

# Exact sampling of determinantal point processes with sublinear time preprocessing

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## Abstract

We study the complexity of sampling from a distribution over all index subsets of the set  $\{1, \dots, n\}$  with the probability of a subset  $S$  proportional to the determinant of the submatrix  $\mathbf{L}_S$  of some  $n \times n$  p.s.d. matrix  $\mathbf{L}$ , where  $\mathbf{L}_S$  corresponds to the entries of  $\mathbf{L}$  indexed by  $S$ . Known as a determinantal point process, this distribution is used in machine learning to induce diversity in subset selection. In practice, we often wish to sample *multiple* subsets  $S$  with small expected size  $k \triangleq \mathbb{E}[|S|] \ll n$  from a very large matrix  $\mathbf{L}$ , so it is important to minimize the preprocessing cost of the procedure (performed once) as well as the sampling cost (performed repeatedly). For this purpose, we propose a new algorithm which, given access to  $\mathbf{L}$ , samples *exactly* from a determinantal point process while satisfying the following two properties: (1) its preprocessing cost is  $n \cdot \text{poly}(k)$ , i.e., *sublinear* in the size of  $\mathbf{L}$ , and (2) its sampling cost is  $\text{poly}(k)$ , i.e., *independent* of the size of  $\mathbf{L}$ . Prior to our results, state-of-the-art exact samplers required  $\mathcal{O}(n^3)$  preprocessing time and sampling time linear in  $n$  or dependent on the spectral properties of  $\mathbf{L}$ . We also give a reduction which allows using our algorithm for exact sampling from cardinality constrained determinantal point processes with  $n \cdot \text{poly}(k)$  time preprocessing.

## 1 Introduction

Given a positive semi-definite (psd)  $n \times n$  matrix  $\mathbf{L}$ , a determinantal point process  $\text{DPP}(\mathbf{L})$  (also known as an  $L$ -ensemble) is a distribution over all  $2^n$  index subsets  $S \subseteq \{1, \dots, n\}$  such that

$$\Pr(S) \triangleq \frac{\det(\mathbf{L}_S)}{\det(\mathbf{I} + \mathbf{L})},$$

where  $\mathbf{L}_S$  denotes the  $|S| \times |S|$  submatrix of  $\mathbf{L}$  with rows and columns indexed by  $S$ . Determinantal point processes naturally appear across many scientific domains [Mac75,

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BLMV17, Gue83], while also being used as a tool in machine learning and recommender systems [KT12] for inducing diversity in subset selection and as a variance reduction approach. In this context, we often wish to efficiently produce many DPP samples of small expected size<sup>1</sup>  $k \triangleq \mathbb{E}[|S|]$  given a large matrix  $\mathbf{L}$ . Sometimes the distribution is restricted to subsets of fixed size  $|S| = k \ll n$ , denoted  $k$ -DPP( $\mathbf{L}$ ). [HKP<sup>+</sup>06] gave an algorithm for drawing samples from DPP( $\mathbf{L}$ ) distributed exactly, later adapted to  $k$ -DPP( $\mathbf{L}$ ) by [KT11], which can be implemented to run in polynomial time. In many applications, however, sampling is still a computational bottleneck because the algorithm requires performing the eigendecomposition of matrix  $\mathbf{L}$  at the cost of  $\mathcal{O}(n^3)$ . In addition to that initial cost, producing many independent samples  $S_1, S_2, \dots$  at high frequency poses a challenge because the cost of each sample is at least linear in  $n$ . Many alternative algorithms have been considered for both DPPs and  $k$ -DPPs to reduce the computational cost of preprocessing and/or sampling, including many approximate and heuristic approaches. Contrary to approximate solutions, we present an algorithm which samples *exactly* from a DPP or a  $k$ -DPP with the initial preprocessing cost *sublinear* in the size of  $\mathbf{L}$  and the sampling cost *independent* of the size of  $\mathbf{L}$ .

**Theorem 1** *For a psd  $n \times n$  matrix  $\mathbf{L}$ , let  $S_1, S_2, \dots$  be i.i.d. random sets from DPP( $\mathbf{L}$ ) or from any  $k$ -DPP( $\mathbf{L}$ ). Then, there is an algorithm which, given access to  $\mathbf{L}$ , returns*

- a) *the first subset,  $S_1$ , in:  $n \cdot \text{poly}(k) \text{polylog}(n)$  time,*
- b) *each subsequent  $S_i$  in:  $\text{poly}(k)$  time.*

We refer to this algorithm as the very fast and exact DPP sampler, or DPP-VFX. Table 1 compares DPP-VFX with other DPP and  $k$ -DPP sampling algorithms. In this comparison, we focus on the methods that provide strong accuracy guarantees. As seen from the table, our algorithm is the first exact sampler to achieve sublinear overall runtime. Only the approximate MCMC sampler of [AGR16] matches our  $n \cdot \text{poly}(k)$  complexity (and only for a  $k$ -DPP), but for this method every next sample is equally expensive, making it less practical when repeated sampling is needed. In fact, to our knowledge, no other exact or approximate method (with rigorous approximation guarantees) achieves  $\text{poly}(k)$  sampling time of this paper.

Our method is based on a technique developed recently by [DWH18, DWH19] and later extended by [Der18]. In this approach, we carefully downsample the index set  $[n] = \{1, \dots, n\}$  to a sample  $\sigma = (\sigma_1, \dots, \sigma_t) \in [n]^t$  that is small but still sufficiently larger than the expected target size  $k$ , and then run a DPP on  $\sigma$ . As the downsampling distribution we use a *regularized* determinantal point process (R-DPP), proposed by [Der18], which (informally) samples  $\sigma$  with probability  $\Pr(\sigma) \sim \det(\mathbf{I} + \tilde{\mathbf{L}}_\sigma)$ , where  $\tilde{\mathbf{L}}$  is a rescaled version of  $\mathbf{L}$ . Overall, the approach is described in the diagram below, where  $|S| \leq t \ll n$ ,

$$\{1, \dots, n\} \xrightarrow{\sigma \sim \text{R-DPP}} (\sigma_1, \dots, \sigma_t) \xrightarrow{\tilde{S} \sim \text{DPP}} S = \{\sigma_i : i \in \tilde{S}\}.$$

The DPP algorithm proposed by [Der18] follows the same diagram, however it requires that the size of the intermediate sample  $\sigma$  be  $\Omega(\text{rank}(\mathbf{L}) \cdot k)$ . This means that their method

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<sup>1</sup> To avoid complicating the exposition with edge cases, we assume  $k \geq 1$ . Note that this can be always satisfied without distorting the distribution by rescaling  $\mathbf{L}$  by a constant, and is without loss of generality, as our analysis can be trivially extended to the case  $0 \leq k < 1$  with some additional notation.

	exact	DPP	$k$ -DPP	first sample	subsequent samples
[HKP <sup>+</sup> 06, KT11]	✓	✓	✓	$n^3$	$nk^2$
[AGR16]	✗	✗	✓	$n \cdot \text{poly}(k)$	$n \cdot \text{poly}(k)$
[LJS16b]	✗	✓	✗	$n^2 \cdot \text{poly}(k)$	$n^2 \cdot \text{poly}(k)$
[LGD18]	✓	✓	✗	$n^3$	$\text{poly}(k \cdot (1 + \ \mathbf{L}\ ))$
[Der18]	✓	✓	✗	$n^3$	$\text{poly}(\text{rank}(\mathbf{L}))$
DPP-VFX (this paper)	✓	✓	✓	$n \cdot \text{poly}(k)$	$\text{poly}(k)$

Table 1: Comparison of DPP and  $k$ -DPP algorithms using the  $\mathbf{L}$ -ensemble representation. For a DPP,  $k$  denotes the expected subset size. Note that  $k \leq \text{rank}(\mathbf{L}) \leq n$ . We omit log terms for clarity.

provides improvement over [HKP<sup>+</sup>06] only when  $\mathbf{L}$  can be decomposed as  $\mathbf{X}\mathbf{X}^\top$  for some  $n \times r$  matrix  $\mathbf{X}$ , with  $r \ll n$ . However, in practice, matrix  $\mathbf{L}$  is often only *approximately low-rank*, i.e., it exhibits some form of eigenvalue decay but it does not have a low-rank factorization. In this case, the results of [Der18] are vacuous both in terms of the preprocessing cost and the sampling cost, in that obtaining *every* sample would take  $\Omega(n^3)$ . We propose a different R-DPP implementation (see DPP-VFX as Algorithm 1) where the expected size of  $\sigma$  is  $\mathcal{O}(k^2)$ . To make the algorithm efficient, we use new connections between determinantal point processes, ridge leverage scores, and Nyström approximation.

**Definition 1** Given a psd matrix  $\mathbf{L}$ , its  $i$ th  $\lambda$ -ridge leverage score (RLS)  $\tau_i(\lambda)$  is the  $i$ th diagonal entry of  $\mathbf{L}(\lambda\mathbf{I} + \mathbf{L})^{-1}$ . The  $\lambda$ -effective dimension  $d_{\text{eff}}(\lambda)$  is the sum of the leverage scores,  $\sum_i \tau_i(\lambda)$ .

An important connection between RLSs and DPPs is that when  $S \sim \text{DPP}(\mathbf{L})$ , the marginal probability of index  $i$  being sampled into  $S$  is equal to the  $i$ th 1-ridge leverage score of  $\mathbf{L}$ , and the expected size  $k$  of  $S$  is equal to the 1-effective dimension:

$$\Pr(i \in S) = [\mathbf{L}(\mathbf{I} + \mathbf{L})^{-1}]_{ii} = \tau_i(1), \quad k \triangleq \mathbb{E}[|S|] = \text{tr}(\mathbf{L}(\mathbf{I} + \mathbf{L})^{-1}) = d_{\text{eff}}(1).$$

Intuitively, if the marginal probability of  $i$  is high, then this index should likely make it into the intermediate sample  $\sigma$ . This suggests that i.i.d. sampling of the indices  $\sigma_1, \dots, \sigma_t$  proportionally to 1-ridge leverage scores, i.e.  $\Pr(\sigma_1 = i) \propto \tau_i(1)$ , should serve as a reasonable and cheap heuristic for constructing  $\sigma$ . In fact, we can show that this distribution can be easily corrected by rejection sampling to become the R-DPP that we need. Computing ridge leverage scores exactly costs  $\mathcal{O}(n^3)$ , so instead we compute them approximately by first constructing a Nyström approximation of  $\mathbf{L}$ .

**Definition 2** Let  $\mathbf{L}$  be a psd matrix and  $C$  a subset of its row/column indices with size  $m \triangleq |C|$ . Then we define the Nyström approximation of  $\mathbf{L}$  based on  $C$  as the  $n \times n$  matrix  $\hat{\mathbf{L}} \triangleq (\mathbf{L}_{C,\mathcal{I}})^\top \mathbf{L}_C^+ \mathbf{L}_{C,\mathcal{I}}$ .

Here,  $\mathbf{L}_{C,\mathcal{I}}$  denotes an  $m \times n$  matrix consisting of (entire) rows of  $\mathbf{L}$  indexed by  $C$  and  $(\cdot)^+$  denotes the Moore-Penrose pseudoinverse. Since we use rejection sampling to achieve the right intermediate distribution, the correctness of our algorithm does not depend on which Nyström approximation is chosen. However, the subset  $C$  greatly influences the

computational cost of the sampling through the rank of  $\widehat{\mathbf{L}}$  and the probability of rejecting a sample. Since  $\text{rank}(\widehat{\mathbf{L}}) = |C|$ , operations such as multiplication and inversion involving the Nyström approximation will scale with  $m$ , and therefore a small subset increases efficiency. However, if  $\widehat{\mathbf{L}}$  is too different from  $\mathbf{L}$ , the probability of rejecting the sample will be very high and the algorithm inefficient. In this case, a slightly larger subset could improve accuracy and acceptance rate without increasing too much the cost of handling  $\widehat{\mathbf{L}}$ . Therefore, subset  $C$  has to be selected so that it is both small and accurately represents the matrix  $\mathbf{L}$ . Here, we once again rely on ridge leverage score sampling which has been effectively used for obtaining good Nyström approximations in a number of prior works such as [AM15, CLV17, RCCR18].

While our main algorithm can sample only from the *random-size* DPP, and not from the *fixed-size  $k$ -DPP*, we present a rigorous reduction argument which lets us use our DPP algorithm to sample exactly from a  $k$ -DPP (for any  $k$ ) with a small computational overhead.

**Related work** Prior to our work, fast exact sampling from generic DPPs has been considered out of reach. The first procedure to sample general DPPs was given by [HKP<sup>+</sup>06] and even most recent exact refinements [LGD18, Der18, Pou19], when the DPP is represented in the form of an  $L$ -ensemble, require preprocessing that amounts to an expensive  $n \times n$  matrix diagonalization at the cost  $\mathcal{O}(n^3)$ , which is shown as the *first-sample* complexity column in Table 1.

Nonetheless, there are well-known samplers for very specific DPPs that are both fast and exact, for instance for sampling uniform spanning trees [Ald90, Bro89, PW98a], which leaves the possibility of a more generic fast sampler open. Since the sampling from DPPs has several practical large scale machine learning applications [KT12], there are now a number of methods known to be able to sample from a DPP *approximately*, outlined in the following paragraphs.

As DPPs can be specified by kernels ( $L$ -kernels or  $K$ -kernels), a natural approximation strategy is to resort to low-rank approximations [KT11, GKT12, AKFT13, LJS16a]. For example, [AKFT13] provides approximate guarantee for the probability of any subset being sampled as a function of eigengaps of the  $L$ -kernel. Next, [LJS16a] construct *coresets* approximating a given  $k$ -DPP and then use them for sampling. In their Section 4.1, [LJS16a] show in which cases we can hope for a good approximation. These guarantees become tight if these approximations (Nyström subspace, coresets) are aligned with data. In our work, we aim for an *adaptive* approach that is able to provide a good approximation for *any* DPP.

The second class of approaches are based on Markov chain Monte-Carlo [MU49] techniques [Kan13, RK15, AGR16, LJS16b, GBV17]. There are known polynomial bounds on the mixing rates [DS91] of MCMC chains with arbitrary DPPs as their limiting measure. In particular, [AGR16] showed them for cardinality-constrained DPPs and [LJS16b] for the general case. The two chains have mixing times which are, respectively, linear and quadratic in  $n$  (see Table 1). Unfortunately, for any subsequent sample we need to wait until the chain *mixes again*.

Neither the known low-rank approximations or the known MCMC methods are able to provide samples that are *exactly* distributed (also called *perfect sampling*) according to a DPP. This is not surprising as having *scalable and exact* sampling is very challenging in general. For example, methods based on rejection sampling are *always exact*, but they typically do not scale with the dimension and are adversely affected by the spikes in the

distribution [EVCM16], resulting in high rejection rate and inefficiency. Surprisingly, our method is based on both low-rank approximation (a source of inaccuracy) and rejection sampling (a common source of inefficiency). In the following section, we show how to obtain a *perfect DPP sampler* from a Nyström approximation of the  $L$ -kernel. Then, to guarantee efficiency, in Section 3 we bound the number of rejections, which is possible thanks to the use of intermediate downsampling.

## 2 Exact sampling using any Nyström approximation

**Notation** We use  $[n]$  to denote the set  $\{1, \dots, n\}$ . For a matrix  $\mathbf{B} \in \mathbb{R}^{n \times m}$  and index sets  $C, D$ , we use  $\mathbf{B}_{C,D}$  to denote the submatrix of  $\mathbf{B}$  consisting of the intersection of rows indexed by  $C$  with columns indexed by  $D$ . If  $C = D$ , we use a shorthand  $\mathbf{B}_C$  and if  $D = [m]$ , we may write  $\mathbf{B}_{C,\mathcal{I}}$ . Finally, we also allow  $C, D$  to be multisets (or sequences), in which case each entry is rescaled by the multiplicities of its row and column indices as follows: the entry at the intersection of the  $i$ th row with the  $j$ th column becomes  $\sqrt{n_i m_j} \cdot B_{ij}$ , where  $n_i$  is the multiplicity of  $i$  in  $C$  and  $m_j$  is the multiplicity of  $j$  in  $D$ . Such a rescaling has the property that if  $\mathbf{L} = \mathbf{B}\mathbf{B}^\top$  then  $\mathbf{L}_{C,D} = \mathbf{B}_{C,\mathcal{I}}\mathbf{B}_{D,\mathcal{I}}^\top$ .

As discussed in the introduction, our method relies on an intermediate downsampling distribution to reduce the size of the problem. The exactness of our sampler relies on the careful choice of that intermediate distribution. To that end, we use regularized determinantal processes, introduced by [Der18]. In the below definition, we adapt them to the kernel setting.

**Definition 3** Given an  $n \times n$  psd matrix  $\mathbf{L}$ , distribution  $p \triangleq (p_1, \dots, p_n)$  and  $r > 0$ , let  $\tilde{\mathbf{L}}$  denote an  $n \times n$  matrix such that  $\tilde{L}_{ij} \triangleq \frac{1}{r\sqrt{p_i p_j}} L_{ij}$  for all  $i, j \in [n]$ . We define  $\text{R-DPP}_p^r(\mathbf{L})$  as a distribution over events  $A \subseteq \bigcup_{k=0}^{\infty} [n]^k$ , where

$$\Pr(A) = \frac{\mathbb{E}_\sigma [\mathbf{1}_{[\sigma \in A]} \det(\mathbf{I} + \tilde{\mathbf{L}}_\sigma)]}{\det(\mathbf{I} + \mathbf{L})}, \quad \text{for } \sigma = (\sigma_1, \dots, \sigma_t) \stackrel{\text{i.i.d.}}{\sim} p, \quad t \sim \text{Poisson}(r).$$

Since the term  $\det(\mathbf{I} + \tilde{\mathbf{L}}_\sigma)$  has the same form as the normalization constant of  $\text{DPP}(\tilde{\mathbf{L}}_\sigma)$ , an easy calculation shows that the R-DPP can be used as an intermediate distribution in our algorithm without introducing any distortion in the sampling.

**Proposition 1 (Der18, Theorem 8)** For any  $\mathbf{L}$ ,  $p$ ,  $r$  and  $\tilde{\mathbf{L}}$  defined as in Definition 3,

$$\text{if } \sigma \sim \text{R-DPP}_p^r(\mathbf{L}) \quad \text{and} \quad S \sim \text{DPP}(\tilde{\mathbf{L}}_\sigma) \quad \text{then} \quad \{\sigma_i : i \in S\} \sim \text{DPP}(\mathbf{L}).$$

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### Algorithm 1 DPP-VFX sampling $S \sim \text{DPP}(\mathbf{L})$

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**input:**

$\mathbf{L} \in \mathbb{R}^{n \times n}$ , its Nyström approximation  $\hat{\mathbf{L}}$ ,  $q > 0$   
 $l_i = [(\mathbf{L} - \hat{\mathbf{L}}) + \hat{\mathbf{L}}(\mathbf{I} + \hat{\mathbf{L}})^{-1}]_{ii} \approx \Pr(i \in S)$ ,  
 $s = \sum_i l_i$ ,  $z = \text{tr}(\hat{\mathbf{L}}(\mathbf{I} + \hat{\mathbf{L}})^{-1})$ ,  
 $\tilde{\mathbf{L}} = \frac{s}{q} \left[ \frac{1}{\sqrt{l_i l_j}} L_{ij} \right]_{ij}$

1: **repeat**

2:   sample  $t \sim \text{Poisson}(q e^{s/q})$

3:   sample  $\sigma_1, \dots, \sigma_t \stackrel{\text{i.i.d.}}{\sim} (\frac{l_1}{s}, \dots, \frac{l_n}{s})$ ,

4:   sample  $Acc \sim \text{Bernoulli}\left(\frac{e^z \det(\mathbf{I} + \tilde{\mathbf{L}}_\sigma)}{e^{ts/q} \det(\mathbf{I} + \tilde{\mathbf{L}})}\right)$

5:   **until**  $Acc = \text{true}$

6:   sample  $\tilde{S} \sim \text{DPP}(\tilde{\mathbf{L}}_\sigma)$

7:   **return**  $S = \{\sigma_i : i \in \tilde{S}\}$

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To sample from the R-DPP, DPP-VFX uses rejection sampling, where the proposal distribution is sampling i.i.d. proportionally to the approximate 1-ridge leverage scores  $l_i \approx \tau_i(1)$  (see Definition 1 and the following discussion), computed using any Nyström approximation  $\widehat{\mathbf{L}}$  of matrix  $\mathbf{L}$ . Apart from  $\widehat{\mathbf{L}}$ , the algorithm also requires an additional parameter  $q$ , which controls the size of the intermediate sample. Because of rejection sampling and Proposition 1, the correctness of the algorithm *does not depend* on the choice of  $\widehat{\mathbf{L}}$  and  $q$ , as demonstrated in the following result. The key part of the proof involves showing that the acceptance probability in Line 4 is bounded by 1. Here, we obtain a considerably tighter bound than the one achieved by [Der18], which allows us to use a much smaller intermediate sample  $\sigma$  (see Section 3) while maintaining the efficiency of rejection sampling.

**Theorem 2** *Given a psd matrix  $\mathbf{L}$ , any one of its Nyström approximations  $\widehat{\mathbf{L}}$  and any positive  $q$ , DPP-VFX returns  $S \sim \text{DPP}(\mathbf{L})$ .*

**Proof** We start by showing that the Bernoulli probability in Line 4 is bounded by 1. Note that this is important not only to sample correctly, but also when we later establish the efficiency of the algorithm. If we showed a weaker upper bound, say  $c > 1$ , we could always divide the expression by  $c$  and retain the correctness, however it would also be  $c$  times less likely that  $\text{Acc} = 1$ .

Since  $\widehat{\mathbf{L}}$  is a Nyström approximation for some  $C \subseteq \mathcal{I}$ , it can be written as

$$\widehat{\mathbf{L}} = \mathbf{L}_{\mathcal{I},C} \mathbf{L}_C^+ \mathbf{L}_{C,\mathcal{I}} = \mathbf{B} \mathbf{B}_{C,\mathcal{I}}^\top \mathbf{L}_C^+ \mathbf{B}_{C,\mathcal{I}} \mathbf{B}^\top = \mathbf{B} \mathbf{P} \mathbf{B}^\top,$$

for any  $\mathbf{B}$  such that  $\mathbf{L} = \mathbf{B} \mathbf{B}^\top$ , where  $\mathbf{P} \triangleq \mathbf{B}_{C,\mathcal{I}}^\top \mathbf{L}_C^+ \mathbf{B}_{C,\mathcal{I}}$  is a projection (so that  $\mathbf{P}^2 = \mathbf{P}$ ). Let  $\widetilde{\mathbf{L}} \triangleq \widetilde{\mathbf{B}} \widetilde{\mathbf{B}}^\top$ , where the  $i$ th row of  $\widetilde{\mathbf{B}}$  is the rescaled  $i$ th row of  $\mathbf{B}$ , i.e.  $\widetilde{\mathbf{b}}_i^\top \triangleq \sqrt{\frac{s}{ql_i}} \mathbf{b}_i^\top$ . Then, we have

$$\begin{aligned} \frac{\det(\mathbf{I} + \widetilde{\mathbf{L}}_\sigma)}{\det(\mathbf{I} + \widehat{\mathbf{L}})} &= \frac{\det(\mathbf{I} + \widetilde{\mathbf{B}}_{\sigma,\mathcal{I}}^\top \widetilde{\mathbf{B}}_{\sigma,\mathcal{I}})}{\det(\mathbf{I} + \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})} = \det((\mathbf{I} + \widetilde{\mathbf{B}}_{\sigma,\mathcal{I}}^\top \widetilde{\mathbf{B}}_{\sigma,\mathcal{I}})(\mathbf{I} + \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})^{-1}) \\ &= \det(\mathbf{I} + (\widetilde{\mathbf{B}}_{\sigma,\mathcal{I}}^\top \widetilde{\mathbf{B}}_{\sigma,\mathcal{I}} - \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})(\mathbf{I} + \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})^{-1}) \\ &\leq \exp\left(\text{tr}\left((\widetilde{\mathbf{B}}_{\sigma,\mathcal{I}}^\top \widetilde{\mathbf{B}}_{\sigma,\mathcal{I}} - \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})(\mathbf{I} + \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})^{-1}\right)\right) \\ &= \exp\left(\sum_{i=1}^t \frac{s}{ql_{\sigma_i}} [\mathbf{B}(\mathbf{I} + \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})^{-1} \mathbf{B}^\top]_{\sigma_i \sigma_i}\right) \cdot e^{-z} = e^{ts/q} e^{-z}, \end{aligned}$$

where the last equality follows because

$$\begin{aligned} \mathbf{B}(\mathbf{I} + \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})^{-1} \mathbf{B}^\top &= \mathbf{B}(\mathbf{I} - \mathbf{P} \mathbf{B}^\top (\mathbf{I} + \mathbf{B} \mathbf{P} \mathbf{B}^\top)^{-1} \mathbf{B} \mathbf{P}) \mathbf{B}^\top \\ &= \mathbf{L} - \widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1} \widehat{\mathbf{L}} = \mathbf{L} - \widehat{\mathbf{L}} + \widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1}. \end{aligned}$$

Thus, we showed that the expression in Line 4 is valid. Let  $\widetilde{\sigma}$  denote the random variable distributed as  $\sigma$  is after exiting the repeat loop. It follows that

$$\begin{aligned} \Pr(\widetilde{\sigma} \in A) &\propto \mathbb{E}_\sigma \left[ \mathbf{1}_{[\sigma \in A]} \frac{e^z \det(\mathbf{I} + \widetilde{\mathbf{L}}_\sigma)}{e^{ts/q} \det(\mathbf{I} + \widehat{\mathbf{L}})} \right] \propto \sum_{t=0}^{\infty} \frac{(q e^{s/q})^t}{e^{q e^{s/q}} t!} \cdot e^{-ts/q} \mathbb{E}_\sigma [\mathbf{1}_{[\sigma \in A]} \det(\mathbf{I} + \widetilde{\mathbf{L}}_\sigma) \mid t] \\ &\propto \mathbb{E}_{t'} \left[ \mathbb{E}_\sigma [\mathbf{1}_{[\sigma \in A]} \det(\mathbf{I} + \widetilde{\mathbf{L}}_\sigma) \mid t = t'] \right] \quad \text{for } t' \sim \text{Poisson}(q), \end{aligned}$$

which shows that  $\tilde{\sigma} \sim \text{R-DPP}_l^q(\mathbf{L})$  for  $l = (\frac{l_1}{s}, \dots, \frac{l_n}{s})$ . The claim follows from Proposition 1.  $\blacksquare$

Even though the choice of  $\widehat{\mathbf{L}}$  affects the overall execution of the algorithm, it does not affect the output so we can reuse the same  $\widehat{\mathbf{L}}$  to produce multiple independent samples  $S_1, S_2, \dots \sim \text{DPP}(\mathbf{L})$  (proof in Appendix A).

**Lemma 1** *Let  $C \subseteq [n]$  be a random set variable with any distribution. Suppose that  $S_1$  and  $S_2$  are returned by two executions of DPP-VFX, both using inputs constructed from the same  $\mathbf{L}$  and  $\widehat{\mathbf{L}} = \mathbf{L}_{\mathcal{I},C} \mathbf{L}_C^+ \mathbf{L}_{C,\mathcal{I}}$ . Then  $S_1$  and  $S_2$  are (unconditionally) independent.*

### 3 Conditions for fast sampling

The complexity cost of DPP-VFX can be roughly summarized as follows: we pay a large one-time cost to precompute  $\widehat{\mathbf{L}}$  and all its associated quantities, and then we pay a smaller cost in the rejection sampling scheme which must be multiplied by the number of times we repeat the loop until acceptance. We first show that if the sum of the approximate RLS (i.e.,  $\sum_i l_i$ , denoted by  $s$ ) is sufficiently close to  $k$ , then we will exit the loop with high probability. We then analyze how accurate the precomputing step needs to be to satisfy this condition.

**Bounding the number of rejections.** The following result presents the two conditions needed for achieving efficient rejection sampling in DPP-VFX. First, the Nyström approximation needs to be accurate enough, and second, the intermediate sample size (controlled by parameter  $q$ ) needs to be  $\Omega(k^2)$ . This is a significant improvement over the guarantee of [Der18] where the intermediate sample size is  $\Omega(\text{rank}(\mathbf{L}) \cdot k)$ , which is only meaningful for low-rank kernels. The main novelty in this proof comes from showing the following lower bound on the ratio of the determinants of  $\mathbf{I} + \mathbf{L}$  and  $\mathbf{I} + \widehat{\mathbf{L}}$ , when  $\widehat{\mathbf{L}}$  is a Nyström approximation:  $\det(\mathbf{I} + \mathbf{L}) / \det(\mathbf{I} + \widehat{\mathbf{L}}) \geq e^{k-z}$ , where  $z \triangleq \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1})$ . Remarkably, this bound exploits the fact that any Nyström approximation of  $\mathbf{L} = \mathbf{B}\mathbf{B}^\top$  can be written as  $\widehat{\mathbf{L}} = \mathbf{B}\mathbf{P}\mathbf{B}^\top$ , where  $\mathbf{P}$  is a projection matrix. Note that while our result holds in the worst-case, in practice the conditions on  $\widehat{\mathbf{L}}$  and on  $q$  can be considerably relaxed.

**Theorem 3** *If the Nyström approximation  $\widehat{\mathbf{L}}$  and the intermediate sample size parameter  $q$  satisfy*

$$\text{tr}(\mathbf{L}(\mathbf{I} + \mathbf{L})^{-1} \mathbf{L} - \widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1} \widehat{\mathbf{L}}) \leq 1 \quad \text{and} \quad q \geq \max\{s^2, s\},$$

then  $\Pr(\text{Acc} = \text{true}) \geq e^{-2}$ . Therefore, with probability  $1 - \delta$  Algorithm 1 exits the rejection sampling loop after at most  $O(\log \delta^{-1})$  iterations and, after precomputing all of the inputs, the time complexity of the rejection sampling loop is  $O(k^6 \log \delta^{-1} + \log^4 \delta^{-1})$ .

**Proof** Let  $\sigma$  be distributed as in Line 3. The probability of exiting the repeat loop at each iteration is

$$\begin{aligned} P &\triangleq \mathbb{E}_\sigma \left[ \frac{e^z \det(\mathbf{I} + \widetilde{\mathbf{L}}_\sigma)}{e^{ts/q} \det(\mathbf{I} + \widehat{\mathbf{L}})} \right] = \sum_{t=0}^{\infty} \frac{(q e^{s/q})^t}{e^{q e^{s/q}} t!} \cdot \frac{e^{z-ts/q}}{\det(\mathbf{I} + \widehat{\mathbf{L}})} \mathbb{E}_\sigma [\det(\mathbf{I} + \widetilde{\mathbf{L}}_\sigma) \mid t] \\ &= \frac{e^{q-q e^{s/q}+z}}{\det(\mathbf{I} + \widehat{\mathbf{L}})} \sum_{t=0}^{\infty} \frac{q^t}{e^{qt!}} \mathbb{E}_\sigma [\det(\mathbf{I} + \widetilde{\mathbf{L}}_\sigma) \mid t] = e^{q-q e^{s/q}+z} \frac{\det(\mathbf{I} + \mathbf{L})}{\det(\mathbf{I} + \widehat{\mathbf{L}})}, \end{aligned}$$

where the last equality follows because the infinite series computes the normalization constant of  $\text{R-DPP}_l^q(\mathbf{L})$  given in Definition 3. If  $s \geq 1$  then  $q = s^2$  and the inequality  $e^x \leq 1 + x + x^2$  for  $x \in [0, 1]$  implies that  $q - qe^{s/q} + z = s^2(1 - e^{1/s} + 1/s) + z - s \geq -1 + z - s$ . On the other hand, if  $q = s \in [0, 1]$ , then  $q - qe^{s/q} + z = (1 - e)s + z \geq -1 + z - s$ . We proceed to lower bound the determinantal ratio. Here, let  $\mathbf{L} = \mathbf{B}\mathbf{B}^\top$  and  $\widehat{\mathbf{L}} = \mathbf{B}\mathbf{P}\mathbf{B}^\top$ , where  $\mathbf{P}$  is a projection matrix. Then,

$$\begin{aligned}
\frac{\det(\mathbf{I} + \mathbf{L})}{\det(\mathbf{I} + \widehat{\mathbf{L}})} &= \frac{\det(\mathbf{I} + \mathbf{B}^\top \mathbf{B})}{\det(\mathbf{I} + \mathbf{P}\mathbf{B}^\top \mathbf{B}\mathbf{P})} = \det(\mathbf{I} - (\mathbf{B}^\top \mathbf{B} - \mathbf{P}\mathbf{B}^\top \mathbf{B}\mathbf{P})(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1})^{-1} \\
&\geq \exp\left(\text{tr}\left((\mathbf{B}^\top \mathbf{B} - \mathbf{P}\mathbf{B}^\top \mathbf{B}\mathbf{P})(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1}\right)\right) \\
&= \exp\left(\text{tr}(\mathbf{B}(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1} \mathbf{B}^\top) - \text{tr}(\mathbf{B}\mathbf{P}(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1} \mathbf{P}\mathbf{B}^\top)\right) \\
&= \exp\left(k - \text{tr}(\mathbf{B}\mathbf{P}(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1} \mathbf{P}\mathbf{B}^\top)\right) \\
&= \exp\left(k - \text{tr}(\mathbf{B}\mathbf{P}(\mathbf{I} + \mathbf{B}^\top \mathbf{B} - \mathbf{B}^\top \mathbf{B})(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1} \mathbf{P}\mathbf{B}^\top)\right) \\
&= \exp\left(k - \text{tr}(\widehat{\mathbf{L}}) + \text{tr}(\mathbf{B}\mathbf{P}\mathbf{B}^\top \mathbf{B}(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1} \mathbf{P}\mathbf{B}^\top)\right) \\
&= \exp\left(k - \text{tr}(\widehat{\mathbf{L}}) + \text{tr}(\mathbf{B}\mathbf{P}\mathbf{B}^\top (\mathbf{I} + \mathbf{B}\mathbf{B}^\top)^{-1} \mathbf{B}\mathbf{P}\mathbf{B}^\top)\right) \\
&= \exp\left(k - \text{tr}(\widehat{\mathbf{L}}) + \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \mathbf{L})^{-1} \widehat{\mathbf{L}})\right) \\
&= \exp\left(k - \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1} (\mathbf{I} + \widehat{\mathbf{L}})) + \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \mathbf{L})^{-1} \widehat{\mathbf{L}})\right) \\
&= \exp\left(k - z - \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1} \widehat{\mathbf{L}}) + \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \mathbf{L})^{-1} \widehat{\mathbf{L}})\right),
\end{aligned}$$

where by definition  $k = \text{tr}(\mathbf{L}(\mathbf{I} + \mathbf{L})^{-1})$  and  $z = \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1})$ . Putting all together,

$$e^{q-qe^{s/q}+z} \frac{\det(\mathbf{I} + \mathbf{L})}{\det(\mathbf{I} + \widehat{\mathbf{L}})} \geq \exp\left(-1 + z - s + k - z - \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1} \widehat{\mathbf{L}}) + \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \mathbf{L})^{-1} \widehat{\mathbf{L}})\right).$$

Here, crucially, the two terms compensated for one another by eliminating  $z$  from the bound, which would otherwise be difficult to control. Rewriting

$$k - s = \text{tr}(\mathbf{L}(\mathbf{I} + \mathbf{L})^{-1} \mathbf{L}) - \text{tr}(\widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1} \widehat{\mathbf{L}}),$$

we obtain our condition. Thus, with probability  $1 - \delta$  the main loop will be repeated  $\mathcal{O}(\log \delta^{-1})$  times. Since the number of samples  $t_i$  drawn from  $l$  in the  $i$ th iteration of the loop is a Poisson distributed random variable, a standard Poisson tail bound implies that with probability  $1 - \delta$  all iterations will satisfy  $t_i = \mathcal{O}(k^2 + \log \delta^{-1})$ . Since the dominant cost is computing the determinant of the matrix  $\mathbf{I} + \widetilde{\mathbf{L}}_\sigma$  in time  $\mathcal{O}(t_i^3)$ , and the final step,  $\text{DPP}(\widetilde{\mathbf{L}}_\sigma)$ , requires its eigendecomposition (with the same time complexity), the result follows.  $\blacksquare$

**Bounding the precompute cost.** All that is left now is to control the cost of the precomputation phase. We will separate the analysis into two steps: how much it costs to choose  $\widehat{\mathbf{L}}$  to satisfy the condition  $s - k \leq 1$ , and how much it costs to compute everything else given  $\widehat{\mathbf{L}}$  (see Appendix A).



**Lemma 2** Let  $\widehat{\mathbf{L}}$  be constructed by sampling  $m = \mathcal{O}(k^3 \log \frac{n}{\delta})$  columns proportionally to their RLS. Then, with probability  $1 - \delta$ ,  $\widehat{\mathbf{L}}$  satisfies Theorem 3.

There exist many algorithms to sample columns proportionally to their RLS. For example, we can take the BLESS algorithm from [RCCR18] with the following guarantee.

**Proposition 2 (RCCR18, Theorem 1)** *There exists an algorithm that with probability  $1 - \delta$  samples  $m$  columns proportionally to their RLS in  $\mathcal{O}(nk^2 \log^2 \frac{n}{\delta} + k^3 \log^4 \frac{n}{\delta} + m)$  time.*

We can now compute the remaining preprocessing costs, given a Nyström approximation  $\widehat{\mathbf{L}}$ .

**Lemma 3** *Given  $\widehat{\mathbf{L}}$  with rank  $m$ , we can compute  $l_i, s, z$ , and  $\widetilde{\mathbf{L}}$  in  $\mathcal{O}(nm^2 + m^3)$  time.*

We are finally ready to combine these results to fully characterize the computational cost.

**Theorem 1 (restated for DPPs only)** *For a psd  $n \times n$  matrix  $\mathbf{L}$ , let  $S_1, S_2$  be i.i.d. random sets from  $\text{DPP}(\mathbf{L})$ . Denote with  $\widehat{\mathbf{L}}$  a Nyström approximation of  $\mathbf{L}$  obtained by sampling  $m = \mathcal{O}(k^3 \log(n/\delta))$  of its columns proportionally to their RLS. Then, with probability  $1 - \delta$ , DPP-VFX returns*

- a) subset  $S_1$  in:  $\mathcal{O}(nk^6 \log^2 \frac{n}{\delta} + k^9 \log^3 \frac{n}{\delta} + k^3 \log^4 \frac{n}{\delta})$  time,
- b) then,  $S_2$  in:  $\mathcal{O}(k^6 \log \frac{1}{\delta} + \log^4 \frac{1}{\delta})$  time.

**Discussion.** Due to the nature of rejection sampling, as long as we exit the loop, i.e., we accept the sample, the output of DPP-VFX is guaranteed to follow the DPP distribution for any value of  $m$ . In Theorem 1 we set  $m = (k^3 \log \frac{n}{\delta})$  to satisfy Theorem 3 and guarantee a constant acceptance probability in the rejection sampling loop, but this might not be necessary or even desirable in practice. Experimentally, much smaller values of  $m$ , starting from  $m = \Omega(k \log \frac{n}{\delta})$  seem to be sufficient to accept the sample, while at the same time a smaller  $m$  greatly reduces the preprocessing costs. In general, we recommend to separate DPP-VFX in three phases. First, compute an accurate estimate of the RLS using off-the-shelf algorithms in  $\mathcal{O}(nk^2 \log^2 \frac{n}{\delta} + k^3 \log^4 \frac{n}{\delta})$  time. Then, sample a small number  $m$  of columns to construct an explorative  $\widehat{\mathbf{L}}$ , and try to run DPP-VFX. If the rejection sampling loop does not terminate sufficiently fast, then we can reuse the RLS estimates to compute a more accurate  $\widehat{\mathbf{L}}$  for a larger  $m$ . Using a simple doubling schedule for  $m$ , this procedure will quickly reach a regime where DPP-VFX is guaranteed to accept w.h.p., maintaining its asymptotic complexity, while at the same time resulting in faster sampling in practice.

## 4 Reduction from DPPs to k-DPPs

We next show that with a simple extra rejection sampling step we can efficiently transform any exact DPP sampler into an exact  $k$ -DPP sampler.

A common heuristic to sample  $S$  from a  $k$ -DPP is to first sample  $S$  from a DPP, and then reject the sample if the size of  $S$  is not exactly  $k$ . The success probability of this procedure can be improved by appropriately rescaling  $\mathbf{L}$  by a constant factor  $\alpha$ ,

$$\text{sample } S_\alpha \sim \text{DPP}(\alpha \mathbf{L}), \quad \text{accept if } |S_\alpha| = k.$$

Note that rescaling the DPP by a constant  $\alpha$  only changes the expected size of the set  $S_\alpha$ , and not its distribution. Therefore, if we accept only sets with size  $k$ , we will be sampling

exactly from our  $k$ -DPP. Moreover, if  $k_\alpha = \mathbb{E}[|S_\alpha|]$  is close to  $k$ , the success probability will improve. With a slight abuse of notation, in the context of  $k$ -DPPs we will indicate with  $k$  the desired size of  $S_\alpha$ , i.e., the final output size at acceptance, and with  $k_\alpha = \mathbb{E}[|S_\alpha|]$  the expected size of the scaled DPP.

While this rejection sampling heuristic is widespread in the literature, until now there has been no proof that the process can be provably made efficient. We solve this open question with two new results. First we show that for an appropriate rescaling  $\alpha^*$  we only reject  $S_{\alpha^*}$  roughly  $O(\sqrt{k})$  times. Then, we show how we can find such an  $\alpha^*$  with a  $\tilde{O}(n \cdot \text{poly}(k))$  time preprocessing step.

**Theorem 4** *There exists constant  $C > 0$  such that for any rank  $n$  psd matrix  $\mathbf{L}$  and  $k \in [n]$ , there is  $\alpha^* > 0$  with the following property: if we sample  $S_{\alpha^*} \sim \text{DPP}(\alpha^* \mathbf{L})$ , then  $\Pr(|S_{\alpha^*}| = k) \geq \frac{1}{C\sqrt{k}}$ .*

The proof (see Appendix B) relies on a known Chernoff bound for the sample size  $|S_\alpha|$  of a DPP. When applied naïvely, the inequality does not offer a lower bound on the probability of any single sample size, however we can show that the probability mass is concentrated on  $O(\sqrt{k_\alpha})$  sizes. This leads to a lower bound on the sample size with the largest probability, i.e., the mode of the distribution. Then, it remains to observe that for any  $k \in [n]$  we can always find  $\alpha^*$  for which  $k$  is the mode of  $|S_{\alpha^*}|$ . We conclude that given  $\alpha^*$ , the rejection sampling scheme described above transforms any  $\text{poly}(k)$  time DPP sampler into a  $\text{poly}(k)$  time  $k$ -DPP sampler. It remains to find  $\alpha^*$  efficiently, which once again relies on using a Nyström approximation of  $\mathbf{L}$ .

**Lemma 4** *If  $k \geq 1$ , then there is an algorithm that finds  $\alpha^*$  in  $\tilde{O}(n \cdot \text{poly}(k))$  time.*

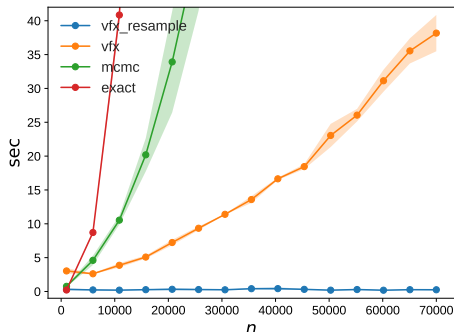


Figure 1: *First-sample cost for DPP-VFX against other DPP samplers ( $n$  is data size).*

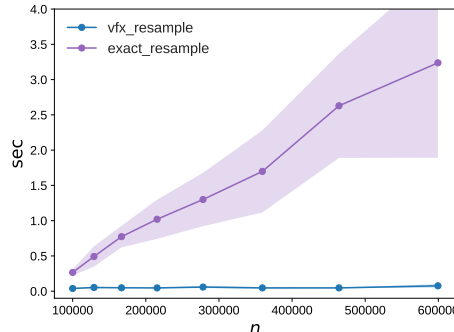


Figure 2: *Resampling cost for DPP-VFX compared to the exact sampler of [HKP<sup>+</sup>06].*

## 5 Experiments

In this section, we experimentally evaluate the performance of DPP-VFX compared to exact sampling [HKP<sup>+</sup>06] and MCMC-based approaches [AGR16]. In particular, since Section 2 proves that DPP-VFX samples exactly from the DPP, we are interested in evaluating computational performance. This will be characterized by showing how DPP-VFX and

baselines scale with the size  $n$  of the matrix  $\mathbf{L}$  when taking a first sample, and how DPP-VFX achieves constant time when resampling.

To construct  $\mathbf{L}$ , we use random subsets of the infinite MNIST digits dataset [LCB07], where  $n$  varies up to  $10^6$  and  $d = 784$ . We use an RBF kernel with  $\sigma = \sqrt{3d}$  to construct  $\mathbf{L}$ . All algorithms are implemented in `python`. For exact and MCMC sampling we used the DPPy library, [GBV18], while for DPP-VFX we reimplemented BLESS [RCCR18], and used DPPy to perform exact sampling on the intermediate subset. All experiments are carried out on a 24-core CPU and fully take advantage of potential parallelization. For the Nyström approximation we set  $m = 10d_{\text{eff}}(1) \approx 10k$ . While this is much lower than the  $\mathcal{O}(k^3)$  value suggested by the theory, as we will see it is already accurate enough to result in drastic runtime improvements over exact and MCMC. For each algorithm we control<sup>2</sup> the size of the output set by rescaling the input matrix  $\mathbf{L}$  by a constant, following the strategy of Section 4. In Figure 1 we report our results, means and 95% confidence interval over 10 runs, for subsets of MNIST that go from  $n = 10^3$  to  $n = 7 \cdot 10^4$ , i.e., the whole original MNIST dataset.

Exact sampling is clearly cubic in  $n$ , and we cannot push our sampling beyond  $n = 1.5 \cdot 10^4$ . For MCMC, we enforce mixing by running the chain for  $nk$  steps, the minimum recommended by [AGR16]. However, for  $n = 7 \cdot 10^5$  the MCMC runtime is 358 seconds and cannot be included in the plot, while DPP-VFX completes in 38 seconds, an order of magnitude faster. Moreover, DPP-VFX rarely rejects more than 10 times, and the mode of the rejections up to  $n = 7 \cdot 10^5$  is 1, that is we mostly accept at the first iteration. Figure 2 reports the cost of the second sample, i.e., of resampling. For exact sampling, this means that an eigendecomposition of  $\mathbf{L}$  is already available, but as the plot shows the resampling process still scales with  $n$ . On the other hand, DPP-VFX’s complexity (after preprocessing) scales only with  $k$  and remains constant regardless of  $n$ .

Finally, we scaled DPP-VFX to  $n = 10^6$  points, a regime where neither exact nor MCMC approaches are feasible. We report runtime and average rejections, with mean and 95% confidence interval over 5 runs. DPP-VFX draws its first sample in  $68.479 \pm 2.63$  seconds, with only  $9 \pm 4.5$  rejections.

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<sup>2</sup>For simplicity we do not perform the full  $k$ -DPP rejection step, but only adjust the expected size of the set.

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## A Omitted proofs for the main algorithm

In this section we present the proofs omitted from Sections 2 and 3, which regarded the correctness and efficiency of DPP-VFX. We start by showing that multiple samples drawn using the same Nyström approximation are independent.

**Lemma 5 (restated Lemma 1)** *Let  $C \subseteq [n]$  be a random set variable with any distribution. Suppose that  $S_1$  and  $S_2$  are returned by two executions of DPP-VFX, both using inputs constructed from the same  $\mathbf{L}$  and  $\widehat{\mathbf{L}} = \mathbf{L}_{\mathcal{I},C} \mathbf{L}_C^+ \mathbf{L}_{C,\mathcal{I}}$ . Then  $S_1$  and  $S_2$  are (unconditionally) independent.*

**Proof** Let  $A$  and  $B$  be two subsets of  $[n]$  representing elementary events for  $S_1$  and  $C$ , respectively. Theorem 2 implies that

$$\Pr(S_1 = A \mid C = B) = \frac{\det(\mathbf{L}_A)}{\det(\mathbf{I} + \mathbf{L})} = \Pr(S_1 = A).$$

Now, for any  $A_1, A_2 \subseteq [n]$  representing elementary events for  $S_1$  and  $S_2$  we have that

$$\begin{aligned} \Pr(S_1 = A_1 \wedge S_2 = A_2) &= \sum_{B \in [n]} \Pr(S_1 = A_1 \wedge S_2 = A_2 \mid C = B) \Pr(C = B) \\ &= \sum_{B \in [n]} \Pr(S_1 = A_1 \mid C = B) \Pr(S_2 = A_2 \mid C = B) \Pr(C = B) \\ &= \Pr(S_1 = A_1) \Pr(S_2 = A_2) \sum_{B \in [n]} \Pr(C = B). \end{aligned}$$

Since  $\sum_{B \in [n]} \Pr(C = B) = 1$ , we get that  $S_1$  and  $S_2$  are independent. ■

We now bound the precompute cost, starting with the construction of the Nyström approximation  $\widehat{\mathbf{L}}$ .

**Lemma 6 (restated Lemma 2)** *Let  $\widehat{\mathbf{L}}$  be constructed by sampling  $m = \mathcal{O}(k^3 \log \frac{n}{\delta})$  columns proportionally to their RLS. Then, with probability  $1 - \delta$ ,  $\widehat{\mathbf{L}}$  satisfies Theorem 3.*

**Proof** Let  $\mathbf{L} = \mathbf{B}\mathbf{B}^\top$  and  $\widehat{\mathbf{L}} = \mathbf{B}\mathbf{P}\mathbf{B}^\top$  (where  $\mathbf{P}$  is a projection matrix). Using algebraic manipulation, we can write

$$s = \text{tr}(\mathbf{L} - \widehat{\mathbf{L}} + \widehat{\mathbf{L}}(\mathbf{I} + \widehat{\mathbf{L}})^{-1}) = \text{tr}(\mathbf{B}(\mathbf{P}\mathbf{B}^\top\mathbf{B}\mathbf{P} + \mathbf{I})^{-1}\mathbf{B}).$$

The  $\mathbf{P}\mathbf{B}^\top\mathbf{B}\mathbf{P}$  matrix in the above expression been recently analyzed by [CCL<sup>+</sup>19] in the context of RLS sampling who gave the following result that we use in the proof.

**Proposition 3 (CCL<sup>+</sup>19, Lemma 6)** *Let the projection matrix  $\mathbf{P}$  be constructed by sampling  $\mathcal{O}(k \log(\frac{n}{\delta})/\varepsilon^2)$  columns proportionally to their RLS. Then,*

$$(1 - \varepsilon)(\mathbf{B}^\top\mathbf{B} + \mathbf{I}) \preceq \mathbf{P}\mathbf{B}^\top\mathbf{B}\mathbf{P} + \mathbf{I} \preceq (1 + \varepsilon)(\mathbf{B}^\top\mathbf{B} + \mathbf{I}).$$

We will decompose the condition in two parts. First we bound  $k - s \leq 1/2$ , and then bound  $z - \text{tr}(\mathbf{B}(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1} \mathbf{P} \mathbf{B}^\top) \leq 1/2$  (see the proof of Theorem 3 for more details). It is easy to see that applying the construction from Proposition 3 leads to the following bound on  $s$ ,

$$s = \text{tr}(\mathbf{B}(\mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P} + \mathbf{I})^{-1} \mathbf{B}) \leq \frac{1}{1 - \varepsilon} \text{tr}(\mathbf{B}(\mathbf{B}^\top \mathbf{B} + \mathbf{I})^{-1} \mathbf{B}) = \frac{1}{1 - \varepsilon} k = k + \frac{\varepsilon}{1 - \varepsilon} k.$$

Tuning  $\varepsilon = 1/(2k + 2)$  we obtain  $s \leq k + 1/2$  and reordering gives us the desired accuracy result. Similarly, we can invert the bound of Proposition 3 to obtain

$$(\mathbf{B}^\top \mathbf{B} + \mathbf{I})^{-1} \preceq (1 + \varepsilon)(\mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P} + \mathbf{I})^{-1}$$

and therefore

$$\text{tr}(\mathbf{B}(\mathbf{I} + \mathbf{B}^\top \mathbf{B})^{-1} \mathbf{P} \mathbf{B}^\top) \leq (1 + \varepsilon) \text{tr}(\mathbf{B}(\mathbf{I} + \mathbf{P} \mathbf{B}^\top \mathbf{B} \mathbf{P})^{-1} \mathbf{P} \mathbf{B}^\top) = (1 + \varepsilon) z \leq (1 + \varepsilon) k,$$

where the last inequality is due to the fact that  $\widehat{\mathbf{L}} \preceq \mathbf{L}$  since it is a Nyström approximation and that the operator  $\text{tr}(\mathbf{L}(\mathbf{L} + \mathbf{I})^{-1})$  is monotone. With the same  $\varepsilon$  as before, we obtain the bound. Summing the two  $1/2$  bounds gives us the result.  $\blacksquare$

Finally, we show how to compute the remaining quantities needed for DPP-VFX (Algorithm 1).

**Lemma 7 (restated Lemma 3)** *Given  $\mathbf{L}$  and an arbitrary Nyström approximation  $\widehat{\mathbf{L}}$  of rank  $m$ , computing  $l_i$ ,  $s$ ,  $z$ , and  $\widehat{\mathbf{L}}$  requires  $\mathcal{O}(nm^2 + m^3)$  time.*

**Proof** Given the Nyström set  $C$ , let us define the matrix  $\overline{\mathbf{B}} \triangleq \mathbf{L}_{\mathcal{I}, C} \mathbf{L}_C^{+1/2} \in \mathbb{R}^{n \times m}$  such that  $\widehat{\mathbf{L}} = \overline{\mathbf{B}} \overline{\mathbf{B}}^\top$ . We also introduce  $\widehat{\mathbf{L}}_m \triangleq \overline{\mathbf{B}}^\top \overline{\mathbf{B}}$  to act as a  $\mathbb{R}^{m \times m}$  counterpart to  $\widehat{\mathbf{L}}$ . Denote with  $\mathbf{e}_i$  the  $i$ -th indicator vector. Then, exploiting the fact that  $\overline{\mathbf{B}} \overline{\mathbf{B}}^\top (\mathbf{I} + \overline{\mathbf{B}} \overline{\mathbf{B}}^\top)^{-1} = \overline{\mathbf{B}} (\mathbf{I} + \widehat{\mathbf{L}}_m)^{-1} \overline{\mathbf{B}}^\top$  for any matrix, we can compute  $l_i$  as

$$l_i = [\mathbf{L} - \widehat{\mathbf{L}} + \overline{\mathbf{B}} \overline{\mathbf{B}}^\top (\mathbf{I} + \overline{\mathbf{B}} \overline{\mathbf{B}}^\top)^{-1}]_{ii} = [\mathbf{L} - \widehat{\mathbf{L}}]_{ii} + \|(\mathbf{I} + \widehat{\mathbf{L}}_m)^{-1/2} \overline{\mathbf{B}}^\top \mathbf{e}_i\|_2^2.$$

Computationally, this means that we first need to compute  $\overline{\mathbf{B}}$ , which takes  $\mathcal{O}(m^3)$  time to compute  $\mathbf{L}_{C, C}^{+1/2}$ , and  $\mathcal{O}(nm^2)$  time for the matrix multiplication. Then,  $[\widehat{\mathbf{L}}]_{ii}$  is the  $\ell_2$  norm of the  $i$ -th row of  $\overline{\mathbf{B}}$  which can be computed in  $nm$  time. Similarly,  $\|(\mathbf{I} + \widehat{\mathbf{L}}_m)^{-1/2} \overline{\mathbf{B}}^\top \mathbf{e}_i\|_2^2$  requires  $\mathcal{O}(m^3 + nm^2)$  time. To compute  $s$ , we simply sum  $l_i$ , while to compute  $z$  we first compute the eigenvalues of  $\widehat{\mathbf{L}}_m$ ,  $a_i = \lambda(\widehat{\mathbf{L}}_m)_i$ , in  $\mathcal{O}(m^3)$  time, and then compute  $z = \sum_i a_i / (a_i + 1)$ . We can also recycle the eigenvalues to precompute  $\log \det(\mathbf{I} + \widehat{\mathbf{L}}) = \log \det(\mathbf{I} + \widehat{\mathbf{L}}_m) = \sum_i \log(a_i + 1)$ .  $\blacksquare$

## B Omitted proofs for the reduction to k-DPPs

In this section we present the proofs omitted from Section 4. Recall that our approach is based on the following rejection sampling strategy:

$$\text{sample } S_\alpha \sim \text{DPP}(\alpha \mathbf{L}), \quad \text{accept if } |S_\alpha| = k.$$

First, we show the existence of the factor  $\alpha^*$  for which the rejection sampling is efficient.



**Theorem 5 (restated Theorem 4)** *There exists constant  $C > 0$  such that for any rank  $n$  PSD matrix  $\mathbf{L}$  and  $k \in [n]$ , there is  $\alpha^* > 0$  with the following property: if we sample  $S_{\alpha^*} \sim \text{DPP}(\alpha^* \mathbf{L})$ , then*

$$\Pr(|S_{\alpha^*}| = k) \geq \frac{1}{C\sqrt{k}}. \quad (1)$$

**Proof** W.l.o.g. assume that  $\mathbf{L}$  is non-zero, and remember  $S_\alpha \sim \text{DPP}(\alpha \mathbf{L})$  with  $k_\alpha = \mathbb{E}[|S_\alpha|]$ . At a high level, the proof proceeds as follows. We first prove that the probability that the size of the subset  $|S_\alpha|$  is equal to its *mode*  $M_\alpha$ , i.e.,  $\Pr(|S_\alpha| = M_\alpha)$  is large enough. Then we show that varying  $\alpha$  can make  $M_\alpha = k$  for any  $k$ , and therefore we can find an  $\alpha^*$  s.t.  $\Pr(|S_{\alpha^*}| = M_{\alpha^*}) = \Pr(|S_{\alpha^*}| = k)$  is large enough. In other words, rescaling  $\text{DPP}(\alpha \mathbf{L})$  to make sure that its mean  $k_\alpha$  is close to  $k$  is sufficient to guarantee that  $|S_\alpha| = k$  with high enough probability.

Our starting point is a standard Chernoff bound for  $|S_\alpha|$ .

**Proposition 4 (PP14)** *Given any PSD matrix  $\mathbf{L}$ , if  $S_\alpha \sim \text{DPP}(\alpha \mathbf{L})$ , then for any  $a > 0$ , we have*

$$\Pr\left(\left||S_\alpha| - \mathbb{E}[|S_\alpha|]\right| \geq a\right) \leq 5 \exp\left(-\frac{a^2}{16(a + 2\mathbb{E}[|S_\alpha|])}\right).$$

Note that Proposition 4 is not sufficiently strong by itself, i.e., if we tried to bound the distance  $||S_\alpha| - \mathbb{E}[|S_\alpha|]|$  to be smaller than 1 we would get vacuous bounds. However, Proposition 4 implies that there is a constant  $C > 0$  independent of  $\mathbf{L}$  such that  $\Pr(|S_\alpha| - k_\alpha| \geq C\sqrt{k_\alpha} + 1) \leq \frac{1}{2}$  for all  $\alpha > 0$ . In particular, this means that the mode of  $|S_\alpha|$ , i.e.  $M_\alpha = \arg\max_i \Pr(|S_\alpha| = i)$  satisfies

$$\Pr(|S_\alpha| = M_\alpha) \geq \frac{1}{2C\sqrt{k_\alpha}} \sum_{i=-\lceil C\sqrt{k_\alpha} \rceil}^{\lceil C\sqrt{k_\alpha} \rceil} \Pr(|S_\alpha| = k_\alpha + i) \geq \frac{1}{4C\sqrt{k_\alpha}}. \quad (2)$$

The distribution of  $|S_\alpha|$  is given by  $\Pr(|S_\alpha| = i) \propto e_i(\alpha \mathbf{L})$ , where  $e_i(\cdot)$  is the  $i$ th elementary symmetric polynomial of the eigenvalues of a matrix. Denoting  $\lambda_1, \dots, \lambda_n$  as the eigenvalues of  $\mathbf{L}$ , we can express the elementary symmetric polynomials as the coefficients of the following univariate polynomial with real non-positive roots,

$$\prod_{i=1}^n (x + \alpha \lambda_i) = \sum_{k=0}^n x^k e_{n-k}(\alpha \mathbf{L}).$$

The non-negative coefficients of such a real-rooted polynomial form a unimodal sequence (Lemma 1.1 in [Bra14]), i.e.,  $e_0(\alpha \mathbf{L}) \leq \dots \leq e_{M_\alpha}(\alpha \mathbf{L}) \geq \dots \geq e_n(\alpha \mathbf{L})$ , with the mode (shared between no more than two positions  $k, k+1$ ) being close to the mean  $k_\alpha$ :  $|M_\alpha - k_\alpha| \leq 1$  (Theorem 2.2 in [Bra14]). Moreover, it is easy to see that  $M_0 = 0$  and  $M_\alpha = n$  for large enough  $\alpha$ , so since the sequence is continuous w.r.t.  $\alpha$ , for every  $k \in [n]$  there is an  $\alpha^*$  such that  $\Pr(|S_{\alpha^*}| = k) = \Pr(|S_{\alpha^*}| = M_{\alpha^*})$  (every  $k$  can become one of the modes). In light of (2), this means that

$$\Pr(|S_{\alpha^*}| = k) \geq \frac{1}{4C\sqrt{k_{\alpha^*}}} \geq \frac{1}{4C\sqrt{k+1}},$$

where the last inequality holds because  $|k - k_{\alpha^*}| \leq 1$ . ■

Finally, we show how to find  $\alpha^*$  efficiently.

**Lemma 8** *If  $k \geq 1$  there is an algorithm that finds  $\alpha^*$  in  $\mathcal{O}(n \cdot \text{poly}(k))$  time.*

**Proof** In order to leverage Theorem 4, we need to find an  $\alpha^*$  such that  $k = M_{\alpha^*}$ , that is such that the mode of  $\text{DPP}(\alpha^* \mathbf{L})$  is equal to  $k$ . Unfortunately simple unimodality is not sufficient to control  $M_{\alpha^*}$  when  $\alpha^*$  is perturbed, as it happens during an approximate optimization of  $\alpha$ . We will now characterize more in detail the distribution of  $|S_\alpha|$ .

In particular,  $|S_\alpha|$  can be defined as the sum of Bernoullis  $|S_\alpha| = \sum_{i=1}^n b_{\alpha,i}$  each distributed according to  $b_{\alpha,i} \sim \text{Bernoulli}(\lambda_i(\alpha \mathbf{L}) / (1 + \lambda_i(\alpha \mathbf{L})))$  [HKP<sup>+</sup>06]. The sum of independent but not identically distributed Bernoullis is a so-called Poisson binomial random variable [H<sup>+</sup>56]. More importantly, the following result holds for Poisson binomial random variable.

**Proposition 5 (D<sup>+</sup>64, Thm. 4)** *Given a Poisson binomial r.v.  $|S_\alpha|$  with mean  $k_\alpha$ , let  $k \triangleq \lfloor k_\alpha \rfloor$ . The mode  $M_\alpha$  is*

$$M_\alpha = \begin{cases} k & \text{if } k \leq k_\alpha < k + \frac{1}{k+2}, \\ k \text{ or } k+1 & \text{if } k + \frac{1}{k+2} \leq k_\alpha \leq k + 1 - \frac{1}{n-k+1}, \\ k+1 & \text{if } k + 1 - \frac{1}{n-k+1} < k_\alpha \leq k + 1. \end{cases}$$

Therefore it is sufficient to find any constant  $\alpha^*$  that places  $k_{\alpha^*}$  in the interval  $[k, k + \frac{1}{k+2})$ . Unfortunately, while the formula for  $k_\alpha = \sum_{i=1}^n \lambda_i(\mathbf{L}) / (1/\alpha + \lambda_i(\mathbf{L}))$  is a unimodal function of the eigenvalues of  $\mathbf{L}$  which is easy to optimize, the eigenvalues themselves are still very expensive to compute. For efficiency, we can optimize it instead on the eigenvalues of a Nyström approximation  $\widehat{\mathbf{L}}$ , but we have to be careful to control the error. In particular, remember that  $k_\alpha = \mathbb{E}[|S_\alpha|]$  when  $S \sim \text{DPP}(\alpha \mathbf{L})$ , so given a Nyström approximation  $\widehat{\mathbf{L}}$  we can define  $s_\alpha \triangleq \text{tr}(\alpha(\mathbf{L} - \widehat{\mathbf{L}}) + \widehat{\mathbf{L}}(\widehat{\mathbf{L}} + \mathbf{I}/\alpha)^{-1})$  as a quantity analogous to  $s$  from DPP-VFX. Then, we can strengthen Lemma 2 as follows.

**Lemma 9 (crf. Lemma 2)** *Let  $\widehat{\mathbf{L}}$  be constructed by sampling  $m = \mathcal{O}((k_\alpha/\varepsilon^2) \log(n/\delta))$  columns proportionally to their RLS. Then with probability  $1 - \delta$*

$$\frac{1}{1+\varepsilon} k_\alpha \leq s_\alpha \leq \frac{1}{1-\varepsilon} k_\alpha.$$

**Proof of Lemma 9** We simply apply the same reasoning of Lemma 2 on both sides. ■

Let  $(1 - \varepsilon)s_{\alpha^*} = k$ , with  $\varepsilon$  that will be tuned shortly. Then proving the first inequality to satisfy Proposition 5 is straightforward:  $k = (1 - \varepsilon)s_{\alpha^*} \leq k_{\alpha^*}$ . To satisfy the other side we upper bound  $k_{\alpha^*} \leq (1 + \varepsilon)s_{\alpha^*} = (1 - \varepsilon)s_{\alpha^*} + 2\varepsilon s_{\alpha^*}$ . We must now choose  $\varepsilon$  such that  $2\varepsilon s_{\alpha^*} = 1/(k+3) < 1/(k+2)$ . Substituting, we obtain  $\varepsilon = \frac{1}{2(k+3)s_{\alpha^*}}$ . Plugging this in the definition of  $s_{\alpha^*}$  we obtain that  $\alpha^*$  must be optimized to satisfy

$$s_{\alpha^*} = \frac{2k^2 + 6k + 1}{2k + 6},$$

which we plug in the definition of  $\varepsilon$  obtaining our necessary accuracy  $\varepsilon = 1/(2k^2 + 6k + 1)$ . Therefore, sampling  $m = \tilde{\mathcal{O}}(k_{\alpha^*} k^4)$  columns gives us a  $s_\alpha$  sufficiently accurate to be optimized. However, we still need to bound  $k_{\alpha^*}$ , which we can do as follows using Lemma 9 and  $k \geq 1$

$$\begin{aligned} k_{\alpha^*} &\leq \left(1 + \frac{1}{2k^2 + 6k + 1}\right) s_{\alpha^*} \leq \left(1 + \frac{1}{9}\right) s_{\alpha^*} = \frac{10}{9} s_{\alpha^*} \\ &\leq \frac{10}{9} \left(\frac{2k^2 + 6k + 1}{2k + 6}\right) = \frac{10}{9} \left(1 + \frac{1}{k(2k + 6)}\right) k = \frac{10}{9} \frac{9}{8} k = \frac{5}{4} k. \end{aligned}$$

Therefore  $m = \tilde{\mathcal{O}}(k_{\alpha^*} k^4) \leq \tilde{\mathcal{O}}(k^5)$  suffices accuracy wise. Moreover, since  $s_\alpha$  is parametrized only in terms of the eigenvalues of  $\hat{\mathbf{L}}$ , which can be found in  $\tilde{\mathcal{O}}(nm^2 + m^3)$  time, we can compute an  $\alpha^*$  such that  $s_{\alpha^*} = \frac{2k^2 + 6k + 1}{2k + 6}$  in  $\tilde{\mathcal{O}}(nk^{10} + k^{15})$  time, which guarantees  $k \leq k_{\alpha^*} < k + \frac{1}{k+2}$ .  $\blacksquare$

Finally, note that these bounds on the accuracy of  $\hat{\mathbf{L}}$  are extremely conservative. In practice, it is much faster to try to optimize  $\alpha^*$  on a much coarser  $\hat{\mathbf{L}}$  first, e.g., for  $m = \mathcal{O}(k_1)$ , and only if this approach fails to increase the accuracy of  $\hat{\mathbf{L}}$ .