Abstract

In this note we consider sampling from (non-homogeneous) strongly Rayleigh probability measures. As an important corollary, we obtain a fast mixing Markov Chain sampler for Determinantal Point Processes.

1 Introduction

Probability distributions over combinatorial families of subsets are important to a variety of problems in machine learning and related areas. Notable examples include discrete probabilistic models \cite{11, 22, 26, 37, 40} for use in computer vision, computational biology, and Natural Language Processing; combinatorial bandit learning \cite{14}; model compression \cite{34}; and low-rank matrix approximations \cite{27}. Consequently, significant recent attention has been paid to sampling rapidly from certain structured discrete distributions \cite{21, 36}, as well as from determinantal point processes \cite{3, 27, 28} and progress on sampling by optimization \cite{16, 32}.

Amongst these distributions, a widely used class is that of log-submodular measures. Formally, for sets $S, T \subseteq V$, a log-submodular measure $\pi : 2^V \rightarrow \mathbb{R}_+$ satisfies the inequality

$$\log \pi(S) + \log \pi(T) \geq \log \pi(S \cup T) + \log \pi(S \cap T). \quad (1.1)$$

Log-submodular measures are useful to several applications in machine learning and computer vision \cite{5, 26}; more generally, submodular functions are widely important across machine learning \cite{4, 6, 25}.

In this note, we focus on a specific subclass of log-submodular measures, namely, strongly Rayleigh (SR) measures. These measures are intimately related to stable polynomials, a viewpoint first established in \cite{7}, which has proved key to uncovering their remarkable properties, both for modeling as well as for fast sampling. For instance, these measures exhibit negative association, a strong, “robust” notion of negative dependence (we formally define SR measures in Section 2).

We mention below some important examples of SR measures.

**Determinantal Point Processes.** A Determinantal Point Process (DPP) is a measure over subsets given by the principal minors of a positive semidefinite matrix $K \in \mathbb{R}^{N \times N}$ with eigenvalues in $[0,1]$. Its marginal probabilities satisfy

$$\Pr(S \subseteq T) = \det(K_S), \quad (1.2)$$

where $K_S$ is the submatrix indexed by the elements in $S$, and $T$ is the random set distributed as a DPP. DPPs arise in random matrix theory, combinatorics, machine learning, matrix approximations, and many other areas; see e.g., \cite{8–10, 13, 23, 26, 28–31, 38}.

**Weighted) regular and balanced matroids.** The uniform distribution over the bases of certain matroids (regular matroids and balanced matroids \cite{17, 35}) is SR, most notably, the uniform distribution over spanning trees in a graph. Here, spanning trees are viewed as subsets of edges, and the distribution is over subsets of edges.
Processes. A natural MCMC sampler for these processes takes swapping steps: given a current set only for some sets of a fixed cardinality \( k \), \( \pi'(S) = \pi(S \mid |S| = k) \) or \( \pi'(S) = 0 \) if \( |S| \neq k \), and \( \pi'(S) \propto \pi(S) \) otherwise.

Strongly Rayleigh measures have been underlying recent progress in approximation algorithms [1, 15, 20, 27], graph sparsification [18, 39], extensions to the Kadison-Singer problem [2], finite extensions to free probability [33], and concentration of measure results [35].

Contributions. Despite their importance, efficient sampling methods are only known for special cases of SR measures. In this note, we derive a provably fast mixing Markov Chain for efficiently sampling general SR measures. For our analysis, we use the recent result of [3] (that analyzes fast mixing for the subclass of \( k \)-homogeneous SR measures), along with the closedness properties of SR measures established in the landmark work [7].

2 Sampling from Strongly Rayleigh Distributions

Strongly Rayleigh (SR) distributions capture the strongest form of negative dependence, while enjoying a host of other notable properties [7]. Several important distributions exhibit the strong Rayleigh property, for example, uniform distributions over spanning trees in graphs, and more generally, the widely occurring Determinantal Point Processes. A distribution is strongly Rayleigh if its generating polynomial \( p_\pi : \mathbb{C}^N \to \mathbb{C} \),

\[
p_\pi(z) = \sum_{S \subseteq V} \pi(S) \prod_{i \in S} z_i
\]

(2.1)
is real stable. This means that if \( \Im(z_i) > 0 \) for all arguments \( z_i \) of \( p_\pi(z) \), then \( p_\pi(z) \neq 0 \).

Markov Chain Sampling. We sample from \( \pi \) via a Markov Chain Monte Carlo method (MCMC), i.e., we run a Markov Chain with state space \( 2^V \) (the power set of \( V \)). All the chains discussed here are ergodic. The mixing time of the chain indicates the number of iterations \( t \) that we must perform (after starting from an arbitrary set \( S_0 \in 2^V \)) before we can consider \( S_t \) a valid sample from \( \pi \). Formally, if \( \delta_{S_0}(t) \) is the total variation distance between the distribution of \( S_t \) and \( \pi \) after \( t \) steps, then \( \tau_{S_0}(\epsilon) = \min\{ t : \delta_{S_0}(t') \leq \epsilon, \forall t' \geq t \} \) is the mixing time to sample from a distribution \( \epsilon \)-close to \( \pi \) in terms of total variation distance. We say that the chain mixes fast if \( \tau_{S_0} \) is polynomial in \( N \).

Existing samplers. Efficient sampling techniques have been studied for special cases of SR distributions. A popular method for sampling from Determinantal Point Processes uses the spectrum of the defining kernel [23]. Generic MCMC samplers can also be derived, for example, previous work used a simple add-delete Metropolis-Hasting chain [24]. Starting with an arbitrary set \( S \subseteq V \), we sample a point \( t \in V \) uniformly at random. If \( t \in S \), we remove \( t \) with probability \( \min\{1, \pi(S \setminus \{t\}) / \pi(S)\} \); if \( t \notin S \), we add it to \( S \) with probability \( \min\{1, \pi(S \cup \{t\}) / \pi(S)\} \). Algorithm 1 shows the (lazy) Markov chain.

The add-delete chain can work well in practice [24], however, it does not always mix fast. An elementary Determinantal Point Process has non-zero measure only on sets of a fixed cardinality; for such a process (or a process close to it), the chain will stall or mix slowly.

Another special case of SR distributions are homogeneous SR measures. These measures are nonzero only for some sets of a fixed cardinality \( k \). Examples include Bernoulli distributions conditioned on cardinality, uniform distributions on the bases of balanced matroids [17], and \( k \)-Determinantal Point Processes. A natural MCMC sampler for these processes takes swapping steps: given a current set \( S \subseteq V \), it picks, uniformly at random, points \( s \in S \) and \( t \notin S \), and swaps them with probability \( \min\{1, \pi(S \cup \{t\} \setminus \{s\}) / \pi(S)\} \). Algorithm 2 formalizes this procedure. Building upon results in [17],

Product measures / Bernoullis conditioned on their sum. Assume there is a weight \( q_i \in [0,1] \) for each element \( i \in V \). The product measure \( \pi(S) = \prod_{i \in S} q_i \prod_{i \notin S} (1 - q_i) \) is SR, as is its conditioning on sets of a specific cardinality \( k \), i.e., \( \pi'(S) = \pi(S \mid |S| = k) \) or \( \pi'(S) = 0 \) if \( |S| \neq k \), and \( \pi'(S) \propto \pi(S) \) otherwise.
Algorithm 1 Add/delete (Metropolis-Hasting) sampler

Require: SR distribution $\pi$
Initialize $S \subseteq V$
while not mixed do
  Let $b = 1$ with probability $\frac{1}{2}$
  if $b = 1$ then
    Pick $t \in V$ uniformly at random
    if $t \in S$ then
      $S = S \setminus \{t\}$ with probability $\min\{1, \pi(S \setminus \{t\})/\pi(S)\}$
    else
      $S = S \cup \{t\}$ with probability $\min\{1, \pi(S \cup \{t\})/\pi(S)\}$
  end if
  else
    Do nothing
  end if
end while

Algorithm 2 Gibbs exchange sampler

Require: Homogeneous SR distribution $\pi$
Initialize $S \subseteq V$, $\pi(S) > 0$
while not mixed do
  Let $b = 1$ with probability $\frac{1}{2}$
  if $b = 1$ then
    Pick $s \in S$ and $t \not\in S$ uniformly randomly
    $S = S \cup \{t\} \setminus \{s\}$ with probability $\min\{1, \pi(S \cup \{t\} \setminus \{s\})/\pi(S)\}$
  else
    Do nothing
  end if
end while

Anari et al. [3] recently showed that the mixing time for the swap sampler for homogeneous SR measures is polynomial in $N$, $k$, and $\log(\frac{1}{\epsilon \pi(S_0)})$. These results are restricted to homogeneous SR measures, and do not hold for arbitrary SR measures.

2.1 A fast mixing chain for general SR measures

In this note, we define a projection chain that works for arbitrary SR measures, and whose mixing time is polynomial in $N$, $k$, and $\log(\frac{1}{\epsilon \pi(S_0)})$. In particular, we make the results in [3, 17] accessible to general SR measures by using specific closure properties [7].

The resulting Markov Chain is shown in Algorithm 3. Interestingly, this sampler uses a mixture of add-delete and swap steps. Hence, intuitively, it preserves the good properties of either type of step. In general the sampled sets can have arbitrary cardinality, and hence add-delete steps are needed. If the distribution concentrates on a certain cardinality, the swap steps gain importance.

This intuition is supported by the following theorem.

Theorem 1. If $\pi$ is a SR measure, the mixing time $\tau_{S_0}(\epsilon)$ of the Markov chain in Algorithm 3 is given by

$$\tau_{S_0}(\epsilon) \leq 2N^2 \left( \log \left( \frac{N}{|S_0|} \right) + \log(\pi(S_0))^{-1} + \log \epsilon^{-1} \right).$$  (2.2)
Algorithm 3 Markov Chain for Strongly Rayleigh Distribution

Require: SR distribution $\pi$

Initialize $R_0 \subseteq [2N]$ where $|R_0| = N$ and take $S = R_0 \cap V$

while not mixed do
  draw $q \sim \text{Unif}[0,1]$
  draw $t \in V \setminus S$ and $s \in S$ uniformly randomly
  if $q \in \left[0, \frac{(N-|S|)^2}{2N^2}\right]$ then
    $S = S \cup \{t\}$ with probability $\min\{1, \frac{\pi(s \cup \{t\})}{\pi(s)} \times \frac{|S|+1}{N-|S|}\}$ \hfill $\triangleright$ Add $t$
  else if $q \in \left(\frac{(N-|S|)^2}{2N^2}, \frac{N-|S|}{2N}\right)$ then
    $S = S \cup \{t\} \setminus \{s\}$ with probability $\min\{1, \frac{\pi(s \cup \{t\} \setminus \{s\})}{\pi(s)}\}$ \hfill $\triangleright$ Exchange $s$ with $t$
  else if $q \in \left(\frac{N-|S|}{2N}, \frac{|S|^2 + N(N-|S|)}{2N^2}\right)$ then
    $S = S \setminus \{s\}$ with probability $\min\{1, \frac{\pi(s \setminus \{s\})}{\pi(s)} \times \frac{|S|}{N-|S|+1}\}$ \hfill $\triangleright$ Delete $s$
  else
    Do nothing
  end if
end while

We may choose the initial set such that $S_0$ makes the first term in the sum logarithmic in $N$ ($S_0 = R_0 \cap V$ in Algorithm 3).

Theorem 1 and Algorithm 3 make use of the closure of SR measures under symmetric homogenization [7]. The idea underlying this construction is to introduce a “shadow” $V'$ of the ground set $V$, and to construct an $N$-homogeneous SR measure $\pi_{sh}$ on this joint ground set $V \cup V'$. Importantly, the marginal distribution on $V$ under this joint measure is exactly $\pi$. The homogeneous measure $\pi_{sh}$ leads to a fast mixing chain that is, however, not practical to implement. Hence, we reduce it to an equivalent, more efficient chain.

Proof. First, we construct a symmetric homogenization of $\pi$, a measure $\pi_{sh}$ on $V \cup V'$:

$$\pi_{sh}(R) = \begin{cases} 
\pi(R \cap [N])(\binom{N}{|R \cap [N]|})^{-1} & \text{if } |R| = N; \\
0 & \text{otherwise}.
\end{cases}$$

If $\pi$ is SR, so is its symmetric homogenization $\pi_{sh}$. We use this property to derive a fast-mixing chain.

The results in [3] show that a Markov Chain with swap steps mixes rapidly for $\pi_{sh}$. Precisely, they show that for any $k$-homogeneous SR distribution on a ground set of size $M$, a Gibbs-exchange sampler has mixing time

$$\tau_{R_0}(\epsilon) \leq 2k(M-k)(\log \pi_{sh}(R_0))^{-1} + \log \epsilon^{-1}).$$

Here, $M = 2N$ and $k = N$, leading to a mixing time of $2N^2 (\log \pi_{sh}(T_0))^{-1} + \log \epsilon^{-1}$, or, equivalently,

$$\tau_{S_0}(\epsilon) \leq 2N^2 \left(\log \left(\frac{N}{|S_0|}\right) + \log(\pi(S_0))^{-1} + \log \epsilon^{-1} \right). \quad (2.3)$$

It remains to show that the chain in Algorithm 3 is equivalent to the Gibbs-exchange sampler for $\pi_{sh}$. In fact, one may be tempted to implement the exchange sampler directly. However, it doubles the size of the ground set to $2N$, and always maintains a set of size $N$. If $N$ is large, this can be impractical.

Claim 1. The mixing time of Markov chain in Algorithm 3 has the same bound as Eq. (2.3).

Our exchange sampler maintains a set $R$ of cardinality $|R| = N$. In each iteration, with probability $\frac{1}{2}$, the sampler does nothing, otherwise it proceeds. If it proceeds, it picks $s \in R$ and $t \in [2N] \setminus R$
uniformly at random, and exchanges them with probability

$$\min \left\{ 1, \frac{\pi_{sh}(R \cup \{t\} \setminus \{s\})}{\pi_{sh}(R)} \right\}.$$  \hfill (2.4)

If the exchange is accepted, then the new set is $R \cup \{t\} \setminus \{s\}$.

To consider the projection of this chain onto $V$, let $S = R \cap V$, and $T = V \setminus R$. There are in total four possibilities for locations of $s$ and $t$:

1. With probability $\frac{|S|(N-|S|)}{N^2}$, $s \in S$ and $t \in T$, and we switch assignment of $s$ and $t$ with probability $\min\{1, \frac{\pi_{sh}(R \cup \{t\} \setminus \{s\})}{\pi_{sh}(R)} \} = \min\{1, \frac{\pi(s \cup \{t\} \setminus \{s\})}{\pi(S)} \}$. This is equivalent to switching elements between $S$ and $T$, i.e., an exchange step on $V$.

2. With probability $\frac{|S|(N-|S|)}{N^2}$, we have $s \not\in S$ and $t \not\in T$. In this case, independent of whether we exchange $s$ and $t$ or not, the set $S = R \cap V$ remains the same. Hence, in this step, $S$ remains unchanged.

3. With probability $\frac{|S|^2}{N^2}$, we have $s \in S$ and $t \not\in T$, and we switch with probability $\min\{1, \frac{\pi(s \cup \{t\} \setminus \{s\})}{\pi(S)} \} \times \frac{|S|}{N-|S|+1}$. This is equivalent to deleting element $s$ from $S$.

4. With probability $\frac{(N-|S|)^2}{N^2}$, we have $s \not\in S$ and $t \in T$, and switch with probability $\min\{1, \frac{\pi(s \cup \{t\} \setminus \{s\})}{\pi(S)} \} \times \frac{|S|+1}{N-|S|}$. This is equivalent to adding element $t$ to $S$.

Algorithm 3 performs those steps with exactly the same probabilities; hence, it is a projection of the exchange chain for $\pi_{sh}$ and has the same mixing time.

Remarks. By using the SR property, we obtain a clean bound for fast mixing. In certain cases, the above chain may mix slower in practice than a pure add-delete chain, since it is “lazier”, i.e., its probability of stalling is higher. However, it is guaranteed to mix well, and, in other cases, can mix much faster than the pure add-delete chain in [21, 24]. We observe both phenomena in our experiments.

3 Experiments

Next, we empirically study the how fast our samplers converge. We compare the strongly-Rayleigh chain in Algorithm 3 (Mix) against a simple add-delete chain (Add-Delete). To monitor the convergence...
of these Markov chains, we use potential scale reduction factor (PSRF) [12, 19] that runs several chains in parallel and compares within-chain variances to between-chain variances. Typically, PSRF is greater than 1 and will converge to 1 in the limit; if it is close to 1 we empirically conclude that chains have mixed. Throughout experiments we run 10 chains in parallel for estimation, and declare “convergence” at a PSRF of 1.05.

We use a DPP on Ailerons data1 of size 200, and the corresponding PSRF is shown in Fig. 1b. We observe that Mix converges slightly slower than Add-Delete since it is lazier. However, the Add-Delete chain does not always mix fast. Fig. 1c illustrates a different setting, where we modify the eigenspectrum of the kernel matrix: the first 100 eigenvalues are 500 and others 1/500. Such a kernel corresponds to almost an elementary DPP, where the size of the observed subsets sharply concentrates around 100. Here, Add-Delete moves very slowly. Mix, in contrast, has the ability to exchange elements and thus converges much faster than Add-Delete.

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