Fast DPP Sampling for Nyström
with Application to Kernel Methods

Chengtao Li
ctli@mit.edu
Stefanie Jegelka
stefje@csail.mit.edu
Suvrit Sra
suvrit@mit.edu
Massachusetts Institute of Technology

Abstract

The Nyström method has long been popular for scaling up kernel methods. However, successful use of Nyström depends crucially on the selected landmarks. We consider landmark selection by using a Determinantal Point Process (DPP) to tractably select a diverse subset from the columns of an input kernel matrix. We prove that the landmarks selected using DPP sampling enjoy guaranteed error bounds; subsequently, we illustrate impact of DPP-sampled landmarks on kernel ridge regression. Moreover, we show how to efficiently sample from a DPP in linear time using a fast mixing (under certain constraints) Markov chain, which makes the overall procedure practical. Empirical results support our theoretical analysis: DPP-based landmark selection shows performance superior to existing approaches.

1 Introduction

An important ingredient in many machine learning methods is the low-rank approximation of matrices. Such approximations are attractive when the default method uses matrix operations quadratic or cubic in the number of input data points, clearly prohibitive for large-data. By working with low-rank approximations one can reduce running times by trading off accuracy for scalability.

A key example of this idea is the Nyström method [8, 31], which takes as input a positive semidefinite matrix \( K \in \mathbb{R}^{N \times N} \) and from it selects a small subset \( C \) of columns \( K_{\cdot C} \) to construct the approximation \( \tilde{K} = K_{\cdot C} K_{C \cdot}^+ K_{\cdot C} \) (\( X^+ \) denotes the Moore-Penrose Pseudoinverse of \( X \)). The matrix \( \tilde{K} \), in its factored form, is then used in place of \( K \). If the number \( |C| \) of selected columns is small, then using \( \tilde{K} \) can dramatically reduce runtimes from (cubic) \( O(N^3) \) to (linear) \( O(N |C|^3) \).

Consequently, the Nyström method has been used to scale up several kernel methods, for instance kernel ICA [6, 35], kernel and spectral methods in computer vision [9, 19], manifold learning [38, 39], regularization [34], and efficient approximate sampling [1]. Recent work [2, 5, 13] also studies risk bounds for Nyström applied to various kernel methods.

The most important step of the Nyström method is the selection of the subset \( C \) of columns, also called landmarks. The choice of landmarks governs the quality of approximation offered by Nyström and thus its subsequent impact on the learning task [13]. A basic choice is to pick landmarks uniformly at random [42]. Several more sophisticated selection strategies have also been proposed, including deterministic greedy schemes [36], incomplete Cholesky decomposition [7, 18], sampling with probabilities proportional to diagonal values [15], to column norms [16], based on leverage scores [20], via K-means [43], and using determinants [10].

In this paper, we study landmark selection using Determinantal Point Processes (DPP), discrete probability models that allow tractable sampling of diverse non-independent subsets [27, 30]. Our work (discovered independently) is related to determinantal sampling scheme of Belabbas and Wolfe [10]'s, but is more general. We refer to our sampling scheme as DPP-Nyström, and analyze it from various perspectives including efficient implementation.

\[ \text{Surprisingly, they do not make an explicit connection to DPPs.} \]
1.1 Overview

We analyze our DPP-Nyström’s performance using its approximation error. Suppose \( k \) is the target rank; then for selecting \( c \geq k \) landmarks, Nyström’s error is typically measured using the Frobenius or spectral norm, relative to the best achievable error via rank-\( k \) SVD \( K_k \). In other words, we measure the relative errors

\[
\frac{\| K - K_{c,C} K_{C,C}^T K_{C} \|_F}{\| K - K_k \|_F} \quad \text{or} \quad \frac{\| K - K_{c,C} K_{C,C}^T K_{C} \|_2}{\| K - K_k \|_2}. \tag{1.1}
\]

Several authors also use additive instead of relative bounds. However, such bounds are very sensitive to scaling, and become loose even if a single entry of the matrix is large. Thus, we focus on the relative error bounds (1.1).

In Section 3 we analyze this error for DPP-Nyström. Previous analysis [10] assumes cardinality \(|C| = k\) in Nyström; we go beyond this limitation and analyze the general case that permits using \(|C| \geq k\) columns, by exploiting properties of the characteristic polynomial of \( K \). Empirically DPP-Nyström is seen to obtain approximations superior to other state-of-art methods.

In Section 4 we consider the impact of DPP-Nyström on kernel methods by focusing on Nyström-based kernel approximations for kernel ridge regression (a task that is also a main application in [2, 5]). We show risk bounds of DPP-Nyström that hold in expectation. Empirically, DPP-Nyström is seen to again obtain the best performance among competing methods.

Section 5 considers the key question of computational efficiency of DPP-Nyström. In particular, we consider efficient realization of determinantal sampling: since its proposal in [10], determinantal sampling (also realized as \( k \)-DPP) has not yet been widely adopted due to concerns about its scalability. To that end, we address a Gibbs sampler for \( k \)-DPP, and analyze its mixing time using a path coupling [12] argument. We prove that under certain conditions the chain is fast mixing, which implies a linear running time for DPP sampling of landmarks. Empirical results (Section 6) indicate that the chain yields favorable results within a small number of iterations as well as the best efficiency-accuracy tradeoffs compared to state-of-art methods (Figure 6).

2 Background and Notation

Let \( K \in \mathbb{R}^{N \times N} \) be positive semidefinite (PSD) with the eigendecomposition \( K = U \Lambda U^T \) where the eigenvalues \( \{ \lambda_i \}_{i=1}^N \) are arranged decreasingly. We use \( K_{i,}\) for the \( i \)-th row and \( K_{j,} \) for the \( j \)-th column; likewise, \( K_{C,} \) denotes rows of \( K \) and \( K_{C,} \) the columns of \( K \) indexed by \( C \subseteq [N] := \{1, 2, \ldots, N\} \). Finally, \( K_{C,C} \) denotes the submatrix of \( K \) with rows and columns indexed by \( C \). In this notation, \( K_k = U_{\cdot,k} \Lambda U_{\cdot,k}^T U_{\cdot,k}^T \) is the best rank-\( k \) approximation to \( K \) in both Frobenius and spectral norm. We write \( r(\cdot) \) for the rank and \( (\cdot)^+ \) for the pseudoinverse, and denote the decomposition of \( K \) by \( B^T B \), where \( B \in \mathbb{R}^{r(k) \times N} \).

The Nyström Method. The standard Nyström method selects a subset \( C \subseteq [N] \) of \( c := |C| \) landmarks, and approximates \( K \) with \( K_{C,K_{C,C}K_{C}} \). The choice of landmarks affects the approximation quality, and has been the subject of a substantial body of research [7, 10, 13, 15, 16, 18, 20, 36, 43]. Besides various landmark selection methods, there exist variants of the standard Nyström method, such as the ensemble Nyström method [28] that uses a weighted combination of approximations and the modified Nyström method that constructs an approximation \( K_{C,K_{C,C}K_{C}} \) [37]. We consider only the standard Nyström method.
Determinantal Point Processes. A determinantal point process $\text{DPP}(K)$ is a distribution over all subsets of a ground set $\mathcal{Y}$ of cardinality $N$ that is determined by a PSD kernel $K \in \mathbb{R}^{N \times N}$. In particular, the probability of observing a subset $C \subseteq [N]$ is proportional to $\det(K_{C,C})$, so that

$$\Pr(C) = \frac{\det(K_{C,C})}{\det(K+I)}.$$  (2.1)

When conditioning on a fixed cardinality $|C| = c$, one obtains a $k$-$\text{DPP}$ [26]:

$$\Pr(C | |C| = c) = \det(K_{C,C})e_c(K)^{-1}1[|C| = c],$$

where $e_c(L)$ is the $c$-th coefficient of the characteristic polynomial $\det(\lambda I - L) = \sum_{i=0}^{N} (-1)^i e_i(L)\lambda^{N-i}$. Sampling from a $(k)$-$\text{DPP}$ can be done in polynomial time, but requires a full eigen-decomposition of $K$ [24], which is prohibitive for large $N$. A number of approaches have been proposed for more efficient sampling [1, 29, 41]. We follow an alternative approach based on Gibbs sampling and show that it can offer fast polynomial-time $\text{DPP}$ sampling under certain constraints.

## 3 DPP for the Nyström Method

In this section we consider sampling landmarks $C \subseteq [N]$ using a $k$-$\text{DPP}(K)$, resulting in the approximation $\hat{K} = K_{C,C}K_{C,C}^T K_{C,C}$. We refer to this procedure as $\text{DPP-Nyström}$, and note that it was essentially introduced by Belbachas and Wolfe [10], though without making an explicit connection to $\text{DPP}$s. Our analysis builds on this connection to $\text{DPP}$s and subsumes existing results which only apply to $|C| = c = k$ (recall that, $k$ is the rank of the target approximation).

In the remainder of this section, we prove the following main result.

**Theorem 1** (Relative Error). If $C \sim k$-$\text{DPP}(K)$, then $\text{DPP-Nyström}$ satisfies the relative errors bounds

$$\mathbb{E}_C \left[ \frac{\|K - K_{C}(KCC)^\dagger K_{C} \|_F}{\|K-K_k\|_F} \right] \leq \left( \frac{c+1}{c+1-k} \right) \sqrt{N-k},$$

$$\mathbb{E}_C \left[ \frac{\|K - K_{C}(KCC)^\dagger K_{C} \|_2}{\|K-K_k\|_2} \right] \leq \left( \frac{c+1}{c+1-k} \right) (N-k).$$

These bounds hold only in expectation; however, a short additional argument based on [32] yields bounds that hold with high probability.

**Corollary 2** (Relative Error w.h.p.). When sampling $C \sim k$-$\text{DPP}(K)$, for any $\delta \in (0,1)$, with probability at least $1 - \delta$ we have

$$\frac{\|K - K_{C}(KCC)^\dagger K_{C} \|_F}{\|K-K_k\|_F} \leq \left( \frac{c+1}{c+1-k} \right) \sqrt{N-k} + \sqrt{8c \log(1/\delta)} \frac{\lambda_1}{\sqrt{\sum_{i=k+1}^{N} \lambda_i}},$$

$$\frac{\|K - K_{C}(KCC)^\dagger K_{C} \|_2}{\|K-K_k\|_2} \leq \left( \frac{c+1}{c+1-k} \right) (N-k) + \sqrt{8c \log(1/\delta)} \frac{\lambda_1}{\lambda_k},$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$ are the eigenvalues of $K$.

We first prove Theorem 1. Our analysis exploits a property of characteristic polynomials observed in [23]. Recall that coefficients of the characteristic polynomial are sums over submatrix determinants, that is

$$e_k(K) = \sum_{|S|=k} \det(B_S^TB_S) = e_k(\Lambda).$$  (3.1)

The following lemma bounds a ratio of consecutive such coefficients.
Lemma 3 (Guruswami and Sinop [23]). Let \( K = U \Lambda U^T \). Then, for any \( c \geq k > 0 \), it holds that

\[
\frac{e_{c+1}(K)}{e_c(K)} \leq \frac{1}{c + 1 - k} \sum_{i > k} \lambda_i.
\]

With Lemma 3 in hand we are ready to prove Theorem 1.

Proof (Theorem 1). We begin with the Frobenius norm error, and then show the spectral norm result. Writing \( K = B^T B \), we see that

\[
\begin{align*}
\mathbb{E}_C \left[ \| K - K_c K^t C C \|_F \right] &= \mathbb{E}_C \left[ \| B^T B - B^T (B C (B^t C)^t B) \|_F \right] \\
&= \mathbb{E}_C \left[ \| B^T (I - B C (B^t C)^t B) \|_F \right] = \mathbb{E}_C \left[ \| B^T (I - U C U^t C) \|_F \right],
\end{align*}
\]

where \( U C \Sigma_C V_C^t \) is the SVD of \( B C \). Next, we extend \( U C \) to a full basis \( U = [U C \ U_C^t] \). Since \( U \) is orthonormal, we have \( U U^T = I \) and \( I - U C U^t C = U_C^t (U_C^t)^t \). Plugging in this identity and applying Cauchy-Schwarz yields

\[
\begin{align*}
\mathbb{E}_C \left[ \| B^T (I - U C U^t C) \|_F \right] &= \mathbb{E}_C \left[ \| B^T U_C^t (U_C^t)^t B \|_F \right] \\
&\leq \mathbb{E}_C \left[ \sum_{i,j} \| b_i^t C \|_2 \| b_j^t U_C^t C \|_2 \right] = \mathbb{E}_C \left[ \sum_i \| b_i^t C \|_2 \right] \\
&= \frac{1}{e_c(K)} \sum_{|C| = c} \mathbb{E}_C \left[ \sum_i \det(B_{C \cup \{i\}} B_{C \cup \{i\}}^t) \right] \\
&= (c + 1) e_{c+1}(K) e_c(K).
\end{align*}
\]

From identity (3.1) and Lemma 3 it follows that

\[
(c + 1) \frac{e_{c+1}(K)}{e_c(K)} \leq \frac{c+1}{c+1-k} \sum_{i > k} \lambda_i \leq \frac{c+1}{c+1-k} \sqrt{N-k} \sqrt{\sum_{i > k} \lambda_i^2} \\
= \frac{c+1}{c+1-k} \sqrt{N-k} \| K - K_k \|_F.
\]

The bound on the Frobenius norm immediately implies the bound on the spectral norm:

\[
\begin{align*}
\mathbb{E}_C \left[ \| K - K C (K C^t) K C \|_2 \right] &\leq \mathbb{E}_C \left[ \| K - K C K^t C \|_F \right] \\
&\leq \frac{c+1}{c+1-k} \sqrt{N-k} \| K - K_k \|_F \leq \frac{c+1}{c+1-k} (N-k) \| K - K_k \|_2.
\end{align*}
\]

To show high probability bounds we employ concentration results on homogeneous strongly Rayleigh measures. Specifically, we use the following theorem.

Theorem 4 (Pemantle and Peres [32]). Let \( P \) be a \( k \)-homogeneous strongly Rayleigh probability measure on \( \{0,1\}^N \) and \( f \) an \( \ell \)-Lipschitz function on \( \{0,1\}^N \), then

\[
P(f - \mathbb{E}[f] \geq a \ell) \leq \exp\{-a^2/8k\}.
\]

Proof (Corollary 2). It is known that a DPP is a strongly Rayleigh measure on \( \{0,1\}^N \). Since a k-DPP is its truncation to a probability measure on cardinality k subsets of \( \{0,1\}^N \), it is still strongly Rayleigh, and hence Theorem 4 applies. Corollary 2 follows since the Lipschitz constant for the relative error is \( \ell = \lambda_1/\lambda_{k+1} \) for the spectral norm, and \( \ell = \lambda_1/\sqrt{\sum_{i=k+1}^{N} \lambda_i} \) for the Frobenius norm. \( \square \)
Remarks. Our bounds are not directly comparable to previous bounds (e.g., [20] on uniform and leverage score sampling). However, in Sec. 6.1 we extensively experiment with DpN-Nyström on various datasets and observe superior accuracies against various existing state-of-the-art methods.

4 Low-rank Kernel Ridge Regression

The theoretical results in Section 3 suggest that DpN-Nyström may be suitable for scaling kernel learning methods. In this section, we analyze DpN-Nyström’s implications on kernel ridge regression. In Section 6 we present empirical results that DpN-Nyström is indeed very effective.

Suppose we have $N$ training samples $\{(x_i, y_i)\}_{i=1}^N$, where $y_i = z_i + \epsilon_i$ are the observed labels under zero-mean noise with finite covariance. We minimize a regularized empirical loss

$$\min_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^N \ell(y_i, f(x_i)) + \frac{\gamma}{2} \|f\|^2$$

over an RKHS $\mathcal{F}$; equivalently we solve

$$\min_{\alpha \in \mathbb{R}^N} \frac{1}{N} \sum_{i=1}^N \ell(y_i, (K\alpha)_i) + \frac{\gamma}{2} \alpha^T K \alpha,$$

using the corresponding kernel matrix $K$. Under the squared loss $\ell(y, f(x)) = \frac{1}{2} (y - f(x))^2$, we can minimize (4.1) to obtain the estimator

$$\hat{f}(x) = \sum_{i=1}^N \alpha_i k(x, x_i), \quad \alpha = (K + N\gamma I)^{-1} y.$$

Thus, we predict $\hat{y} = K(K + N\gamma I)^{-1} y$ for $\{x_i\}_{i=1}^N$. If $F$ is the noise covariance we obtain the risk

$$\mathcal{R}(\hat{y}) = \frac{1}{N} \mathbb{E}_x \|\hat{x} - x\|^2 = N\gamma^2 (K + N\gamma I)^{-2} + \frac{1}{N} \text{tr}(FK^2(K + N\gamma I)^{-2})$$

$$= \text{bias}(K) + \text{var}(K).$$

Observe that the bias term is matrix-decreasing (in $K$) while the variance term is matrix-increasing. Since the estimator (4.2) requires expensive matrix inversions, it is common to replace $K$ in (4.2) by an approximation $\hat{K}$. A $\hat{K}$ constructed via Nyström satisfies $\hat{K} \preceq K$, whereby the variance shrinks upon using $\hat{K}$ while the bias increases. Denoting the predictions corresponding to $\hat{K}$ by $\hat{y}_{\hat{K}}$, Theorem 5 completes the picture of how using $\hat{K}$ affects the risk.

Theorem 5. If $\hat{K}$ is constructed via DpN-Nyström and $\gamma \geq \frac{1}{N} \text{tr}(K)$, then

$$\mathbb{E}_C \left[ \sqrt{\frac{\mathcal{R}(\hat{y})}{\mathcal{R}(\hat{y}_{\hat{K}})}} \right] \geq 1 - \frac{(c + 1) \epsilon_{c+1}(K)}{N\gamma} \epsilon_c(K).$$

Proof. We build upon [5]. Knowing that $\text{Var}(\hat{K}) \preceq \text{Var}(K)$ as $\hat{K} \preceq K$, it remains to bound the bias. We write $K = B^T B$ and $\hat{K} = B^T B_C (B_C^T B_C)^{-1} B_C^T B$, and bound the difference $K - \hat{K}$ as

$$K - \hat{K} = B^T (I - B_C (B_C^T B_C)^{-1} B_C^T) B = B^T U_C^T (U_C^T)^T B$$

$$\leq \|B^T U_C^T (U_C^T)^T B\|_F I = \sqrt{\sum_{i,j} \|b_i^T U_C^T (U_C^T)^T b_j\|^2 I}$$

$$\leq \sqrt{\sum_{i,j} \|b_i^T U_C^T\|_2^2 \|b_j^T U_C^T\|_2^2} I = \sum_i \|b_i^T U_C^T\|_2^2 I = \nu_C I,$$
where \( v_C = \sum_i \| b_i^T U_{C,i} \|^2 \leq \sum_i \| b_i \|^2 = \text{tr}(K) \). By assumption \( \frac{1}{N} \text{tr}(K) < \gamma \), so that \( \frac{v_C}{N\gamma} < 1 \); thus

\[
(\hat{K} + N\gamma I)^{-1} \leq (K - v_C I + N\gamma I)^{-1} \leq (1 - \frac{v_C}{N\gamma})^{-1}(K + N\gamma I)^{-1}.
\]

Finally, this matrix inequality implies that

\[
\sqrt{\frac{\text{bias}(K)}{\text{bias}(\hat{K})}} \geq 1 - \frac{v_C}{N\gamma}.
\]

Taking expectation over \( C \sim k\text{-DrP}(K) \) yields

\[
\mathbb{E}_C \left[ \sqrt{\frac{\text{bias}(K)}{\text{bias}(\hat{K})}} \right] \geq 1 - \mathbb{E}_C \left[ \frac{v_C}{N\gamma} \right] = 1 - \frac{(c + 1) e_{c+1}(K)}{N\gamma e_c(K)}.
\]

Together with the fact that \( \text{var}(\hat{K}) \geq \text{var}(K) \), we obtain

\[
\mathbb{E}_C \left[ \sqrt{\frac{\mathcal{R}(\hat{z})}{\mathcal{R}(z_K)}} \right] = \mathbb{E}_C \left[ \sqrt{\frac{\text{bias}(K) + \text{var}(K)}{\text{bias}(\hat{K}) + \text{var}(\hat{K})}} \right] \\
\geq 1 - \frac{(c + 1) e_{c+1}(K)}{N\gamma e_c(K)} \\
\geq 1 - \frac{c + 1}{c + 1 - k} \frac{\sum_{i > k} \lambda_i}{\sum_{i} \lambda_i}, \tag{4.4}
\]

for any \( k \leq c \), where the last inequality follows from Lemma 3 and \( \gamma \geq \frac{1}{N} \text{tr}(K) \).

By employing Theorem 4 we obtain the following bounds that hold with high probability:

**Corollary 6.** If \( \hat{K} \) is constructed via \( \text{DPP-Nyström} \) and \( \gamma \geq \frac{1}{N} \text{tr}(K) \), then with probability at least \( 1 - \delta \)

\[
\sqrt{\frac{\text{bias}(K)}{\text{bias}(\hat{K})}} \geq 1 - \frac{1}{N\gamma} \left( \frac{(c + 1) e_{c+1}(K)}{e_c(K)} + \sqrt{8c \log(1/\delta) \text{tr}(K)} \right).
\]

*Proof.* Consider the function \( f_C(K) = v_C = \sum_i \| b_i^T U_{C,i} \|^2 \). Since \( 0 \leq f_C(K) \leq \text{tr}(K) \), it follows that the Lipschitz constant for \( f_C \) is at most \( \text{tr}(K) \). Thus when \( C \sim k\text{-DrP} \) and \( \delta \in (0, 1) \), by applying Theorem 4 we see that the inequality \( v_C \leq \mathbb{E} \left[ v_C \right] + \sqrt{8c \log(1/\delta) \text{tr}(K)} \) holds with probability at least \( 1 - \delta \). Thus, it follows that the bound

\[
\sqrt{\frac{\text{bias}(K)}{\text{bias}(\hat{K})}} \geq 1 - \mathbb{E} \left[ \frac{v_C}{N\gamma} \right] - \sqrt{8c \log(1/\delta) \text{tr}(K)} \frac{1}{N\gamma} \\
= 1 - \frac{1}{N\gamma} \left( \frac{(c + 1) e_{c+1}(K)}{e_c(K)} + \sqrt{8c \log(1/\delta) \text{tr}(K)} \right)
\]

holds with probability at least \( 1 - \delta \). \( \Box \)

**Remarks.** Theorem 5 quantifies how the learning results rely on the decay of the spectrum of \( K \). In particular, the ratio \( e_{c+1}(K)/e_c(K) \) closely relates to the effective rank of \( K \): if \( \lambda_c > a \) and \( \lambda_{c+1} \leq a \), this ratio becomes almost zero, resulting in near-perfect approximations and no loss in learning. This conclusion is also evident from (4.5).

There exist works considering Nyström methods in this scenario \([2, 5]\). Although our bounds are not directly comparable to the existing ones, we do extensive experiments against other state-of-art methods in Sec. 6.2 and observe superior performances of \( \text{DPP-Nyström} \).
5 Fast Mixing Markov Chain for DPP

Despite its excellent empirical performance and strong theoretical results, determinantal sampling for Nyström has rarely been used in applications due to the computational cost of $O(N^3)$ for exactly sampling from a DPP, which relies on eigendecomposition. Instead, we resort to using an MCMC sampler, which offers a promising alternative if the chain mixes fast enough. Recent empirical results provide initial evidence [25], but without a theoretical analysis; other recent works [22, 33] do not apply to our setting which deals with cardinality constrained $k$-DPP. We offer the theoretical analysis that confirms fast mixing (i.e., polynomial or even linear-time sampling) under certain conditions and connect it to our empirical results. (We note in a time period overlapping with completion of our proofs, [4] have independently obtained an elegant polynomial mixing time analysis that does not place additional restrictions.) The empirical results in Section 6 illustrate the favorable performance of DPP-Nyström in trading off time and error.

Algorithm 1 presents a Gibbs sampler for $k$-DPPs. Starting with a uniformly random set $Y_0$, at iteration $t$ the sampler tries to swap an element $y^{\text{in}} \in Y_t$ with an element $y^{\text{out}} \notin Y_t$, according to the probabilities of the sets $Y_t$ and $Y_t \cup \{y^{\text{out}}\} \setminus \{y^{\text{in}}\}$. The stationary distribution of the corresponding Markov chain is exactly the desired $k$-DPP $(K)$.

**Algorithm 1** Gibbs sampler for $k$-DPP

**Require:** $K$ the kernel matrix, $\mathcal{Y} = [N]$ the ground set

**Ensure:** $Y$ sampled from exact $k$-DPP $(K)$

Randomly Initialize $Y \subseteq \mathcal{Y}$

while not mixed do

Sample $b$ from uniform Bernoulli distribution

if $b = 1$ then

Pick $y^{\text{in}} \in Y$ and $y^{\text{out}} \in \mathcal{Y} \setminus Y$ uniformly randomly

\[
q(y^{\text{in}}, y^{\text{out}}, Y) \leftarrow \frac{\det(L_{Y \cup \{y^{\text{out}}\} \setminus \{y^{\text{in}}\}})}{\det(L_{Y \cup \{y^{\text{out}}\} \setminus \{y^{\text{in}}\}} + \det(L_Y))
\]

\[Y \leftarrow Y \cup \{y^{\text{out}}\} \setminus \{y^{\text{in}}\}\] with probability $q(y^{\text{in}}, y^{\text{out}}, Y)$

end if

end while

The mixing time $\tau(\varepsilon)$ of the Markov chain is the number of iterations it takes until the distribution over the states is $\varepsilon$-close to the target in total variation, i.e., $\tau(\varepsilon) := \min\{t: \max_{Y_0} TV(Y_t, \pi) \leq \varepsilon\}$. We show a bound on this mixing time via coupling techniques.

Given a Markov chain $(Y_t)$ on a state space $\Omega$ with transition matrix $P$, a coupling is a new chain $(Y_t, Z_t)$ on $\Omega \times \Omega$ such that both $(Y_t)$ and $(Z_t)$, if considered marginally, are Markov chains with the same transition matrices $P$. The key point of coupling is to construct such a new chain to encourage $Y_t$ and $Z_t$ to coalesce quickly. If in the new chain $\Pr(Y_t = Z_t) \leq \varepsilon$ for some fixed $t$ regardless of the starting state $(Y_0, Z_0)$, then the mixing time $\tau(\varepsilon) \leq t$ [3].

Such coalescing chains can be difficult to construct. Path coupling [12] relieves this burden by reducing the coupling to adjacent states in an appropriately constructed state graph. The coupling of arbitrary states follows by aggregation over a path between the two. Path coupling is formalized in the following lemma.

**Lemma 7** ([12, 17]). Let $\delta$ be an integer-valued metric on $\Omega \times \Omega$ where $\delta(\cdot, \cdot) \leq D$. Let $E$ be a subset of $\Omega \times \Omega$ such that for all $(Y_t, Z_t) \in E$ there exists a path $Y_t = X_0, \ldots, X_r = Z_t$ between $Y_t$ and $Z_t$. Then the mixing time $\tau(\varepsilon)$ of $(Y_t)$ is bounded by $\tau(\varepsilon) \leq t$. 

The analysis in [25] is not correct.
and $Z_i$ where $(X_i, X_{i+1}) \in E$ for $i \in [r - 1]$ and $\sum_i \delta(X_i, X_{i+1}) = \delta(Y_i, Z_i)$. Suppose a coupling $(R, T) \rightarrow (R', T')$ of the Markov chain is defined on all pairs in $E$ such that there exists a scalar $\alpha < 1$ such that $\mathbb{E}[\delta(R', T')] \leq \alpha \delta(R, T)$ for all $(R, T) \in E$. Then, for any $\epsilon > 0$ we have the following bound:

$$\tau(\epsilon) \leq \frac{\log(D\epsilon^{-1})}{(1 - \alpha)}.$$ 

The lemma says that if we have a contraction of the two chains in expectation ($\alpha < 1$), then the chain mixes fast. With the path coupling lemma, we obtain a bound on the mixing time that can be linear in the data set size $N$.

The actual result depends on three quantities that relate to how sensitive the transition probabilities are to swapping a single element in a set of size $k$. Consider an arbitrary set $S$ of columns, $|S| = k - 1$, and complete it to two $k$-sets $R = S \cup \{r\}$ and $T = S \cup \{t\}$ that differ in exactly one element. Our quantities are, for $u \notin R \cup T, v \in S$ and $q$ defined as in Algorithm 1:

$$p_1(S, r, t, u) = \min\{q(r, u, R), q(t, u, T)\}$$

$$p_2(S, r, t, u) = \min\{q(v, t, R), q(v, u, T)\}$$

$$p_3(S, r, t, v, u) = |q(v, u, R) - q(v, u, T)|.$$ 

**Theorem 8.** Let

$$\alpha = \max_{|S| = k - 1, r \notin [n]} \sum_{u_1 \notin S, u_2 \notin \{r, t\}} p_3(S, r, t, u_3, u_4) - \sum_{u_1 \notin S \cup \{r\}} p_3(S, r, t, u_1) - \sum_{u_2 \in S} p_2(S, r, t, u_2).$$

Given $\alpha < 1$, the mixing time for the Gibbs sampler in Algorithm 1 is bounded as

$$\tau(\epsilon) \leq \frac{2k(N - k) \log(k\epsilon^{-1})}{(1 - \alpha)}.$$ 

**Proof.** We bound the mixing time via path coupling. Let $\delta(R, T) = |R \oplus T|/2$ be half the Hamming distance on the state space, and define $E$ to consist of all state pairs $(R, T)$ in $\Omega \times \Omega$ such that $\delta(R, T) = 1$. We intend to show that for all states $(R, T) \in E$ and next states $(R', T') \in E$, we have $\mathbb{E}[\delta(R', T')] \leq \alpha \delta(R, T)$ for an appropriate $\alpha$.

Since $\delta(R, T) = 1$, the sets $R$ and $T$ differ in only two entries. Let $S = R \cap T$, so $|S| = k - 1$ and $R = S \cup \{r\}$ and $T = S \cup \{t\}$. For a state transition, we sample an element $r_{in} \in R$ and $r_{out} \in [n] \setminus R$ as switching candidates for $R$, and elements $t_{in} \in T$ and $t_{out} \in [n] \setminus T$ as switching candidates for $T$. Let $b_R$ and $b_T$ be the Bernoulli random variables indicating whether to try to make a transition. In our coupling we always set $b_R = b_T$. Hence, if $b_R = 0$ then both chains will not transition and the distance of states remains. For $b_R = b_T = 1$, we distinguish four cases:

**Case C1.** If $r_{in} = r$ and $r_{out} = t$, we let $t_{in} = t$ and $t_{out} = r$. As a result, $\delta(R', T') = 0$.

**Case C2.** If $r_{in} = r$ and $r_{out} = u_1 \notin S \cup \{r, t\}$, we let $t_{in} = t$ and $t_{out} = u_1$. In this case, if both chains transition, then the resulting distance is zero, otherwise it remains one. With probability $p_1(S, r, t, u_1) = \min\{q(r, u_1, R), q(t, u_1, T)\}$ both chains transit.

**Case C3.** If $r_{in} = u_2 \in S$ and $r_{out} = t$, we let $t_{in} = u_2$ and $t_{out} = r$. Again, if both chains transition, then the resulting distance is $\delta(R', T') = 0$, otherwise it remains one. With probability $p_2(S, r, t, u_2) = \min\{q(u_2, t, R), q(u_2, u_1, T)\}$ both chains transit.
Case C4. If \( r^{in} = u_3 \in S \) and \( r^{out} = u_4 \notin S \cup \{r, t\} \), we let \( t^{in} = u_3 \) and \( t^{out} = u_4 \). If both chains make the same transition (both move or do not move), the resulting distance is one, otherwise it increases to 2. The distance increases with probability \( p_3(S, r, t, u_3, u_4) = |q(u_3, u_4, R) - q(u_3, u_4, T)| \).

With those four cases, we can now bound \( E[\delta(R', T')] \). For all \((R, T) \in E\), i.e., \( \delta(R, T) = 1 \):

\[
\frac{E[\delta(R', T')]}{E[\delta(R, T)]]} = \frac{1}{2} + \Pr(C2)E[\delta(R', T')|C2] + \Pr(C3)E[\delta(R', T')|C3] + \Pr(C4)E[\delta(R', T')|C4]
\]

\[
= \frac{1}{2} + \frac{1}{2k(n - k)} \left( \sum_{u_1 \notin S \cup \{r, t\}} (1 - p_1(u_1)) + \sum_{u_2 \in S} (1 - p_2(u_2)) + \sum_{u_3 \in S, u_4 \notin S \cup \{r, t\}} (1 + p_3(u_3, u_4)) \right)
\]

\[
= \frac{1}{2} + \frac{1}{2k(n - k)} \left( 2k(n - 1) + \sum_{u_3 \in S, u_4 \notin S \cup \{r, t\}} p_3(u_3, u_4) - \sum_{u_1 \notin S \cup \{r, t\}} p_1(u_1) + \sum_{u_2 \in S} p_2(u_2) - 1 \right),
\]

where we did not explicitly write the arguments \( S, r, t \) to \( p_1, p_2, p_3 \). For

\[
\alpha = \max_{|S| = k - 1, r, t \in [n] \setminus S, u_4 \notin S \cup \{r, t\}} \frac{p_3(u_3, u_4)}{p_1(u_1)} - \frac{p_2(u_2)}{1 - \alpha}
\]

and \( \alpha < 1 \) the path coupling lemma 7 implies that

\[
\tau(\epsilon) \leq \frac{2k(N - k) \log(k \epsilon^{-1})}{(1 - \alpha)}.
\]

**Remarks.** If \( \alpha < 1 \) is fixed, then the mixing time depends only linearly on \( N \). The quantity \( \alpha \) itself depends on our three quantities. In particular, fast mixing requires \( p_3 \) (the difference between transition probabilities) to be very small compared to \( p_1, p_2 \), at least on average. The difference \( p_3 \) measures how exchangeable two points \( r \) and \( t \) are. This notion of symmetry is closely related to a symmetry that determines the complexity of submodular maximization [40] (indeed, \( F(S) = \log \det K_S \) is a submodular function). This symmetry only needs to hold for most pairs \( r, t \), and most swapping points \( u, v \). It holds for kernels with sufficiently fast-decaying similarities, similar to the conditions in [33] for unconstrained sampling.

Finally, we note that a single iteration of the sampler can be implemented to run in \( O(k^2) \) time using block inversion [21]. Together with fast mixing, this leads to an efficient sampler for \( k\)-DPPs.

### 6 Experiments

In our experiments, we evaluate the performance of \( \text{DPP-Nyström} \) on both kernel approximation and kernel learning tasks; we report both running times and accuracy.

We use 8 datasets: Abalone, Ailerons, Elevators, CompAct, CompAct(s), Bank32NH, Bank8FM and California Housing\(^3\). We truncated each dataset to 4,000 samples (3,000 training and 1,000 testing). Throughout our experiments we use an RBF kernel and choose the bandwidth parameter \( \sigma \) and regularization parameter \( \lambda \) for each dataset by 10-fold cross-validation. We initialize the Gibbs sampler via Kmeans++ and run for 3,000 iterations. Results are averaged over 3 random subsets of data.

\(^3\)The data is available at [http://www.dcc.fc.up.pt/~ltorgo/Regression/DataSets.html](http://www.dcc.fc.up.pt/~ltorgo/Regression/DataSets.html)
6.1 Kernel Approximation

We first explore DPP-Nyström (kDPP in the figures) for approximating kernel matrices. We compare against the following methods:

- Uniform sampling (Unif);
- Leverage score sampling (Lév) [20];
- AdapFull (kAdapFull) [14];
- Sampling with regularized leverage scores (RegLév) [2].

Unif and Lév serve as baseline landmark selection methods. Though AdapFull performs quite well in terms of accuracy, it scales poorly, as $O(N^2)$, with the size of dataset. We note that RegLév is not originally designed for kernel approximation, but we include its results to see how regularization impacts leverage score sampling.

Figure 1 shows example results on the Ailerons data, further experiments may be found in the appendix. DPP-Nyström performs well, and achieves the lowest errors as measured in both spectral and Frobenius norm. The only method that is on par in terms of accuracy is AdapFull but with a much higher running time.

For a different view, Figure 2 shows the improvement in error over Unif. Relative improvements are averaged over all data sets. Again, the performance of DPP-Nyström almost always dominates other methods and achieves up to an 80% reduction in error.

6.2 Kernel Ridge Regression

Next, we apply DPP-Nyström to kernel ridge regression, comparing against uniform sampling (Unif) [5] and regularized leverage score sampling (RegLév) [2] which have theoretical guarantees for this task. Figure 3 illustrates an example result: non-uniform sampling greatly improves accuracy, with kDPP improving over regularized leverage scores in particular for a small number of landmarks, where a single column has a larger effect.

Figure 4 displays the average improvement over Unif, averaged over 8 data sets. Again the performances of kDPP dominates those of RegLév and Unif and leads to gains in accuracy. On average kDPP consistently achieve more than 20% improvement over Unif.
6.3 Mixing of the Gibbs Markov Chain

In the next experiment, we empirically study the mixing of the Gibbs chain with respect to matrix approximation error, the ultimate measure that is of interest in our application. We use $c = 50$ and vary $N$ from 500 to 4,000. To exclude impacts of the initialization, we pick the initial state $Y_0$ uniformly at random. We run the chain for 5,000 iterations, monitoring how the error changes with the number of iterations. The example results in Figure 5 show that empirically, the error drops very quickly and afterwards fluctuates only little, indicating a fast convergence of the approximation error (even before the Gibbs chain has truly mixed). Other error measures and larger $c$ confirm this trend. Further results may be found in the supplementary material.

Notably, our empirical results suggest that the mixing time does not increase much even if $N$ increases greatly, suggesting that the Gibbs sampler remains fast even for large $N$.

In Theorem 8, the mixing time depends on the quantity $\alpha$. By subsampling 1,000 random sets $S$ and column indices $r, t$, we approximately computed $\alpha$ on our data sets. We find that, as expected, $\alpha < 1$ in particular for kernels with a smaller bandwidth, and in general $\alpha$ increases with $k$. In accordance with the theory, we found that the mixing time (in terms of error) too increases with $k$. In practice, we observe a fast drop in error even for cases where $\alpha > 1$, indicating that in this regime Theorem 8 is conservative and that the iterative approach is even more widely applicable.
Figure 4: Improvements in training/testing errors (%) over uniform sampling (with corresponding landmark sizes) in kernel ridge regression, averaged over all datasets.

Figure 5: Relative Frobenius norm error of DPP-Nyström with 50 landmarks as changing across iterations of the Markov Chain.

6.4 Time-Error Tradeoffs

Figure 6: Time-Error tradeoffs with 50 landmarks on the Ailerons data truncated at 2,000 samples (1,000 training and 1,000 testing). Errors are shown on a log scale. Bottom left is the best (low error, low running time), top right is the worst.

Iterative methods like the Gibbs sampler offer tradeoffs between time and error. The longer the Markov Chain runs, the closer the sampling distribution is to the desired DPP, and the higher
the accuracy obtained by Nyström. We hence explicitly show the time and accuracy for 0 to 300 iterations of the sampler.

A similar tradeoff occurs with leverage scores. For the experiments in the other sections, we computed the (regularized) leverage scores for $\text{Lev}$ and $\text{RegLev}$ exactly. This requires a full, computationally expensive eigendecomposition. For a fast, rougher approximation, we here compare to an approximation mentioned in [2]. Concretely, we sample $p$ elements with probability proportional to the diagonal entries of kernel matrices $K_{ii}$, and then use a Nyström-like method to construct an approximate low-rank decomposition of $K$, and compute scores based on this approximation. We vary $p$ from 50 to 500 to show the tradeoff for approximated leverage score sampling (AppLev) and regularized leverage score sampling (AppRegLev).

Figure 6 summarizes and compares the tradeoffs offered by these different methods. The x-axis indicates time, the y-axis error, so the lower left is the preferred corner. We see that exact leverage scores are accurate but expensive, whereas the approximate versions empirically lose accuracy. $k\text{dF11}$ is accurate but needs longer time than kDPP. These results are sharpened as $N$ grows. Overall, $D\text{pp}$-Nyström offers the best tradeoff of accuracy versus efficiency.

7 Conclusion

In this paper, we revisited the use of $k$-Determinantal Point Processes for sampling good landmarks for the Nyström method. We theoretically and empirically observe its competitive performance, for both matrix approximation and ridge regression, compared to state-of-the-art methods.

To make this accurate method scalable to large matrices, we consider an iterative approach, and analyze it theoretically as well as empirically. Our results indicate that the iterative approach, a Gibbs sampler, achieves good landmark samples quickly; under certain conditions even in a linear number of iterations, for an $N$ by $N$ matrix. Finally our empirical results demonstrate that among state of the art methods, the iterative sampler yields the best tradeoff between efficiency and accuracy.

References

[1] R. H. Affandi, A. Kulesza, E. Fox, and B. Taskar. Nyström approximation for large-scale determinantal processes. In AISTATS, pages 85–98, 2013.

[2] A. E. Alaoui and M. W. Mahoney. Fast randomized kernel methods with statistical guarantees. NIPS, 2015.

[3] D. J. Aldous. Some inequalities for reversible markov chains. Journal of the London Mathematical Society, pages 564–576, 1982.

[4] N. Anari, S. O. Gharan, and A. Rezaei. Monte Carlo Markov Chain Algorithms for Sampling Strongly Rayleigh distributions and Determinantal Point Processes. arXiv:1602.05242, 2016.

[5] F. Bach. Sharp analysis of low-rank kernel matrix approximations. COLT, 2013.

[6] F. R. Bach and M. I. Jordan. Kernel independent component analysis. JMLR, pages 1–48, 2003.

[7] F. R. Bach and M. I. Jordan. Predictive low-rank decomposition for kernel methods. In ICML, pages 33–40, 2005.

[8] C. T. Baker and C. Baker. The numerical treatment of integral equations. Clarendon press Oxford, 1977.
[9] M.-A. Belabbas and P. J. Wolfe. On landmark selection and sampling in high-dimensional data analysis. *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, pages 4295–4312, 2009.

[10] M.-A. Belabbas and P. J. Wolfe. Spectral methods in machine learning and new strategies for very large datasets. *Proceedings of the National Academy of Sciences*, pages 369–374, 2009.

[11] J. Borcea, P. Brändén, and T. Liggett. Negative dependence and the geometry of polynomials. *Journal of the American Mathematical Society*, pages 521–567, 2009.

[12] R. Bubley and M. Dyer. Path coupling: A technique for proving rapid mixing in markov chains. In *FOCS*, pages 223–231, 1997.

[13] C. Cortes, M. Mohri, and A. Talwalkar. On the impact of kernel approximation on learning accuracy. In *AISTATS*, pages 113–120, 2010.

[14] A. Deshpande, L. Rademacher, S. Vempala, and G. Wang. Matrix approximation and projective clustering via volume sampling. In *SODA*, pages 1117–1126, 2006.

[15] P. Drineas and M. W. Mahoney. On the Nyström method for approximating a gram matrix for improved kernel-based learning. *JMLR*, pages 2153–2175, 2005.

[16] P. Drineas, R. Kannan, and M. W. Mahoney. Fast monte carlo algorithms for matrices II: Computing a low-rank approximation to a matrix. *SIAM Journal on Computing*, pages 158–183, 2006.

[17] M. Dyer and C. Greenhill. A more rapidly mixing markov chain for graph colorings. *Random Structures and Algorithms*, pages 285–317, 1998.

[18] S. Fine and K. Scheinberg. Efficient SVM training using low-rank kernel representations. *JMLR*, pages 243–264, 2002.

[19] C. Fowlkes, S. Belongie, F. Chung, and J. Malik. Spectral grouping using the Nyström method. *TPAMI*, pages 214–225, 2004.

[20] A. Gittens and M. W. Mahoney. Revisiting the Nyström method for improved large-scale machine learning. *ICML*, 2013.

[21] G. H. Golub and C. F. Van Loan. *Matrix computations*. 2012.

[22] A. Gotovos, H. Hassani, and A. Krause. Sampling from probabilistic submodular models. In *NIPS*, pages 1936–1944, 2015.

[23] V. Guruswami and A. K. Sinop. Optimal column-based low-rank matrix reconstruction. In *SODA*, pages 1207–1214, 2012.

[24] J. B. Hough, M. Krishnapur, Y. Peres, B. Virág, et al. Determinantal processes and independence. *Probability Surveys*, pages 206–229, 2006.

[25] B. Kang. Fast determinantal point process sampling with application to clustering. In *NIPS*, pages 2319–2327, 2013.

[26] A. Kulesza and B. Taskar. k-DPPs: Fixed-size determinantal point processes. In *ICML*, pages 1193–1200, 2011.

[27] A. Kulesza and B. Taskar. Determinantal point processes for machine learning. *arXiv preprint arXiv:1207.6083*, 2012.
[28] S. Kumar, M. Mohri, and A. Talwalkar. Ensemble Nyström method. In NIPS, pages 1060–1068, 2009.

[29] C. Li, S. Jegelka, and S. Sra. Efficient sampling for k-determinantal point processes. AISTATS, 2016.

[30] O. Macchi. The coincidence approach to stochastic point processes. Advances in Applied Probability, pages 83–122, 1975.

[31] E. J. Nyström. Über die praktische Auflösung von Integralgleichungen mit Anwendungen auf Randwertaufgaben. Acta Mathematica, pages 185–204, 1930.

[32] R. Pemantle and Y. Peres. Concentration of lipschitz functionals of determinantal and other strong rayleigh measures. Combinatorics, Probability and Computing, pages 140–160, 2014.

[33] P. Rebeschini and A. Karbasi. Fast mixing for discrete point processes. COLT, 2015.

[34] A. Rudi, R. Camoriano, and L. Rosasco. Less is more: Nyström computational regularization. NIPS, 2015.

[35] H. Shen, S. Jegelka, and A. Gretton. Fast kernel-based independent component analysis. Signal Processing, IEEE Transactions on, pages 3498–3511, 2009.

[36] A. J. Smola and B. Schölkopf. Sparse greedy matrix approximation for machine learning. ICML, 2000.

[37] S. Sun, J. Zhao, and J. Zhu. A review of Nyström methods for large-scale machine learning. Information Fusion, pages 36–48, 2015.

[38] A. Talwalkar, S. Kumar, and H. Rowley. Large-scale manifold learning. In CVPR, 2008.

[39] A. Talwalkar, S. Kumar, M. Mohri, and H. Rowley. Large-scale SVD and manifold learning. JMLR, pages 3129–3152, 2013.

[40] J. Vondrák. Symmetry and approximability of submodular maximization problems. SIAM Journal on Computing, 42(1):265–304, 2013.

[41] S. Wang, C. Zhang, H. Qian, and Z. Zhang. Using the matrix ridge approximation to speedup determinantal point processes sampling algorithms. In AAAI, 2014.

[42] C. Williams and M. Seeger. Using the Nyström method to speed up kernel machines. In NIPS, pages 682–688, 2001.

[43] K. Zhang, I. W. Tsang, and J. T. Kwok. Improved Nyström low-rank approximation and error analysis. In ICML, pages 1232–1239, 2008.
A Supplementary Experiments

A.1 Kernel Approximation

Fig. 7 shows the matrix norm relative error of various methods in kernel approximation on the remaining 7 datasets mentioned in the main text.

Figure 7: Relative Frobenius norm and spectral norm error achieved by different kernel approximation algorithms on the remaining 7 data sets.
A.2 Approximated Kernel Ridge Regression

Fig. 8 shows the training and test error of various methods for kernel ridge regression on the remaining 7 datasets.

Figure 8: Training and test error achieved by different Nyström kernel ridge regression algorithms on the remaining 7 regression datasets.
Figure 9: Performance of Markov chain DPP-Nyström with 50 landmarks on Ailerons. Runs for 5,000 iterations.

A.3 Mixing of Markov Chain $k$-Dpp

We show the mixing of the Gibbs DPP-Nyström with 50 landmarks with different performance measures: relative spectral norm error, training error and test error of kernel ridge regression in Fig. 9.

We also show corresponding results with respect to 100 and 200 landmarks in Fig. 10 and Fig. 11, so as to illustrate that for varying number of landmarks the chain is indeed fast mixing and will give reasonably good result within a small number of iterations.

A.4 Running Time Analysis

We show running time comparisons for various sampling methods on the Ailerons dataset with respect to spectral norm error and training error with 50 landmarks and all error measures with 100 landmarks. The result is shown in Fig. 12 and Fig. 13 and similar trends as the example results in the main text could be spotted.
Figure 10: Performance of Markov chain DPP-Nyström with 100 landmarks on Ailerons. Runs for 5,000 iterations.
Figure 11: Performance of Markov chain DPP-Nyström with 200 landmarks on Ailerons. Runs for 5,000 iterations.

Figure 12: Time-Error tradeoff with 50 landmarks on Ailerons. Errors shown in log-scale.
Figure 13: Time-Error tradeoff with 100 landmarks on Ailerons. Errors shown in log-scale.