3}\right)$ 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

$$
K_{i j}=\sum_{d=1}^{D} \frac{\lambda_{d}}{\lambda_{d}+1}\left(\frac{1}{\sqrt{\lambda_{d}}} B_{i}^{T} \hat{v}_{d}\right)^{T}\left(\frac{1}{\sqrt{\lambda_{d}}} B_{j}^{T} \hat{v}_{d}\right) .
$$

One may therefore obtain the marginal probability of an event in time $O\left(D^{2}\right)$. For a $k$ event, this becomes $O\left(D^{2} k^{2}+k^{3}\right)$. This beats the usual $O\left(n^{3}\right)$ 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

$$
V=\left\{B^{T} \hat{v} \mid \hat{v} \in \hat{V}\right\}
$$

One may implicitly obtain linear combinations of vectors in $V$ by performing actions on their preimages: $v_{1}+v_{2}=B^{T}\left(\hat{v}_{1}+\hat{v}_{2}\right)$. Moreover,

$$
v_{1}^{T} v_{2}=\left(B^{T} \hat{v}_{1}\right)^{T}\left(B^{T} \hat{v}_{2}\right)=\hat{v}_{1}^{T} C \hat{v}_{2}
$$

so we can compute dot products of elements in $V$ in time $O\left(D^{2}\right)$. 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 \(\left\{\left(\boldsymbol{v}_{n}, \lambda_{n}\right)\right\}_{n=1}^{N}\) 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
    \(V \leftarrow\left\{\boldsymbol{v}_{n}\right\}_{n \in J}\)
    \(Y \leftarrow \emptyset\)
    while \(|V|>0\) do
        Select \(i\) from \(\mathcal{Y}\) with \(\operatorname{Pr}(i)=\frac{1}{|V|} \sum_{\boldsymbol{v} \in V}\left(\boldsymbol{v}^{\top} \boldsymbol{e}_{i}\right)^{2}\)
        \(Y \leftarrow Y \cup i\)
        \(V \leftarrow V_{\perp}\), 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:

$$
\begin{aligned}
\operatorname{Pr}(i) & =\frac{1}{|V|} \sum_{v \in V}\left(v^{T} e_{i}\right)^{2}=\frac{1}{|\hat{V}|} \sum_{\hat{v} \in \hat{V}}\left(\left(B^{T} \hat{v}\right)^{T} e_{i}\right)^{2} \\
& =\frac{1}{|\hat{V}|} \sum_{\hat{v} \in \hat{V}}\left(B_{i}^{T} \hat{v}\right)^{2}
\end{aligned}
$$

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

## Sampling DPPs

```
Algorithm 3 Sampling from a DPP (dual representation)
    Input: eigendecomposition \(\left\{\left(\hat{\boldsymbol{v}}_{n}, \lambda_{n}\right)\right\}_{n=1}^{N}\) of \(C\)
    \(J \leftarrow \emptyset\)
    for \(n=1,2, \ldots, N\) do
        \(J \leftarrow J \cup\{n\}\) with prob. \(\frac{\lambda_{n}}{\lambda_{n}+1}\)
    end for
    \(\hat{V} \leftarrow\left\{\frac{\hat{\boldsymbol{v}}_{n}}{\sqrt{\hat{\boldsymbol{v}}_{n}^{T} C \hat{\boldsymbol{v}}_{n}}}\right\}_{n \in J}\)
    \(Y \leftarrow \emptyset\)
    while \(|\hat{V}|>0\) do
        Select \(i\) from \(\mathcal{Y}\) with \(\operatorname{Pr}(i)=\frac{1}{|\hat{V}|} \sum_{\hat{\boldsymbol{v}} \in \hat{V}}\left(\hat{\boldsymbol{v}}^{\top} B_{i}\right)^{2}\)
        \(Y \leftarrow Y \cup i\)
        Let \(\hat{\boldsymbol{v}}_{0}\) be a vector in \(\hat{V}\) with \(B_{i}^{\top} \hat{\boldsymbol{v}}_{0} \neq 0\)
        Update \(\hat{V} \leftarrow\left\{\left.\hat{\boldsymbol{v}}-\frac{\hat{\boldsymbol{v}}^{\top} B_{i}}{\hat{\boldsymbol{v}}_{0}^{\top} B_{i}} \hat{\boldsymbol{v}}_{0} \right\rvert\, \hat{\boldsymbol{v}} \in \hat{V}-\left\{\hat{\boldsymbol{v}}_{0}\right\}\right\}\)
        Orthonormalize \(\hat{V}\) with respect to the dot product \(\left\langle\hat{\boldsymbol{v}}_{1}, \hat{\boldsymbol{v}}_{2}\right\rangle=\hat{\boldsymbol{v}}_{1}^{\top} C \hat{\boldsymbol{v}}_{2}\)
    end while
    Output: \(Y\)

\section*{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,
\[
L_{i j}=q_{i} \phi_{i}^{T} \phi_{j} q_{j}
\]

If \(q_{i}\) communicates the 'goodness' of item \(i\), then
\[
S_{i j}=\frac{L_{i j}}{\sqrt{L_{i i} L_{j j}}}
\]

This representation allows one to independently model quality and diversity using the model
\[
\operatorname{Pr}_{L}(Y) \propto\left(\prod_{i \in Y} q_{i}^{2}\right) \operatorname{det}\left(S_{Y}\right)
\]

\section*{Conditional DPPs}
- A conditional DPP takes the form of an L-ensemble
\[
\operatorname{Pr}_{L}(Y \mid X) \propto \operatorname{det}\left(L_{Y}(X)\right)
\]
- \(L\) is a positive semi-definite kernel matrix.
- The normalizing constant takes the form \(\operatorname{det}(L(X)+I)\).
- Using the quality-diversity decomposition, we have
\[
L_{i j}(X)=q_{i}(X) \phi_{i}(X)^{T} \phi_{j}(X) q_{j}(X)
\]
for \(q_{i}>0, \phi_{i} \in \mathbb{R}^{D}\) and \(\left\|\phi_{i}\right\|=1\).

\section*{Supervised learning}

We observe \(\left\{Y_{t}, X_{t}\right\}_{t=1}^{T}\) and assume individual \(Y_{t} s\) generated independently with probabilities
\[
\operatorname{Pr}(Y \mid X, \theta)=\frac{\operatorname{det}\left(L_{Y}(X, \theta)\right)}{\operatorname{det}(L(X, \theta)+I)}
\]

Then the log-likelihood takes the form
\[
\begin{aligned}
\ell(\theta) & =\log \left(\prod_{t=1}^{T} \operatorname{Pr}\left(Y_{t} \mid X_{t}, \theta\right)\right) \\
& =\sum_{t=1}^{T}\left(\log \operatorname{det}\left(L_{Y_{t}}\left(X_{t}, \theta\right)\right)-\log \operatorname{det}\left(L\left(X_{t}, \theta\right)+I\right)\right) .
\end{aligned}
\]

\section*{Supervised learning}

Suppose one keeps the feature functions \(\phi_{i}(X)\) fixed but models the quality scores with the log-linear model
\[
q_{i}(X, \theta)=e^{f_{i}(X)^{\top} \theta}
\]

Then the probability of a single sample can be written
\[
\operatorname{Pr}(Y \mid X, \theta)=\frac{\operatorname{det} S_{Y} \prod_{i \in Y} e^{f_{i}(X)^{T} \theta}}{\sum_{Y^{\prime} \subseteq \mathcal{Y}} \operatorname{det} S_{Y^{\prime}} \prod_{i \in Y^{\prime}} e^{f_{i}(X)^{\top} \theta}}
\]

The resulting log-likelihood is convex in \(\theta\) :
\[
\ell(\theta) \propto \theta^{T} \sum_{i \in Y} f_{i}(X)-\log \sum_{Y^{\prime} \subseteq \mathcal{Y}} \exp \left(\theta^{T} \sum_{i \in Y^{\prime}} f_{i}(X)\right) \operatorname{det} S_{Y^{\prime}}(X)
\]

\section*{k-DPPs}
- A k-DPP on a discrete set \(\mathcal{Y}=\{1,2, \ldots, N\}\) 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
\[
\operatorname{Pr}_{L}^{k}(Y)=\frac{\operatorname{det}\left(L_{Y}\right)}{\sum_{\left|Y^{\prime}\right|=k} \operatorname{det}\left(L_{Y^{\prime}}\right)}
\]

\section*{k-DPPs: normalization}

Define the \(k\) th elementary symmetric polynomial on \(\lambda_{1}, \ldots, \lambda_{N}\)
\[
e_{k}\left(\lambda_{1}, \ldots, \lambda_{N}\right)=\sum_{\substack{J \subseteq\{1, \ldots, N\} \\|J|=k}} \prod_{n \in J} \lambda_{n}
\]

For example,
\[
\begin{aligned}
& e_{1}\left(\lambda_{1}, \lambda_{2}, \lambda_{3}\right)=\lambda_{1}+\lambda_{2}+\lambda_{3} \\
& e_{2}\left(\lambda_{1}, \lambda_{2}, \lambda_{3}\right)=\lambda_{1} \lambda_{2}+\lambda_{1} \lambda_{3}+\lambda_{2} \lambda_{3} \\
& e_{3}\left(\lambda_{1}, \lambda_{2}, \lambda_{3}\right)=\lambda_{1} \lambda_{2} \lambda_{3} .
\end{aligned}
\]

\section*{Proposition 2}

The normalizing constant for a \(k\)-DPP is
\[
Z_{k}=\sum_{\left|Y^{\prime}\right|=k} \operatorname{det}\left(L_{Y^{\prime}}\right)=e_{k}\left(\lambda_{1}, \ldots, \lambda_{N}\right)
\]
where \(\lambda_{n}\) are the eigenvalues of \(L\).

\section*{k-DPPs: normalization}

Proof.
Recalling that
\[
\sum_{Y \subseteq \mathcal{Y}} \operatorname{det}\left(L_{Y}\right)=\operatorname{det}(L+I)
\]
we know
\[
\sum_{\left|Y^{\prime}\right|=k} \operatorname{det}\left(L_{Y^{\prime}}\right)=\operatorname{det}(L+I) \sum_{\left|Y^{\prime}\right|=k} \operatorname{Pr}_{L}\left(Y^{\prime}\right)
\]

Then, because every DPP is a mixture of elementary DPPs:
\[
\begin{aligned}
\operatorname{det}(L+I) \sum_{\left|Y^{\prime}\right|=k} \operatorname{Pr}_{L}\left(Y^{\prime}\right) & =\frac{\operatorname{det}(L+I)}{\operatorname{det}(L+I)} \sum_{\left|Y^{\prime}\right|=k} \sum_{J \subseteq\{1, \ldots, N\}} \operatorname{Pr}^{V_{J}}\left(Y^{\prime}\right) \prod_{n \in J} \lambda_{n} \\
& =\sum_{|J|=k} \sum_{\left|Y^{\prime}\right|=k} \operatorname{Pr}^{V_{J}}\left(Y^{\prime}\right) \prod_{n \in J} \lambda_{n} \\
& =\sum_{|J|=k} \prod_{n \in J} \lambda_{n}
\end{aligned}
\]

\section*{Computing elementary symmetric polynomials}

Use the shorthand \(e_{k}^{N}=e_{K}\left(\lambda_{1}, \ldots, \lambda_{N}\right)\), we have the recursion
\[
e_{k}^{N}=e_{k}^{N-1} \lambda_{N} e_{k-1}^{N-1} .
\]

Thus, the following algorithm computes \(e_{k}^{N}\) in time \(O(N k)\).
```

Algorithm 7 Computing the elementary symmetric polynomials
Input: $k$, eigenvalues $\lambda_{1}, \lambda_{2}, \ldots \lambda_{N}$
$e_{0}^{n} \leftarrow 1 \quad \forall n \in\{0,1,2, \ldots, N\}$
$e_{l}^{0} \leftarrow 0 \quad \forall l \in\{1,2, \ldots, k\}$
for $l=1,2, \ldots k$ do
for $n=1,2, \ldots, N$ do
$e_{l}^{n} \leftarrow e_{l}^{n-1}+\lambda_{n} e_{l-1}^{n-1}$
end for
end for
Output: $e_{k}\left(\lambda_{1}, \lambda_{2}, \ldots, \lambda_{N}\right)=e_{k}^{N}$

```

\section*{k-DPPs: sampling}
- One may use a (slow) rejection sampling approach, sampling DPPs and discarding those for which \(|Y| \neq k\).
- It is more efficient to first recognize that, when \(|Y|=k\)
\[
\operatorname{Pr}_{L}^{k}(Y)=\frac{\operatorname{det}(L+I)}{e_{k}^{N}} \operatorname{Pr}_{L}(Y)
\]
and therefore
\[
\operatorname{Pr}_{L}^{k}(Y)=\frac{1}{e_{k}^{N}} \sum_{|J|=k} \operatorname{Pr}^{V_{J}}(Y) \prod_{n \in J} \lambda_{n}
\]
- A k-DPP is also a mixture of elementary DPPs! So if we can sample \(k\) eigenvalues, we can then use the mixture of elementary DPPs to generate samples.

\section*{k-DPPs: sampling}

The following \(O(N k)\) algorithm samples sets of \(k\) eigenvalues according to desired probabilities
\[
\operatorname{Pr}(J)=\frac{1\{|J|=k\}}{e_{k}^{N}} \prod_{n \in J} \lambda_{n} .
\]
```

Algorithm 8 Sampling $k$ eigenvectors
Input: $k$, eigenvalues $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{N}$
compute $e_{l}^{n}$ for $l=0,1, \ldots, k$ and $n=0,1, \ldots, N$ (Algorithm 7)
$J \leftarrow \emptyset$
$l \leftarrow k$
for $n=N, \ldots, 2,1$ do
if $l=0$ then
break
end if
if $u \sim U[0,1]<\lambda_{n} \frac{e_{l-1}^{n-1}}{e_{l}^{n}}$ then
$J \leftarrow J \cup\{n\}$
$l \leftarrow l-1$
end if
end for
Output: J

```

\section*{k-DPPs: marginalization}

Recall that for a general L-ensemble, we have
\[
\begin{aligned}
\operatorname{Pr}_{L}(B \subseteq Y \mid A \subseteq Y) & =\operatorname{det}\left(\left[I-\left[\left(L+I_{A^{c}}\right)^{-1}\right]_{A^{c}}\right]_{B}\right) \\
& =\operatorname{det}\left(L_{B}^{A}\right)
\end{aligned}
\]

\section*{k-DPPs: marginalization}
k-DPPs are not DPPs and do not have a marginal kernel. But for \(|A| \leq k\), we have:
\[
\begin{aligned}
& \operatorname{Pr}_{L}^{k}(A \subseteq Y)=\sum_{\substack{\left|Y^{\prime}\right|=k-|A| \\
Y^{\prime} \cap A=\emptyset}} \operatorname{Pr}_{L}^{k}\left(Y^{\prime} \cup A\right) \\
& =\frac{\operatorname{det}(L+I)}{Z_{k}} \sum_{\substack{\left|Y^{\prime}\right|=k-|A| \\
Y^{\prime} \cap A=\emptyset}} \operatorname{Pr}_{L}\left(Y^{\prime} \cup A\right) \\
& =\frac{\operatorname{det}(L+I)}{Z_{k}} \sum_{\substack{\left|Y^{\prime}\right|=k-|A| \\
Y^{\prime} \cap A=\emptyset}} \operatorname{Pr}_{L}\left(Y=Y^{\prime} \cup A \mid A \subseteq Y\right) \operatorname{Pr}_{L}(A \subseteq Y) \\
& =\frac{Z_{k-|A|}^{A}}{Z_{k}} \frac{\operatorname{det}(L+I)}{\operatorname{det}\left(L^{A}+I\right)} \operatorname{Pr}_{L}(A \subseteq Y),
\end{aligned}
\]
where
\[
Z_{k-|A|}^{A}=\operatorname{det}\left(L^{A}+1\right) \sum_{\substack{\left|Y^{\prime}\right|=k-|A| \\ Y^{\prime} \cap A=\emptyset}} \operatorname{Pr}\left(Y=Y^{\prime} \cup A \mid A \subseteq Y\right)=\sum_{\substack{\left|Y^{\prime}\right|=k-|A| \\ Y^{\prime} \cap A=\emptyset}} \operatorname{det}\left(L_{Y^{\prime}}^{A}\right)
\]
is the normalizing constant for the \((k-|A|)\)-DPP with kernel \(L^{A}\).

\section*{k-DPPs: marginalization}

Thus, the marginal probabilities for a k-DPP are the same as those of the DPP with the same kernel but properly renormalized. By observing that
\[
\frac{\operatorname{det}\left(L^{A}\right)}{\operatorname{det}(L+I)}=\frac{\operatorname{Pr}_{L}(A \subseteq Y)}{\operatorname{det}\left(L^{A}+I\right)}
\]
(since \(1 / \operatorname{det}\left(L^{A}+I\right)\) is the probability of observing nothing else conditioned on \(A\) ), the equation simplifies further:
\[
\begin{aligned}
\operatorname{Pr}_{L}^{k}(A \subseteq Y) & =\frac{Z_{k-|A|}^{A}}{Z_{k}} \frac{\operatorname{det}(L+I)}{\operatorname{det}\left(L^{A}+I\right)} \operatorname{Pr}_{L}(A \subseteq Y) \\
& =\frac{Z_{k-|A|}^{A}}{Z_{k}} \operatorname{det}\left(L^{A}\right)=Z_{k-|A|}^{A} \operatorname{Pr}_{L}^{k}(A)
\end{aligned}
\]

Computing such a probability is \(O\left((N-|A|)^{3}\right)\) and very inefficient for \(|A|\) small.

\section*{k-DPPs: singleton marginals}

First, write the marginal probability of an item \(i\) using elementary DPPs:
\[
\operatorname{Pr}_{L}^{k}(i \in Y)=\frac{1}{e_{k}^{N}} \sum_{|J|=k} \operatorname{Pr}^{V_{J}}(i \in Y) \prod_{n^{\prime} \in J} \lambda_{n^{\prime}}
\]

But the marginal kernel of an elementary DPP is \(\sum_{n \in J} v_{n} v_{n}^{T}\), so this becomes:
\[
\begin{aligned}
\operatorname{Pr}_{L}^{k}(i \in Y) & =\frac{1}{e_{k}^{N}} \sum_{|J|=k}\left(\sum_{n \in J}\left(e_{i}^{T} v_{n}\right)^{2}\right) \prod_{n^{\prime} \in J} \lambda_{n^{\prime}} \\
& =\frac{1}{e_{k}^{N}} \sum_{n=1}^{N}\left(e_{i}^{T} v_{n}\right)^{2} \sum_{\substack{J \supset\{n\} \\
|J|=k}} \prod_{n^{\prime} \in J} \lambda_{n^{\prime}} \\
& =\sum_{n=1}^{N}\left(e_{i}^{T} v_{n}\right)^{2} \lambda_{n} \frac{e_{k-1}^{-n}}{e_{k}^{N}}
\end{aligned}
\]

If we have the eigendecomposition of \(L\) and know the values \(e_{k-1}^{-n} / e_{k}^{N}\), then we can obtain all singleton marginals in time \(\mathrm{O}\left(N^{2}\right)\). \(e_{k}^{N}\) can be computed in time \(\mathrm{O}(N k)\) and all \(e_{k-1}^{-n}\) can be computed in time \(\mathrm{O}\left(N^{2} k\right)\). This can be improved to \(\mathrm{O}(N \log (N) k)\).

\section*{k-DPPs: conditioning}

For \(|A|+|B|=k\),
\[
\begin{aligned}
\operatorname{Pr}_{L}^{k}(Y=A \cup B \mid A \subseteq Y) & \propto \operatorname{Pr}_{L}^{k}(Y=A \cup B) \\
& \propto \operatorname{Pr}_{L}(Y=A \cup B) \\
& \propto \operatorname{Pr}_{L}(Y=A \cup B \mid A \subseteq Y) \\
& \propto \operatorname{det}\left(L_{B}^{A}\right) .
\end{aligned}
\]

So the conditional \(k\)-DPP is a \((k-|A|)\)-DPP.```

