Large Scale Learning with Kreın Kernels

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Abstract

We extend the Nyström method for low-rank approximation of positive definite Mercer kernels to approximation of indefinite kernel matrices. Our result is the first derivation of the approach that does not require the positive definiteness of the kernel function. Building on this result, we then devise highly scalable methods for learning in reproducing kernel Kreın spaces. The main motivation for our work comes from problems with structured representations (e.g., graphs, strings, time-series), where it is relatively easy to devise a pairwise (dis)similarity function based on intuition/knowledge of a domain expert. Such pairwise functions are typically not positive definite and it is often well beyond the expertise of practitioners to verify this condition. The proposed large scale approaches for learning in reproducing kernel Kreın spaces provide principled and theoretically well-founded means to tackle this class of problems. The effectiveness of the approaches is evaluated empirically using kernels defined on structured and vectorial data representations.

1 Introduction

The Nyström method [21, 32, 31] is an effective approach for low-rank approximation of positive definite kernel matrices that can scale kernel methods to problems with millions of instances. In this paper, we extend it to low-rank approximation and eigendecomposition of indefinite kernel matrices by providing the first derivation that does not require the positive definiteness of the kernel function. Recently, a variant of the approach [27, 28] has been used for approximate eigendecomposition and low-rank approximation of indefinite kernel matrices without showing that the restriction of the original Nyström method to positive definite kernels can be eliminated. In addition to this theoretical result, we also propose a novel approach for finding an approximate eigendecomposition of indefinite kernel matrices that is computationally more efficient than the one from previous work [27, 28].

The main motivation for our work comes from learning problems with structured data (e.g., graphs, strings, time-series), where it is relatively easy to devise a pairwise similarity/dissimilarity function based on intuition/knowledge of a domain expert. Such pairwise functions are typically not positive definite and it is often the case that verifying this condition is well beyond the expertise of practitioners. The problems with indefinite similarity/dissimilarity functions are typically modeled via Kreın spaces [19, 23, 24], which are vector spaces with an indefinite bilinear form [5, 16]. The computational and space complexities of these approaches are similar to those of standard kernel methods that work with positive definite kernels [29]. In order to tackle large scale problems with indefinite kernels, we devise several novel low-rank approaches tailored for learning in reproducing kernel Kreın spaces.

We start by showing that the Nyström method can be used for low-rank approximations of indefinite kernel matrices and provide means for finding their approximate eigendecompositions (Section 2.2). We then devise two landmark sampling strategies based on state-of-the-art techniques [14, 22] used in Nyström approximations of positive definite kernels (Section 2.3). Having described means for finding low-rank factorizations of indefinite kernel matrices, we formulate low-rank variants of two least squares methods [23, 29] for learning in reproducing kernel Kreın spaces (Section 2.4). We also derive
a novel low-rank variant of the support vector machine for large scale learning in reproducing kernel Kre˘ın spaces (Section 2.5), inspired by the considerations in [23]. Having introduced means for large scale learning in reproducing kernel Kre˘ın spaces, we evaluate the effectiveness of these approaches and the Nyström low-rank approximations on datasets from standard machine learning repositories (Section 3). The empirical results demonstrate the effectiveness of the proposed approaches in classification tasks and the Nyström method across different datasets for a variety of kernels. The paper concludes with a discussion where we contrast ours and other relevant approaches (Section 4).

2 Large Scale Learning with Kre˘ın Kernels

We propose here an extension of the Nyström method for low-rank approximation of indefinite kernel matrices and show that the approach can scale Kre˘ın kernel methods to large scale datasets with millions of instances/pairwise (dis)similarities. More specifically, we devise low-rank variants of kernel ridge regression and support vector machines in reproducing kernel Kre˘ın spaces, as well as a low-rank variant of the variance constrained ridge regression proposed in [23]. In addition to this, we also provide effective sampling strategies for landmark selection in the Nyström method.

2.1 Reproducing Kernel Kre˘ın Spaces

In this section, we follow [5, 24] and provide a brief overview of reproducing kernel Kre˘ın spaces. A more extensive study of the properties of these spaces can be found in [7, 16].

Let $\mathcal{K}$ be a vector space defined on the scalar field $\mathbb{R}$. A bilinear form on $\mathcal{K}$ is a function $(\cdot, \cdot)_\mathcal{K} : \mathcal{K} \times \mathcal{K} \to \mathbb{R}$ such that, for all $f, g, h \in \mathcal{K}$ and scalars $\alpha, \beta \in \mathbb{R}$, it holds: i) $(\alpha f + \beta g, h)_\mathcal{K} = \alpha (f, h)_\mathcal{K} + \beta (g, h)_\mathcal{K}$ and ii) $(f, \alpha g + \beta h)_\mathcal{K} = \alpha (f, g)_\mathcal{K} + \beta (f, h)_\mathcal{K}$. For $f \in \mathcal{K}$, if $(f, g)_\mathcal{K} = 0$ for all $g \in \mathcal{K}$ implies that $f = 0$, then the form is non-degenerate. The bilinear form $(\cdot, \cdot)_\mathcal{K}$ is symmetric if, for all $f, g \in \mathcal{K}$, we have $(f, g)_\mathcal{K} = (g, f)_\mathcal{K}$. The form is called indefinite if there exists $f, g \in \mathcal{K}$ such that $(f, f)_\mathcal{K} > 0$ and $(g, g)_\mathcal{K} < 0$. On the other hand, if $(f, f)_\mathcal{K} \geq 0$ for all $f \in \mathcal{K}$, then the form is called positive. A non-degenerate, symmetric, and positive bilinear form on $\mathcal{K}$ is called inner product.

Two elements $f, g \in \mathcal{K}$ that satisfy $(f, g)_\mathcal{K} = 0$ are called $\langle \cdot, \cdot \rangle_\mathcal{K}$-orthogonal. Similarly, any two subspaces $\mathcal{K}_1, \mathcal{K}_2 \subset \mathcal{K}$ that satisfy $(f_1, f_2)_\mathcal{K} = 0$ for all $f_1 \in \mathcal{K}_1$ and $f_2 \in \mathcal{K}_2$ are called $\langle \cdot, \cdot \rangle_\mathcal{K}$-orthogonal. Having reviewed bilinear forms, we are now ready to introduce the notion of a Kre˘ın space.

Definition 1. [5, 7] The vector space $\mathcal{K}$ with a bilinear form $(\cdot, \cdot)_\mathcal{K}$ is called Kre˘ın space if it admits a decomposition into a direct sum $\mathcal{K} = \mathcal{H}_+ \oplus \mathcal{H}_-$ of $(\cdot, \cdot)_\mathcal{K}$-orthogonal Hilbert spaces $\mathcal{H}_\pm$ such that the bilinear form can be written as

$$
(f, g)_\mathcal{K} = (f_+, g_+)_\mathcal{H}_+ - (f_-, g_-)_\mathcal{H}_-,
$$

where $\mathcal{H}_\pm$ are endowed with inner products $(\cdot, \cdot)_{\mathcal{H}_\pm}$, $f = f_+ \oplus f_-$, $g = g_+ \oplus g_-$, and $f_\pm, g_\pm \in \mathcal{H}_\pm$.

Thus, a Kre˘ın space is defined with a non-degenerate, symmetric, and indefinite bilinear form. For a fixed decomposition $\mathcal{K} = \mathcal{H}_+ \oplus \mathcal{H}_-$, the Hilbert space $\mathcal{H}_\mathcal{K} = \mathcal{H}_+ \oplus \mathcal{H}_-$ endowed with inner product

$$
(f, g)_{\mathcal{H}_\mathcal{K}} = (f_+, g_+) + (f_-, g_-) \quad (f_\pm, g_\pm \in \mathcal{H}_\pm)
$$

can be associated with $\mathcal{K}$. For a Kre˘ın space $\mathcal{K}$, the decomposition $\mathcal{K} = \mathcal{H}_+ \oplus \mathcal{H}_-$ is not necessarily unique. Thus, a Kre˘ın space can, in general, be associated with infinitely many Hilbert spaces. However, for any such Hilbert space $\mathcal{H}_\mathcal{K}$ the topology introduced on $\mathcal{K}$ via the norm $||f||_{\mathcal{H}_\mathcal{K}} = \sqrt{(f, f)_{\mathcal{H}_\mathcal{K}}}$ is independent of the decomposition and the associated Hilbert space. More specifically, all norms $||\cdot||_{\mathcal{H}_\mathcal{K}}$ generated by different decompositions of $\mathcal{K}$ into direct sum of Hilbert spaces are topologically equivalent [18]. The topology on $\mathcal{K}$ defined by the norm of an associated Hilbert space is called the strong topology on $\mathcal{K}$. In the remainder, notions of convergence and continuity on a Kre˘ın space are defined with respect to the strong topology. As the strong topology of a Kre˘ın space is a Hilbert space topology, then it can be shown that the Riesz representation theorem holds. More formally, for a continuous linear functional $L$ on a Kre˘ın space $\mathcal{K}$ there exists a unique $q \in \mathcal{K}$ such that the functional $L$, for all $f \in \mathcal{K}$, can be written as $L f = (f, q)_\mathcal{K}$. Having reviewed basic properties of Kre˘ın spaces, we are now ready to introduce a notion of reproducing kernel Kre˘ın space.

Definition 2. [3, 24] A Kre˘ın space $(\mathcal{K}, (\cdot, \cdot)_\mathcal{K})$ is a reproducing kernel Kre˘ın space if $\mathcal{K} \subset \mathbb{R}^{\mathcal{X}}$ and the evaluation functional is continuous on $\mathcal{K}$ with respect to the strong topology.
The following theorem provides a characterization of reproducing kernel Kreın spaces.

**Theorem 1.** [3, 30] Let $k : X \times X \to \mathbb{R}$ be a real-valued symmetric function. Then, there is an associated reproducing kernel Kreın space if and only if $k = k_+ - k_-$, where $k_+$ and $k_-$ are positive definite kernels. When the function $k$ admits such a decomposition, one can choose $k_+$ and $k_-$ such that the corresponding reproducing kernel Hilbert spaces are disjoint.

In contrast to reproducing kernel Hilbert spaces, there is no bijection between reproducing kernel Kreın spaces and indefinite reproducing kernels. Moreover, it is important to note that not every symmetric kernel function admits a representation as a difference between two positive definite kernels. A symmetric function that does not admit such a representation has been constructed by Schwartz [30] and it can also be found in Alpay [Theorem 2.2, 3]. On finite discrete spaces, however, any symmetric kernel function admits a Kreın decomposition.

### 2.2 Nyström Method for Kreın Kernels

Let $X$ be an instance space and $X = \{x_1, \ldots, x_n\}$ an independent sample from a Borel probability measure defined on $X$. Let $K$ be a reproducing kernel Kreın space with an indefinite kernel $k : X \times X \to \mathbb{R}$ and let $H_K$ be an associated reproducing kernel Hilbert space with a positive definite kernel $h : X \times X \to \mathbb{R}$. For a positive definite kernel $h$ and a set of landmarks $Z = \{z_1, \ldots, z_m\} \subset X$, the Nyström method [21, 31, 32] first projects the evaluation functionals $h(x_i, \cdot)$ onto span $\{h(z_1, \cdot), \ldots, h(z_m, \cdot)\}$ and then approximates the kernel matrix $H$ with entries $[H_{ij} = h(x_i, x_j)]_{i,j=1}^n$ by inner products between the projections of the corresponding evaluation functionals. The projections of the evaluation functionals $h(x_i, \cdot)$ are linear combinations of the landmarks and these coefficients are given by the following convex optimization problem

$$
\alpha^* = \arg \min_{\alpha \in \mathbb{R}^{m \times n}} \sum_{i=1}^n \left\| h(x_i, \cdot) - \sum_{j=1}^m \alpha_{j,i} h(z_j, \cdot) \right\|_{H_K}^2 .
$$

While this approach works for positive definite kernels, it cannot be directly applied to reproducing Kreın kernels. In particular, a reproducing Kreın kernel is defined by an indefinite bilinear form $(\cdot, \cdot)_K$ which does not induce a norm on $K$ and for all $a, b \in K$ the value of $(a - b, a - b)_K$ does not capture the distance between these two points (see Section 2.1).

For an evaluation functional $k(x, \cdot) \in K$ and a linear subspace $L_Z \subset K$ spanned by the landmarks $\{k(z_1, \cdot), \ldots, k(z_m, \cdot)\}$, the orthogonal projection $\tilde{k}(x, \cdot)$ of the evaluation functional $k(x, \cdot)$ onto the subspace $L_Z$ satisfies [5, 16]:

$$
k(x, \cdot) = \tilde{k}(x, \cdot) + k^\perp(x, \cdot) ,
$$

where $\langle k^\perp(x, \cdot), L_Z \rangle_K = 0$ and $\tilde{k}(x, \cdot) = \sum_{i=1}^m \alpha_{i,x} k(z_i, \cdot)$ with $\alpha_x \in \mathbb{R}^m$. For a landmark $z \in Z$, the inner product between the corresponding evaluation functional $k(z, \cdot)$ and $k(x, \cdot)$ then gives

$$
k(x, z) = \langle k(x, \cdot), k(z, \cdot) \rangle_K = \sum_{i=1}^m \alpha_{i,x} \tilde{k}(z_i, z) .
$$

Denote with $K_{Z \times Z}$ the block in the kernel matrix $K$ corresponding to landmarks $Z$ and let $k_x = \text{vec} \{k(x, z_1), \ldots, k(x, z_m)\}$. From Eq. (2) it then follows that $k_x = K_{Z \times Z} \alpha_x$. Thus, in Kreın spaces a unique projection point exists only if the matrix $K_{Z \times Z}$ is non-singular. If this condition is satisfied, then the projection point can be computed as

$$
\tilde{k}(x, \cdot) = \sum_{i=1}^m \alpha_{i,x}^* k(z_i, \cdot) \quad \text{with} \quad \alpha_x^* = K_{Z \times Z}^{-1} k_x \in \mathbb{R}^m .
$$

Having computed the projection of a point onto the span of the landmarks in a Kreın space, we now proceed to define the Nyström approximation of the corresponding indefinite kernel matrix. In this, we follow the approach for positive definite kernels [29, 31] and approximate the Kreın kernel matrix $K$ using the bilinear form on the span of the landmarks. More formally,

$$
\tilde{k}(x_i, x_j) = \left\langle \sum_{p=1}^m \alpha_{p,i} k(x_i, \cdot), \sum_{q=1}^m \alpha_{q,j} k(x_j, \cdot) \right\rangle_K = k_{x_i}^T K_{Z \times Z}^{-1} k_{x_j} .
$$
Thus, the low-rank approximation of the Kreĭn kernel matrix $K$ is given by

$$\tilde{K}_{X|Z} = K_{X \times Z} K^{-1}_{Z \times Z} K_{Z \times Z} K^{-1}_{Z \times Z} K_{Z \times X} = K_{X \times Z} K^{-1}_{Z \times Z} K_{Z \times X}.$$  \hspace{1cm} (5)

This approach for low-rank approximation of Kreĭn kernel matrices also provides a direct way for an out-of-sample extension in the non-transductive setting. In particular, for an out-of-sample instance $x \in \mathcal{X}$ we have that if holds

$$\tilde{k}_{x|X} = \text{vec}\left(\tilde{k}(x, x_1), \ldots, \tilde{k}(x, x_n)\right) = K_{X \times Z} K^{-1}_{Z \times Z} k_x.$$  

In applications to estimation problems (see Sections 2.4 and 2.5) the so called one-shot variant of the Nyström method, providing an approximate eigendecomposition of the kernel matrix, is sometimes preferred over the plain Nyström approximation described above. For that, one can first introduce the low-rank approximation of the flipped spectrum kernel matrix

$$\tilde{H}_{X|Z} = K_{X \times Z} H^{-1}_{Z \times Z} K_{Z \times X},$$

with $H_{Z \times Z} = U_{Z \times Z} D_{Z \times Z}^{-1} U_{Z \times Z}^\top$ derived from an eigendecomposition of the block matrix $K_{Z \times Z} = U_{Z \times Z} D_{Z \times Z}^{-1} U_{Z \times Z}^\top$, the flipped spectrum matrix can be factorized as $\tilde{H}_{X|Z} = LL^\top$ with $L = K_{X \times Z} U_{Z \times Z} D_{Z \times Z}^{-\frac{1}{2}}$. Then, from a singular value decomposition of $L = A \Sigma B^\top$, with orthonormal matrices $A \in \mathbb{R}^{n \times m}$ and $B \in \mathbb{R}^{m \times m}$, we derive

$$\tilde{K}_{X|Z} = LSL^\top = A \Sigma B^\top \Sigma A^\top = A \Lambda A^\top.$$  

Thus, $M = \Sigma B^\top \Sigma$ is a symmetric matrix with an eigendecomposition $M = \Lambda P \Lambda^\top$ and

$$\tilde{K}_{X|Z} = (AP) \Lambda (AP)^\top \text{ with } (AP)^\top AP = I_m.$$

As the matrix $\tilde{U} = AP \in \mathbb{R}^{n \times m}$ contains $m$ orthonormal column vectors and $\Lambda$ is a diagonal matrix, we have then derived an approximate eigendecomposition of the Kreĭn kernel matrix $\tilde{K}$.

### 2.3 Landmark Selection for the Nyström Method with Kreĭn Kernels

In this section, we consider the problem of landmark selection in the Nyström method for low-rank approximation of indefinite kernel matrices and adapt two state-of-the-art strategies developed for the approximation of positive definite matrices. In particular, we devise landmark selection strategies for indefinite Kreĭn kernels based on approximate kernel $K$-means++ sampling [22] and statistical leverage scores [2, 10, 11]. In both cases, we propose to first sample a small number of instances uniformly at random and create a flip-spectrum sketch matrix $\tilde{H} = K_{X \times Z} H^{-1}_{Z \times Z} K_{Z \times X}$ from the Kreĭn kernel function by following the procedure described in Section 2.2. Then, using this sketch matrix we propose to approximate: i) statistical leverage scores for all instances, and/or ii) squared distances between instances in the feature space of a factorization $H = LL^\top$.

For landmarks based on statistical leverage score sampling, we first compute the approximate eigenvectors $\tilde{U}_Z$ of the positive definite matrix $\tilde{H}$ using the one-shot Nyström method for positive definite matrices (the only difference compared to Section 2.2 is in the fact that there is no diagonal sign matrix $S_{Z \times Z}$). Then, an approximate leverage score assigned to the $i$-th instance is given as the squared norm of the $i$-th row in the matrix $\tilde{U}_Z$, that is $\ell(x_i) = \|\tilde{U}_Z(i)\|^2$ with $1 \leq i \leq n$. As the two matrices $\tilde{H}$ and $\tilde{K}$ have identical eigenvectors, the approximate leverage scores obtained using $\tilde{H}$ capture the informative part of the eigenspace of the matrix $\tilde{K}$. The landmark selection strategy based on the approximate leverage scores then works by taking a set of independent samples from

$$p_{\ell}(x) = \ell(x) \sum_{i=1}^{n} \ell(x_i).$$

For approximate kernel $K$-means++ landmark selection, we propose to perform $K$-means++ clustering [4] in the feature space defined by the matrix $\tilde{L}$, that is each instance is represented with a row from this matrix. The approach works by first sampling an instance uniformly at random and setting it as the first landmark (i.e., the first cluster centroid). Following this, the
next landmark/centroid is selected by sampling an instance to its probability proportional to its clustering contribution. More formally, assuming that landmarks \( \{ z_1, z_2, \ldots, z_s \} \) have already been selected the \((s+1)\)-st landmark is selected by taking a sample from the distribution

\[
p_{s+1}^X(x) = \frac{\min_{1 \leq i \leq s} \| x - z_i \|^2}{\sum_{i=1}^n \min_{1 \leq j \leq s} \| x_i - z_j \|^2}.
\]

### 2.4 Large Scale Least Squares Methods for Krein Kernels

In this section, we adapt two least squares methods for large scale learning with Krein kernels. Our regularization term is motivated by the considerations in [23] where the authors regularize with respect to a decomposition of the Krein kernel into a direct sum of Hilbert spaces. In particular, we first consider a Krein least squares method (KREIN LSM), which is a variant of kernel ridge regression,

\[
f^* = \arg \min_{f \in \mathcal{K}} \frac{1}{n} \sum_{i=1}^n \left( f(x_i) - y_i \right)^2 + \lambda_+ \| f_+ \|_2^2 + \lambda_- \| f_- \|_2^2,
\]

where \( f = f_+ \oplus f_- \in \mathcal{K}, \mathcal{K} = \mathcal{H}_+ \oplus \mathcal{H}_- \) with disjoint \( \mathcal{H}_\pm \), \( f_\pm \in \mathcal{H}_\pm \), and hyperparameters \( \lambda_\pm \in \mathbb{R}^+ \). This is a convex optimization problem for which the representer theorem holds [23, Appendix A] and \( f^* = \sum_{i=1}^n \alpha_i^* k(x_i, \cdot) \) with \( \alpha^* \in \mathbb{R}^m \). Applying the reproducing property of the Krein kernel and setting the gradient of the objective to zero, we obtain the optimal solution as

\[
\alpha^* = \left( H + n\Lambda_\pm \right)^{-1} P y,
\]

with \( K = UDU^T, S = \text{sign} (D), H = UDSU^T, \Lambda_\pm = \lambda_+ S_+ + \lambda_- |S_-|, S_\pm = \frac{(S_\pm^2)}{2}, \) and \( P = USU^T \). As already mentioned in Section 2.2, the matrix \( H \) is called the flip-spectrum transformation of \( K \) and \( k_{\pm \times \times X}^P \) is the corresponding out-of-sample transformation. Learning with the flip-spectrum transformation of an indefinite kernel matrix was first considered in [15] and the corresponding out-of-sample transformation was first proposed in [8]. The following proposition establishes the equivalence between the least squares method with the flip-spectrum matrix in place of an indefinite kernel matrix and Krein kernel ridge regression regularized with a single hyperparameter.

**Proposition 2.** If the Krein kernel ridge regression problem is regularized via the norm \( \| \cdot \|_{\mathcal{H}_\pm} \) with \( \lambda = \lambda_+ = \lambda_- \), then the optimal hypothesis is equivalent to that obtained with kernel ridge regression and the flip-spectrum matrix in place of an indefinite Krein kernel matrix.

Thus, to obtain a true Krein hypothesis one needs to regularize via decomposition components \( \mathcal{H}_\pm \). Having established this, we now proceed to formulate a Krein regression problem with a low-rank approximation \( \tilde{K}_{\chi|z} \) in place of the indefinite kernel matrix \( K \). More formally, after substituting the low-rank approximation into Krein kernel ridge regression problem we can transform it as

\[
z = [D_{\chi \times z}]^{-1/2} U_{\chi \times z}^T K_{\chi \times \chi} \alpha = L_{\chi|z} \alpha \in \mathbb{R}^m
\]

\[
\Phi = K_{\chi \times z} U_{\chi \times z}^T [D_{\chi \times z}]^{-1/2} S_{\chi \times z} = L_{\chi|z} S_{\chi \times z} \in \mathbb{R}^{n \times m}
\]

\[
\tilde{K}_{\chi|z} \alpha = L_{\chi|\chi} S_{\chi \times z} \alpha = \Phi z
\]

\[
\alpha^T H_\pm \alpha = z^T \alpha.
\]

Hence, we can write a low-rank variant of the Krein kernel ridge regression problem as

\[
z^* = \arg \min_{z \in \mathbb{R}^m} \| \Phi z - y \|^2_2 + n\lambda_+ \| z_+ \|^2_2 + n\lambda_- \| z_- \|^2_2.
\]

The problem is convex in \( z \) and the optimal solution is given by

\[
z^* = \left( \Phi^T \Phi + n\Lambda_\pm \right)^{-1} \Phi^T y.
\]

An out-of-sample extension for this learning problem is given by

\[
\tilde{f}^*(x) = k_{x \times z}^T U_{\chi \times z}^T [D_{\chi \times z}]^{-1/2} S_{\chi \times z} z^*.
\]
We propose the following optimization problem as the Kreăin support vector machine
where \( \Phi \) we can transform this problem into \( K \) without loss of generality assumed that the kernel matrix with hyperparameters \( r \) and \( \lambda_\pm \in \mathbb{R}^+ \). To simplify our derivations [just as in 23], we have without loss of generality assumed that the kernel matrix \( K \) is centered. Then, the hard constraint fixes the variance of the predictor over training instances. Similar to Kreăin kernel ridge regression, we can transform this problem into
\[
\begin{align*}
    z^* &= \arg\min_{z \in \mathbb{R}^m} n \lambda_+ \|z_+\|^2 + n \lambda_- \|z_-\|^2 - 2z^T \Phi^T y \\
    &\text{s.t. } z^T \Phi^T \Phi z = r^2 .
\end{align*}
\]
Now, performing a singular value decomposition of \( \Phi = A \Delta B^T \) and taking \( \gamma = \Delta B^T z \) we obtain
\[
\begin{align*}
    \gamma^* &= \arg\min_{\gamma \in \mathbb{R}^m} n \gamma^T (\Delta^{-1} B^T A \Delta^{-1}) \gamma - 2(A^T y)^T \gamma \\
    &\text{s.t. } \gamma^T \gamma = r^2 .
\end{align*}
\]
A globally optimal solution to this non-convex optimization problem can be computed by following the procedures outlined in [13, 23]. The optimal solution can be computed in time \( O(m^3) \) and the cost for the low-rank transformation of the problem is \( O(m^3 + m^2 n) \). An out-of-sample extension can also be obtained by following the derivation for Kreăin kernel ridge regression.

2.5 Large Scale Support Vector Machines for Kreăin Kernels

In this section, we propose a Kreăin support vector machine for large scale classification with indefinite kernels. Our regularization term is again motivated by the considerations in [23] and that is the main difference compared to Kreăin support vector machine proposed in [19]. Moreover, we show that the latter variant of the support vector machine outputs a hypothesis which can equivalently be obtained using the standard support vector machine with the flip-spectrum kernel matrix combined with the corresponding out-of-sample transformation (introduced in Section 2.4).

We propose the following optimization problem as the Kreăin support vector machine
\[
\begin{align*}
    f^* &= \arg\min_{f \in \mathcal{K}} \frac{1}{n} \sum_{i=1}^{n} \max\{1 - y_i f(x_i), 0\} + \lambda_+ \|f_+\|^2 + \lambda_- \|f_-\|^2 .
\end{align*}
\]
Similar to Section 2.4, the representer theorem holds for this problem and applying the reproducing property of the Kreăin kernel we can transform it to a matrix form. If we again substitute a low-rank approximation \( \widetilde{K}_{X|Z} \) in place of the Kreăin kernel matrix \( K \), we observe that a hypothesis is given by
\[
\begin{align*}
    f(x_i) &= k_i^T \alpha = k_i^T Z x Z K Z x X \alpha = k_i^T \Phi z, \\
    \text{where } \Phi_i \text{ denotes the } i\text{-th row in the matrix } \Phi . \text{ The low-rank variant of the Kreăin support vector machine can be then written as}
\end{align*}
\]
\[
\begin{align*}
    z^* &= \arg\min_{z \in \mathbb{R}^m} \sum_{i=1}^{m} \max\{1 - y_i \Phi_i z, 0\} + n \lambda_+ \|z_+\|^2 + n \lambda_- \|z_-\|^2 .
\end{align*}
\]
The derivation of the solution follows that for the standard support vector machines with the only difference being that the diagonal matrix \( \Lambda_\pm \) is used instead of the scalar hyperparameter controlling the hypothesis complexity [e.g., see 17, 20]. Having introduced a large scale classifier in reproducing kernel Kreăin spaces, we proceed to show that the Kreăin support vector machine proposed in [19] is equivalent to the standard support vector machine with flip-spectrum matrix in place of an indefinite Kreăin kernel matrix, combined with the corresponding out-of-sample transformation.

**Proposition 3.** The Kreăin support vector machine proposed in [19] is equivalent to the standard support vector machine with the flip-spectrum matrix in place of an indefinite Kreăin kernel matrix.
3 Experiments

In this section, we report the results of experiments aimed at demonstrating the effectiveness of: i) the Nyström method in low-rank approximation of indefinite kernel matrices, and ii) the described large scale Krein approaches in classification tasks with pairwise (dis)similarity matrices.

In the first set of experiments, we take several datasets from UCI and LIACC repositories and define kernel matrices on them using the same indefinite kernels as previous work [23, Appendix C]. We use

$$0 \leq t = \sum_{i: \lambda_i < c_0} |\lambda_i| / \sum |\lambda_i| \leq 1$$

to quantify the level of indefiniteness of a kernel matrix. Prior to computation of kernel matrices, all the data matrices were normalized to have mean zero and unit variance across features. Following this, we have applied the Nyström method with landmark selection strategies presented in Section 2.3 to derive approximations of different ranks. We measure the effectiveness of a low-rank approximation with its error in the Frobenius norm. To quantify the effectiveness of the approximate eigendecomposition of the kernel matrix (i.e., the one-shot Nyström method) derived in Section 2.2, we have performed rank $k$ approximations using sets of $k \log n$ landmarks. Figures 1 and 2 summarize the results obtained with an indefinite kernel defined by the difference between two Gaussian kernels. The reported error/time is the median error/time over 10 repetitions of the experiment. Figure 1 indicates a sharp (approximately exponential) decay in the approximation error as the rank of the approximation increases. The devised approximate kernel $K$-means++ sampling strategy performs the best in terms of the accuracy in the experiments where rank $k$ approximations are generated using $k$ landmarks. The approximate leverage score strategy is quite competitive and in rank $k$ approximations generated using $k \log n$ landmarks it performs as good or even better than the approximate kernel $K$-means++ sampling scheme. We also observe the lack of a gap between the two sampling strategies, compared to the results reported in [22] for positive definite kernels. Our hypothesis is that this is due to sub-optimal choices of landmarks that define sketch matrices. In our simulations, we have generated sketches by sampling the corresponding landmarks uniformly at random. In support of this hypothesis, rather large approximation errors for uniformly selected landmarks in approximation of other indefinite kernels can be observed (see Appendix B). Figure 2 reports the time required to
generate a Nyström low-rank approximation and indicates that the considered sampling strategies amount to only a small fraction of the total time required to generate the low-rank approximation.

In the second set of experiments, we evaluate the effectiveness of the proposed large scale Krein least square methods on classification tasks with pairwise dissimilarity matrices [12, 25]. Following the instructions in [26], the dissimilarity matrices are converted to similarities by applying the transformation (i.e., negative centering of the squared dissimilarities) characteristic to multi-dimensional scaling [9]. In each simulation, we perform 10-fold stratified cross-validation and measure the effectiveness of an approach with the average/median percentage of misclassified examples. For multi-class problems, we only evaluate the effectiveness of one-vs-all classifier for the class with label one. Figure 3 shows the reduction in the classification error as the approximation rank increases. The reported error is the median error over 10-folds. Here, SF-LSM represents the baseline in which similarities are used as features and a linear ridge regression model is trained in that instance space [1, 8]. The figure indicates that the baseline is quite competitive, but overall the proposed low-rank variants perform very well across different datasets (additional results are provided in Appendix B). For completeness, we have also included the detailed results over all the datasets in Appendix B.

4 Discussion

The only existing variant of the Nyström method for indefinite kernels can be found in [27, 28]. There are, however, two potential issues with this approach:

1. The original Nyström method applies only to positive definite Mercer kernels [e.g., see 29, 32]. This assumption on the definiteness of the kernel function does not hold for Krein kernels and it is not addressed in [27, 28] where it is just stated that the Nyström approximation of an indefinite kernel matrix \( K \) can be computed as \( \tilde{K}_{SGT}^X \mid Z = K^X \times Z K^{-1} Z \times Z K \times K \).

2. From the presentation of the one-shot Nyström method for indefinite kernels in [27, 28] one could interpret that complex numbers will arise in the process of deriving the Nyström approximation of an indefinite kernel matrix. This would not be desirable from the perspective of numerical stability of the derivation and can be avoided with a slightly better presentation (for the sake of completeness, we cover this in Appendix A).

In addition to these two issues, the approach for derivation of an approximate low-rank eigendecomposition from [27, 28] requires 7 matrix-to-matrix multiplications with computational complexity \( \mathcal{O}(m^2n) \) and 2 eigendecompositions with complexity \( \mathcal{O}(m^3) \). In contrast to this, the approach proposed in Section 2.2 comes with a much better constant and requires \( (3m^2n + 3m^3) \) operations.

Beside the considered low-rank approximations, it is possible to treat indefinite similarity functions as features and learn with linear models [1, 8]. However, Balcan et al. [6] have showed that learning with a positive definite kernel corresponding to a feature space where the target concept is separable by a linear hypothesis yields a larger margin compared to learning with a linear model in a feature space constructed using that kernel function. As a result, if a kernel is used to construct a feature representation the sample complexity of a linear model in that space might be higher compared to learning with a kernelized variant of regularized risk minimization.

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1 http://prtools.org/disdatasets/index.html
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A Proofs

Proposition 2. If the Kreǐn kernel ridge regression problem is regularized via the norm $\|\cdot\|_{\mathcal{H}_K}$ with $\lambda = \lambda_+ = \lambda_-$, then the optimal hypothesis is equivalent to that obtained with kernel ridge regression and the flip-spectrum matrix in place of an indefinite Kreǐn kernel matrix.

Proof. The optimal hypothesis over training instances is given by

$$K\alpha^* = UDU^T (DS + n\lambda I)^{-1} U^T y = UDU^T (DS + n\lambda I)^{-1} U^T y = H (H + n\lambda I)^{-1} y.$$ Thus, if we only regularize with $\|f\|_{\mathcal{H}_K}$, then the Kreǐn kernel ridge regression problem is equivalent to that with the flip-spectrum transformation combined with the corresponding out-of-sample extension.

More formally, if $\alpha_H^* = (H + n\lambda I)^{-1} y$ denotes the optimal solution of the kernel ridge regression with the flip-spectrum matrix $H$ in place of the indefinite kernel matrix $K$ then the predictions at out-of-sample test instances are given by

$$f(x) = k_x^T \alpha_H^*.$$

Proposition 3. The Kreǐn support vector machine proposed in [19] is equivalent to the standard support vector machine with the flip-spectrum matrix in place of an indefinite Kreǐn kernel matrix.

Proof. The optimal hypothesis over training instances in [19] is given by

$$K\alpha^* = KP\alpha_H^* = UDU^T U^T \alpha_H^* = H\alpha_H^*,$$

where $\alpha_H^*$ is the optimal solution for the support vector machine problem with the flip-spectrum transformation of an indefinite kernel matrix.

An out-of-sample extension for a test instance $x$ is given by

$$f(x) = k_x^T \alpha^* = k_x^T P\alpha_H^*.$$

We provide here a brief review of the approach [27, 28] for the approximate eigendecomposition of an indefinite matrix based on the authors’ Matlab implementation\(^\text{2}\). The approach is motivated by the observation that an indefinite symmetric matrix and its square have identical eigenvectors. For this reason, the authors first form the squared low-rank Kreǐn kernel matrix as

$$\tilde{K}^2 = K_{X \times Z} K_{Z \times X}^{-1} K_{X \times Z} K_{Z \times X}^{-1} K_{Z \times Z} K_{X \times X} K_{X \times Z} K_{Z \times X} K_{Z \times Z}^{-1}.$$ The matrix $A = K_{Z \times Z}^{-1} K_{X \times Z} K_{X \times X} K_{X \times Z} K_{Z \times Z} K_{X \times Z} K_{Z \times X} K_{Z \times Z}^{-1}$ is positive definite because it can be written as $LL^T$ (e.g., taking $L = K_{Z \times Z}^{-1/2} K_{Z \times X}$). Thus, all the eigenvalues in an eigendecomposition of $A = VTV^T$ are non-negative and we can set $A = LL^T$ with $L = VT^{1/2}$. From here it then follows that the matrix $\tilde{K}^2$ can be factored as $\tilde{K}^2 = BB^T$ with $B = K_{X \times Z} V T^{1/2}$. Following this, Schleif et al. [27, 28] follow the standard procedure for the derivation of approximate eigenvectors and eigenvalues characteristic to the Nyström method for positive definite kernels [10, 11, 32]. In particular, they first decompose the positive definite matrix $B^T B = Q\Delta Q^T$ and then compute the approximate eigenvectors of $\tilde{K}^2$ as $U = B Q \Delta^{-1/2}$. Now, to obtain an approximate eigendecomposition of the Kreǐn kernel matrix the authors use these eigenvectors in combination with the posited form of the low-rank approximation $\tilde{K} = K_{X \times Z} K_{Z \times Z}^{-1} K_{Z \times X}$ and compute the approximate eigenvalues as $\tilde{D} = \tilde{U}^T \tilde{K} \tilde{U}$. As the diagonal matrix $\Delta$ contains the eigenvalues of $\tilde{K}^2$ this step retrieves the signed eigenvalues of $\tilde{K}$. The one-shot Nyström approximation of the kernel matrix is then given as [27, 28]

$$K_{X \times Z}^{\text{Nyström}} = \tilde{U}^T \tilde{U} = K_{X \times Z} V T^{1/2} \Delta^{-1/2} \tilde{D} \Delta^{-1/2} Q T^{1/2} V^T K_{Z \times X}.$$  

\(^2\)https://www.techfak.uni-bielefeld.de/~fschleif/eigenvalue_corrections_demos.tgz, accessed in May 2018

11
B Additional Experiments

Figure 4: The figure shows the reduction in the approximation error for an indefinite kernel matrix obtained using the SIGMOID kernel [Appendix C, 23] as a result of the increase in the approximation rank.

Figure 5: The figure shows the reduction in the approximation error for an indefinite kernel matrix obtained using the RL-SIGMOID kernel [Appendix C, 23] as a result of the increase in the approximation rank.

Figure 6: The figure shows the reduction in the approximation error for an indefinite kernel matrix obtained using the EPANECHNIKOV kernel [Appendix C, 23] as a result of the increase in the approximation rank.
Table 1: We have evaluated the effectiveness of low-rank variants of Krein least squares methods on classification tasks with pairwise dissimilarity matrices. The reported error is the average classification error obtained after 10-fold stratified cross-validation.

| DATASET       | DISSIMILARITY TYPE                      | RANK 100 APPROXIMATION | SIMILARITY MATRIX (COMPLETE) |
|---------------|----------------------------------------|------------------------|-------------------------------|
| zongker       | Graph matching                         | 32.22% (±2.00)         | 11.21% (±5.28)               |
| chicken25-45  | Shortest distance between balls         | 1.00% (±1.50)          | 0.50% (±1.50)                |
| polydism57    | Structural alignment of proteins        | 0.92% (±0.46)          | 0.92% (±0.46)                |
| chicken25     | String edit distance                   | 16.35% (±4.31)         | 15.69% (±4.97)               |
| protein       | Structural alignment of proteins        | 4.19% (±2.47)          | 3.72% (±2.76)                |
| woody50       | Deformable template matching            | 17.70% (±2.06)         | 17.75% (±2.23)               |
| polydiss57    | String edit distance                   | 19.29% (±4.64)         | 20.41% (±4.09)               |
| prodom        | Hausdorff distance                      | 3.40% (±0.39)          | 3.40% (±0.42)                |
| woody50       | Plant leaves' shape dissimilarity       | 30.84% (±5.25)         | 30.47% (±5.54)               |

Figure 7: The figure shows the reduction in the classification error as the approximation rank increases. The reported error is the median classification error obtained using 10-fold stratified cross-validation.