Learning in Reproducing Kernel Kreın Spaces

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Abstract
We formulate a novel regularized risk minimization problem for learning in reproducing kernel Kreın spaces and show that the strong representer theorem applies to it. As a result of the latter, the learning problem can be expressed as the minimization of a quadratic form over a hypersphere of constant radius. We present an algorithm that can find a globally optimal solution to this non-convex optimization problem in time cubic in the number of instances. Moreover, we derive the gradient of the solution with respect to its hyperparameters and, in this way, provide means for efficient hyperparameter tuning. The approach comes with a generalization bound expressed in terms of the Rademacher complexity of the corresponding hypothesis space. The major advantage over standard kernel methods is the ability to learn with various domain specific similarity measures for which positive definiteness does not hold or is difficult to establish. The approach is evaluated empirically using indefinite kernels defined on structured as well as vectorial data. The empirical results demonstrate a superior performance of our approach over the state-of-the-art baselines.

1. Introduction
We build on the work by Ong et al. (2004) and formulate a novel regularized risk minimization problem for learning in reproducing kernel Kreın spaces (reviewed in Section 2). The proposed risk minimization problem is of interest to several applications of machine learning (Laub & Müller, 2004) where the instance space can be accessed only implicitly, through a kernel function that outputs a real-value for a pair of instances. Typically, for a given set of instances the kernel matrix does not exhibit properties required by standard machine learning algorithms such as positive definiteness or metricity. A common practice in dealing with such data is to map the indefinite kernel matrix to a positive definite one using a spectrum transformation. This conversion can cause information loss and affect our ability to model a functional dependence of interest. In particular, Laub & Müller (2004) have used three real-world datasets to demonstrate that for symmetric kernel functions corresponding to indefinite kernel matrices, the negative parts of their spectra contain useful information which gets discarded by some of the standard procedures that learn by first transforming the indefinite kernel matrix to a positive definite one.

We show that the strong representer theorem applies to the proposed risk minimization problem and utilize this theoretical result to express the learning problem as the minimization of a quadratic form over a hypersphere of constant radius (Section 3.1). The optimization problem is, in general, neither convex nor concave and it can have exponentially many local optima (with respect to the representation size). Despite this, a globally optimal solution to this problem can be found in time cubic in the number of training examples. The algorithm for solving this non-convex problem relies on the work by Forsythe & Golub (1965) and Gander et al. (1989), who were first to consider the optimization of a quadratic form over a hypersphere of constant radius. The proposed risk minimization problem is consistent and comes with a generalization bound expressed in terms of the Rademacher complexity of the corresponding hypothesis space, which is a subset of a reproducing kernel Kreın space of functions (Section 3.2). In Section 3.3, we derive the gradient of an optimal solution to the risk minimization problem with respect to the hyperparameters of the model (e.g., the regularization parameters, hypersphere radius, and/or kernel-specific parameters). The derived solution gradient allows one to tune the hyperparameters of the model using an off-the-shelf optimization algorithm (e.g., L-BFGS-B minimization procedure, available in most numerical packages). In Section 4, we place our work in the context of relevant existing approaches for learning in reproducing kernel Kreın spaces. The effectiveness of the approach is evaluated empirically using indefinite kernels defined on structured and vectorial data. The results show a superior performance of our approach over the state-of-the-art baselines and indicate that on some problems indefinite kernels can be more effective than the positive definite ones.

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2. Reproducing Kernel Kreın Spaces

This section provides a brief overview of reproducing kernel Kreın spaces. The review follows closely the study by Azizov & Iokhvidov (1981) and the work by Ong et al. (2004). For a more extensive introduction, we refer to works by Bognär (1974) and Iokhvidov et al. (1982).

Let \( K \) be a vector space defined on the scalar field \( \mathbb{R} \). A bilinear form on \( K \) is a function \( \langle \cdot, \cdot \rangle_K : K \times K \rightarrow \mathbb{R} \) such that, for all \( f, g, h \in K \) and scalars \( \alpha, \beta \in \mathbb{R} \), it holds:

i) \( \langle \alpha f + \beta g, h \rangle_K = \alpha \langle f, h \rangle_K + \beta \langle g, h \rangle_K \),

ii) \( \langle f, \alpha g + \beta h \rangle_K = \alpha \langle f, g \rangle_K + \beta \langle f, h \rangle_K \).

For \( f \in K \), if \( \langle f, g \rangle_K = 0 \) for all \( g \in K \) implies that \( f = 0 \), then the form is non-degenerate. The bilinear form \( \langle \cdot, \cdot \rangle_K \) is symmetric if, for all \( f, g \in K \), we have \( \langle f, g \rangle_K = \langle g, f \rangle_K \).

The form is called indefinite if there exists \( f, g \in K \) such that \( \langle f, f \rangle_K > 0 \) and \( \langle g, g \rangle_K < 0 \). On the other hand, if \( \langle f, f \rangle_K \geq 0 \) for all \( f \in K \), then the form is called positive.

A non-degenerate, symmetric, and positive bilinear form on \( K \) is called inner product. Any two elements \( f, g \in K \) that satisfy \( \langle f, g \rangle_K = 0 \) are \( \langle \cdot, \cdot \rangle_K \)-orthogonal. Similarly, any two subspaces \( K_1, K_2 \subset K \) that satisfy \( \langle f_1, f_2 \rangle_K = 0 \) for all \( f_1 \in K_1 \) and \( f_2 \in K_2 \) are \( \langle \cdot, \cdot \rangle_K \)-orthogonal.

Having reviewed bilinear forms, we are now ready to introduce the notion of a reproducing Kreın space.

**Definition 1.** (Azizov & Iokhvidov, 1981; Bognär, 1974)
The vector space \( K \) with a bilinear form \( \langle \cdot, \cdot \rangle_K \) is called Kreın space if it admits a decomposition into a direct sum \( K = H_+ \oplus H_- \) of \( \langle \cdot, \cdot \rangle_K \)-orthogonal Hilbert spaces \( H_\pm \) such that the bilinear form can be written as

\[
\langle f, g \rangle_K = \langle f_+, g_+ \rangle_{H_+} - \langle f_-, g_- \rangle_{H_-},
\]

where \( H_\pm \) are endowed with inner products \( \langle \cdot, \cdot \rangle_{H_\pm} \), \( f = f_+ \oplus f_- \), \( g = g_+ \oplus g_- \), and \( f_\pm, g_\pm \in H_\pm \).

Thus, a Kreın space is defined with a non-degenerate, symmetric, and indefinite bilinear form. For a fixed decomposition \( K = H_+ \oplus H_- \), the Hilbert space \( H_K = H_+ \oplus H_- \) endowed with inner product

\[
\langle f, g \rangle_{H_K} = \langle f_+, g_+ \rangle_{H_+} + \langle f_-, g_- \rangle_{H_-} \quad (f_\pm, g_\pm \in H_\pm)
\]

can be associated with \( K \). For a Kreın space \( K \), the decomposition \( K = H_+ \oplus H_- \) is not necessarily unique. Thus, a Kreın space can, in general, be associated with infinitely many Hilbert spaces. However, for any such Hilbert space \( H_K \), the topology introduced on \( K \) via the norm \( \|f\|_{H_K} = \sqrt{\langle f, f \rangle_{H_K}} \) is independent of the decomposition and the associated Hilbert space. More specifically, all the norms \( \|\cdot\|_{H_K} \) generated by different decompositions of \( K \) into direct sums of Hilbert spaces are topologically equivalent (Langer, 1962). The topology on \( K \) defined by the norm of an associated Hilbert space is called the strong topology on \( K \). Henceforth, notions of convergence and continuity on a Kreın space are defined with respect to the strong topology. As the strong topology of a Kreın space is a Hilbert space topology, the Riesz representation theorem holds.

More formally, for a continuous linear functional \( L \) on a Kreın space \( K \), there exists a unique \( g \in K \) such that the functional \( L \), for all \( f \in K \), can be written as \( Lf = \langle f, g \rangle_K \).

Having reviewed basic properties of Kreın spaces, we are now ready to introduce the notion of a reproducing kernel Kreın space.

**Definition 2.** (Alpay, 1991; Ong et al., 2004) A Kreın space \( (K, \langle \cdot, \cdot \rangle_K) \) is a reproducing kernel Kreın space if \( K \subset \mathbb{R}^X \) and the evaluation functional is continuous on \( K \) with respect to the strong topology.

The following theorem provides a characterization of reproducing kernel Kreın spaces.

**Theorem 1.** (Alpay, 1991; Schwartz, 1964) Let \( k : X \times X \rightarrow \mathbb{R} \) 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 (1964) and it can also be found in Alpay (Theorem 2.2, 1991). On finite discrete spaces, however, any symmetric kernel function admits a Kreın decomposition.

3. Regularized Risk Minimization in Reproducing Kernel Kreın Spaces

Building on the work by Ong et al. (2004), we first propose a novel regularized risk minimization problem for learning in reproducing kernel Kreın spaces and then show that the strong representer theorem applies to it (Section 3.1). The main difference compared to previous stabilization approaches due to Ong et al. (2004) is in the way the optimization problem accounts for the complexity of hypotheses. As a result of our representer theorem, the proposed regularized risk minimization problem defined over a reproducing kernel Kreın space can be transformed into a non-convex optimization problem over a Euclidean space. Following
this, we build on the work by Gander et al. (1989) and show how to find a globally optimal solution to the transformed non-convex optimization problem. Having provided means for finding an optimal solution to the learning problem, we present a sample complexity bound (Ong et al., 2004) which shows that learning in a reproducing kernel Kreın space is consistent (Section 3.2). The section concludes with a procedure for the optimization of hyperparameters arising in our regularized risk minimization problem (Section 3.3).

3.1. Optimization Problem

We retain the notation from Section 2 and assume that a sample \( z = \{(x_i, y_i)\}_{i=1}^n \) has been drawn independently from a Borel probability measure \( \rho \) defined on \( \mathcal{Z} = \mathcal{X} \times \mathcal{Y} \), with \( \mathcal{Y} \subset \mathbb{R} \). For an approximation of the target function \( f_\rho(x) = \int y \, d\rho(y \mid x) \), we measure the goodness of fit with the expected squared error in \( \rho \), i.e.,

\[
\mathcal{E}_\rho(f) = \langle f(x) - y \rangle^2 \, d\rho.
\]

The empirical counterpart of the error, defined over a sample \( z \in \mathcal{Z}^n \) is denoted with \( \mathcal{E}_z(f) = \frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2 \).

Early attempts at defining a regularized risk minimization problem for learning in reproducing kernel Kreın spaces are based on the stabilization approach by Ong et al. (2004). We start with an instance of that approach where the stabilization is replaced with minimization over a reproducing kernel space. More formally, we refer to the following risk minimization problem over a reproducing kernel space as the OMCS-Kreın problem (Ong et al., 2004)

\[
\begin{align*}
\min_{f \in \mathcal{K}} & \quad \frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda \langle f, f \rangle_{\mathcal{K}} \\
\text{s.t.} & \quad \frac{1}{n} \sum_{i=1}^n f(x_i) - \frac{1}{n} \sum_{j=1}^n f(x_j)^2 = r^2.
\end{align*}
\]

The empirical squared error depends on \( f \in \mathcal{K} \) only through its evaluations \( f(x_i) \), with \( 1 \leq i \leq n \). Moreover, the squared error loss function is convex and thus, satisfies the requirement on the loss function from the representer theorem for stabilization (Theorem 11, Ong et al., 2004). In Eq. (1), we choose the linear identity function as the stabilizer and constrain the solution space by matching the variance of the estimator \( f \) to an a priori specified hyperparameter. Thus, the OMCS-Kreın problem satisfies the conditions from the representer theorem for stabilization (Ong et al., 2004) and any saddle point of the optimization problem in Eq. (1) admits the expansion as \( f^* = \sum_{i=1}^n \alpha_i k(x_i, \cdot) \) with \( \alpha_i \in \mathbb{R} \). This allows us to express the optimization problem from Eq. (1) in terms of the parameters \( \alpha \in \mathbb{R}^n \). To simplify our derivations, we can without loss of generality assume that the kernel matrix \( K \) is centered, where \( K_{ij} = k(x_i, x_j) \) for \( 1 \leq i, j \leq n \). Then, substituting \( f = \sum_{i=1}^n \alpha_i k(x_i, \cdot) \) and using the reproducing property of the Kreın kernel \( k \) we can rewrite the optimization problem from Eq. (1) as

\[
\begin{align*}
\min_{\alpha \in \mathbb{R}^n} & \quad \|K\alpha - y\|^2_2 + n\lambda^2 \alpha^\top K\alpha \\
\text{s.t.} & \quad \alpha^\top K^2\alpha = nr^2.
\end{align*}
\]

The OMCS-Kreın regularized risk minimization problem is non-convex and can have exponentially many local optima. Despite this, we subsequently show how to find a globally optimal solution to this problem in time cubic in the size of the kernel expansion. However, our empirical evaluation of the approach (presented in Section 5) demonstrates that it fails to generalize to unseen instances. As \( \langle f, f \rangle_{\mathcal{K}} = \|f_+\|^2_{\mathcal{H}_+} - \|f_-\|^2_{\mathcal{H}_-} \) does not define a norm, we suspect that the regularization term does not capture the complexity of hypotheses from the reproducing kernel Kreın space \( \mathcal{K} \). To address this, we propose to penalize the complexity of hypotheses via decomposition components \( \mathcal{H}_\pm \) and/or the strong topology on \( \mathcal{K} \). More formally, we propose the following regularized risk minimization problem for learning in reproducing kernel Kreın spaces and henceforth refer to it as the Kreın problem

\[
\begin{align*}
\min_{f \in \mathcal{K}} & \quad \frac{1}{n} \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda_+ \|f_+\|^2_{\mathcal{H}_+} + \lambda_- \|f_-\|^2_{\mathcal{H}_-} \\
\text{s.t.} & \quad \frac{1}{n} \sum_{i=1}^n f(x_i) - \frac{1}{n} \sum_{j=1}^n f(x_j)^2 = r^2.
\end{align*}
\]

Having introduced our regularized risk minimization problem, we show that the following strong representer theorem applies to it (a proof is provided in Appendix A).

**Theorem 2.** Let \( f^* \in \mathcal{K} \) be an optimal solution to the Kreın optimization problem from Eq. (3). Then, \( f^* \) admits the expansion \( f^* = \sum_{i=1}^n \alpha_i k(x_i, \cdot) \) with \( \alpha_i \in \mathbb{R} \).

The representer theorem allows us to express the regularized risk minimization problem as an optimization problem over a Euclidean space. In particular, substituting \( f = \sum_{i=1}^n \alpha_i k(x_i, \cdot) \) into Eq. (3) we deduce

\[
\begin{align*}
\min_{\alpha \in \mathbb{R}^n} & \quad \|K\alpha - y\|^2_2 + n\alpha^\top (\lambda_+^2 K_+ + \lambda_-^2 K_-) \alpha \\
\text{s.t.} & \quad \alpha^\top K^2\alpha = nr^2,
\end{align*}
\]

where \( K_\pm \) are kernel matrices corresponding to disjoint reproducing kernel Hilbert spaces given by positive definite kernels \( k_\pm \), \( k = k_+ - k_- \), and \( K = K_+ + K_- \).

The optimization problems in Eq. (2) and (4) are minimizing quadratic forms over hyperellipsoids with radius \( r \) and center at the origin. As such, the problems are non-convex even in the cases when the regularization term is defined with a positive definite matrix. Despite this, it is possible to find a globally optimal solution to such a problem using a method proposed by Gander et al. (1989). To simplify our
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presentation, we focus on our regularized risk minimization problem from Eq. (4) and note that the derivation for the OMC-S-Krein problem follows along these lines. First, we provide a proposition which is crucial for finding a globally optimal solution to the problem in Eq. (4). To this end, let us derive the Lagrangian of that optimization problem as

\[ L(\alpha, \mu) = \alpha^\top (\lambda_+^2 K_+ + \lambda_-^2 K_-) \alpha - 2y^\top K \alpha - \mu (\alpha^\top K^2 \alpha - r^2), \]

and denote with \( \Theta(\alpha) \) the optimization objective in problem (4). If we now set the derivative of the Lagrangian to zero, we obtain the following two stationary constraints

\[ (\lambda_+^2 K_+ + \lambda_-^2 K_-) \alpha = Ky + \mu K^2 \alpha, \]

\[ \alpha^\top K^2 \alpha - r^2 = 0. \]  

Having introduced all the relevant terms, we are now ready to characterize a globally optimal solution to problem (4).

**Proposition 3.** (Forsythe & Golub, 1965; Gander et al., 1989) The optimization objective \( \Theta(\alpha) \) attains its minimal value at the tuple \((\alpha^*, \mu^*)\) satisfying the stationary constraints (5) with the smallest value of \( \mu \). Analogously, the maximal value of \( \Theta(\alpha) \) is attained at the tuple with the largest value of the Lagrange multiplier \( \mu \).

Hence, instead of the original optimization problem (4) we can solve the system with two stationary equations (5) and minimal \( \mu \). Gander et al. (1989) propose two methods for solving such problems. In the first approach, the problem is reduced to a quadratic eigenvalue problem and afterwards transformed into a linear eigenvalue problem. In the second approach, the problem is reduced to solving a one-dimensional secular equation. The first approach is more elegant, as it allows us to compute the solution in a closed form. More specifically, the solution to problem (4) is given by (Gander et al., 1989)

\[ \alpha^* = (\lambda_+^2 P_+ - \lambda_+^{2*} P_- - \mu^* K)^{-1} y, \]

where \( \mu^* \) is the smallest real eigenvalue of the matrix

\[ \begin{bmatrix} \lambda_+^2 K_+^\dag + \lambda_-^2 K_-^\dag & -I \\ -y y^\top /r^2 & \lambda_-^2 K_+^\dag + \lambda_+^2 K_-^\dag \end{bmatrix}, \]

\[ P_{\pm} = V I_{\pm} V^\top, K = V \Sigma V^\top \] is an eigendecomposition of \( K \), and \( I_{\pm} \) are diagonal matrices with ones at places corresponding to positive/negative eigenvalues of \( K \).

Despite its elegance, the approach requires us to: i) invert/decompose a positive definite matrix, and ii) decompose a non-symmetric block matrix of dimension \( 2n \), which is not a numerically stable task for every such matrix. Furthermore, the computed solution \( \alpha^* \) highly depends on the precision up to which the optimal \( \mu \) is computed and for an imprecise value the solution might not be on the correct hyperellipsoid at all (e.g., see Gander et al., 1989).

For this reason, we rely on the secular approach in the computation of the optimal solution. Gander et al. (1989) proposed an efficient algorithm for the computation of the optimal Lagrange multiplier to machine precision. For the sake of completeness (and brevity), we review this approach in Appendix B and in the remainder of the section describe how to derive the secular equation required to compute the optimal multiplier. First, we perform the eigendecomposition of the symmetric and indefinite kernel matrix \( K = V \Sigma V^\top \). From this eigendecomposition, we derive the decompositions of matrices \( K_{\pm} = V \Sigma_{\pm} V^\top \), where \( \Sigma_+ / \Sigma_- \) are diagonal matrices with the absolute values of the positive/negative eigenvalues of \( K \) at their respective diagonals, padded with zeros. The decomposition of \( K \) allows us to transform the stationary constraints from Eq. (5) as

\[ V \left( \lambda_+^2 \Sigma_+ + \lambda_-^2 \Sigma_- \right) V^\top u = y + \mu u, \]

where \( u = K \alpha, u^\top u = r^2 \), and \( \Sigma_{\pm} \) denote the pseudo-inverses of the diagonal matrices \( \Sigma_{\pm} \). Then, this resulting equation is multiplied with the orthogonal matrix \( V^\top \) from the left and transformed into

\[ \left( \lambda_+^2 \Sigma_+ + \lambda_-^2 \Sigma_- \right) \hat{u} = \hat{y} + \mu \hat{u}, \]

with \( \hat{y} = V^\top y \) and \( \hat{u} = V^\top u \). From here, we deduce

\[ \hat{u}(\mu) = \sigma_i \hat{v}_i / (\lambda_+^2 \sigma_i - \mu \sigma_i) \quad (i = 1, 2, ..., n), \]

and substitute the computed vector \( \hat{u}(\mu) \in \mathbb{R}^n \) into the second stationary constraint to form the secular equation

\[ g(\mu) = \sigma_i \hat{v}_i / (\lambda_+^2 \sigma_i - \mu \sigma_i) - r^2 = 0. \]

The optimal value of the parameter \( \mu \) is the smallest root of this non-linear secular equation and the optimal solution to problem (4) is given by \( u^* = V \hat{u}(\mu^*) \). Moreover, the interval at which the root lies is known (Gander et al., 1989). In particular, the quadratic term from Eq. (4) is a positive definite matrix and \( \mu^* \in (-\infty, \lambda_+^2 / \sigma_+) \), where \( \sigma_+ \) is the largest eigenvalue of the matrix \( |K| \). On the other hand, the quadratic term from Eq. (2) is an indefinite matrix and \( \mu^* \in (-\infty, \lambda_-^2 / \sigma_-) \), where \( \sigma_- \) is the largest negative eigenvalue of the matrix \( K \). The condition on the interval of the optimal Lagrange multiplier implies that the matrix defining the optimal solution \( u^* \) is positive semidefinite. Thus, the proposed regularized risk minimization problem is well-posed if \( \mu^* \neq \lambda_+^2 / \sigma_+ \). The computational complexity of both approaches (secular and eigenvalue) is \( O(n^3) \).

### 3.2. Generalization Bound

In this section, we present a generalization bound for learning in a reproducing kernel Krein space using the proposed
We now show how to improve the inductive bias (Baxter, 2000) of our approach by automatically tuning the hyperparameters while performing inner cross-validation. In this process, we split the training data into training and validation folds and select a validation function that will be optimized with respect to the hyperparameter vector. The optimization can be performed with an off-the-shelf algorithm (e.g., L-BFGS-B solver) as long as we are able to compute the hyperparameter gradient of the validation function.

Denote the training and validation examples with $F$ and $F^\perp$, respectively. Then, the validation function corresponding to the squared error loss function is given by

$$
\Xi(F, f) = \frac{1}{|F^\perp|} \sum_{(x,y) \in F^\perp} (f(x) - y)^2,
$$

where $f = \sum_{i=1}^n \alpha_i k(x_i, \cdot)$ is a hypothesis from the reproducing kernel Krein space defined by training examples in $F$. Now, denote the hyperparameter vector with $\theta$ consisting of scalars $\lambda_{\pm}$ and $r$ that control the capacity of the hypothesis and a vector $\eta$ parameterizing the kernel function. Then, the gradient of this validation function is given by

$$
\nabla \Xi(F, f) = \frac{2}{|F^\perp|} \sum_{(x,y) \in F^\perp} \left( K_x^\top \alpha - y \right) \cdot \left( (\partial K_x/\partial \theta)^\top \alpha + K_x^\top \partial \alpha/\partial \theta \right).
$$

A globally optimal solution to our regularized risk minimization problem is given in a closed form in Eq. (6). From that solution, we can derive the gradient of $\alpha$ with respect to the hyperparameters. More specifically, we have

$$
\tau \frac{\partial \alpha}{\partial \theta} = - t^\top P_+ \alpha \frac{\partial}{\partial \theta} (\lambda_+)^2 + t^\top P_- \alpha \frac{\partial}{\partial \theta} (\lambda_-)^2 + t^\top \mu^* + \mu^* t^\top \frac{\partial K}{\partial \theta} \alpha,
$$

with $\tau = \frac{2}{|F^\perp|} \sum_{(x,y) \in F_1} (K_x^\top \alpha - y)K_x$, $St = \tau$, and $S = V (\lambda_+^2 \mathbb{I} - \lambda_-^2 \mathbb{I} - \mu^* \Sigma) V^\top$ that can be computed from the eigendecomposition of $K$. Thus, $t$ is the solution of a linear system which can be solved in time quadratic in the number of instances using the eigendecomposition of $S$.

Before we give the gradients of the hyperparameters, we need to find the derivative of the optimal Lagrange multiplier $\mu^*$. In order to do this, we substitute the expression for $u^*$ into the second stationary constraint from Eq. (5) to obtain

$$
y^\top (\lambda_+^2 K_+^{-1} + \lambda_-^2 K_-^{-1} - \mu^*)^{-2} y = r^2.
$$

To find the derivative of $\mu^*$ with respect to $\theta$ we need to implicitly derive the latter equation. In particular, taking the derivative of both sides with respect to $\theta$ we deduce

$$
\frac{\partial}{\partial \theta} \left( \frac{r^2}{2} \right) = - q^\top P_+ u \frac{\partial}{\partial \theta} (\lambda_+^2) + q^\top P_- u \frac{\partial}{\partial \theta} (\lambda_-^2) + u^\top \frac{\partial K}{\partial \theta} \alpha + \mu^* q^\top K \frac{\partial K}{\partial \theta} \alpha + q^\top K u \frac{\partial \mu^*}{\partial \theta},
$$

where $q = \sum_{i=1}^n \alpha_i k(x_i, \cdot)$.
where \( q \) is the solution of the linear system \( Sq = u \) which can again be solved in quadratic time using the eigendecomposition of \( S \). From the latter equation, we derive the gradient of the optimal Lagrange multiplier \( \mu^* \) with respect to the individual hyperparameters (a detailed derivation is provided in Appendix E). If we now substitute the derived gradients of the optimal multiplier \( \mu^* \) into \( \frac{\partial}{\partial \eta} q \), we obtain

\[
\tau^T \frac{\partial \alpha}{\partial \tau} = \tau^T u \frac{t^T K u}{q^T K u},
\]

\[
\tau^T \frac{\partial \alpha}{\partial \eta} = \frac{t^T u}{q^T K u} (-u - \mu^* K q)^T \frac{\partial K}{\partial \eta} \alpha + \mu^* t^T \frac{\partial K}{\partial \eta} \alpha,
\]

\[
\tau^T \frac{\partial \alpha}{\partial \lambda_{\pm}} = 2\lambda_{\pm} \left( \pm \frac{t^T u}{q^T K u} q^T P_{\pm} u \mp t^T P_{\pm} \alpha \right).
\]

Now, the gradient of the validation function \( \Xi(F, f) \) can be derived by substituting the individual gradients into Eq. (8).

### 4. Related Work

From the perspective of practitioners, the main advantage of the proposed regularized risk minimization problem over standard kernel methods is the fact that a kernel function does not need to be positive definite. It is often well beyond the ability of practitioners to verify this condition and many intuitive/interpretable similarity functions are not positive definite. Previous approaches for dealing with indefiniteness of kernel matrices can be divided into three classes: i) transformations of the kernel spectrum, ii) stabilization instead of minimization of a risk functional, and iii) learning with evaluation functionals as features.

The first class of approaches aims at converting an indefinite kernel function, which defines a reproducing kernel Krein space, to a positive definite one. Perhaps the simplest such approach is to clip the spectrum of the kernel matrix, i.e., set the negative eigenvalues to zero (Wu et al., 2005). This corresponds to projecting an indefinite kernel matrix to the cone of positive definite matrices. The approach can be motivated by problems in which negative spectrum amounts to noise, rather than useful information. Another approach from this class, considers shifting the spectrum of the kernel matrix by adding the absolute value of the smallest eigenvalue to the diagonal of the kernel matrix (Roth et al., 2003; Zhang et al., 2006). While spectrum clip changes the kernel matrix, spectrum shift modifies only its diagonal entries. Some approaches consider mapping of an indefinite kernel matrix to its square which is positive definite (Chen et al., 2009; Graepel et al., 1998). Another popular transformation flips the spectrum by taking the absolute value of the eigenvalues (Graepel et al., 1998; Loosli et al., 2016). This transformation is equivalent to learning in an associated Hilbert space corresponding to a decomposition of a Krein kernel. We conclude our brief review of spectral transformations with the work by Ong et al. (2004), which regularizes the risk minimization by setting to zero the eigenvalues with the absolute value below an a priori specified threshold. The hypothesis is then obtained by solving the linear system given by the minimization of the expected squared error.

In the second class of approaches, the minimization of a regularized risk functional is replaced with its stabilization. The stabilization of a risk functional, first proposed by Ong et al. (2004), can intuitively be interpreted as setting with a good stationary point of the regularized risk minimization. Early approaches from this class involved optimization of support vector machines while ignoring the non-convexity of the optimization problem (Lin & Lin, 2003). Recently, Loosli et al. (2016) have proposed a support vector machine for learning in Krein spaces that performs stabilization by finding a hypothesis in a reproducing kernel Krein space \( (H_+, \oplus H_-, \langle \cdot, \cdot \rangle_K) \) that solves the corresponding primal optimization problem by minimizing over \( H_+ \) and maximizing over \( H_- \). As the authors of that work show, this amounts to solving the dual optimization problem over the associated reproducing kernel Hilbert space \( (H_+ \oplus H_-, \langle \cdot, \cdot \rangle_K) \). The approach is related to considerations by Graepel et al. (1998), where the eigenvalues of an indefinite kernel matrix are replaced with their absolute values. Another support vector machine approach for learning in Krein spaces was proposed by Luss & d’Aspremont (2009). A key idea in that work is to first find a positive definite matrix that approximates well the indefinite one and then learn a support vector machine predictor with that positive definite matrix as the kernel matrix. Thus, the approach can be seen as a sophisticated transformation of spectrum, where an indefinite matrix is mapped to a positive definite one using training examples. Chen & Ye (2008) have provided a fast algorithm for this variant of support vector machines in Krein spaces.

The third class of approaches first embeds instances into a feature space defined by kernel values between them and a fixed number of landmarks from the instance space. Following this, a linear model is used in the constructed feature space to learn a target concept. Chen et al. (2009) have considered such an approach for learning with symmetric similarity/kernel functions, providing a detailed empirical study and a generalization bound. Recently, Alabdulmohsin et al. (2015) have reported promising empirical results using support vector machines with \( \ell_1 \)-norm regularization and indefinite kernels as features. Balkan et al. (2008) have studied generalization properties of learning with kernel/similarity functions as features. Their theoretical results demonstrate 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.

An important aspect of learning with indefinite kernels is the consistent treatment of training and test instances known as the *out-of-sample extension*. While this problem does not occur in transductive setting, where the kernel matrix can be constructed using both training and test samples, it affects a number of approaches based on spectral transformations. In particular, Chen et al. (2009) have constructed a linear operator to deal with training and test samples consistently in the case of spectrum clip. In addition to this, the authors of that work have provided an out-of-sample extension for spectrum flip without a theoretical result guaranteeing its consistency. Contrary to some of the previous empirical studies, these out-of-sample extensions are used in our experiments to transform test samples. For other transformations, such as spectrum shift, the described regularization by Ong et al. (2004), and/or matrix inversion no linear transformation exists to consistently deal with training and test samples. In these cases, it is possible to use a heuristic proposed by Wu et al. (2005), that can also be found in Chen et al. (2009). The heuristic first applies the spectral transformation to a kernel matrix comprised of training instances and a test sample and then uses the transformed part of the kernel matrix corresponding to the test sample to define its kernel expansion. In our experiments, we use this heuristic for shift and square transformations of the kernel spectrum.

### 5. Experiments

The presented optimization procedure can compute a globally optimal solution to the regularized risk minimization problem defined by either a positive definite (e.g., regularization via decomposition components $H_\perp$) or an indefinite regularization/quotient term (e.g., regularization via $(\cdot, \cdot)_\perp$). In the first set of experiments, we exploit this to gain an insight into the effectiveness of learning in reproducing kernel Krein spaces using: i) our approach that regularizes via decomposition components (Krein), ii) an approach that regularizes via the strong topology (FLIP), iii) a variant of the stabilization approach (OMCS-Krein) motivated by Ong et al. (2004), and iv) approaches relying on spectral transformations of the kernel matrix (CLIP, SHIFT, SQUARE). In the first case, we find a globally optimal solution to the problem from Eq. (4) and in others we solve the problem from Eq. (2), defined with an indefinite kernel matrix or a spectral transformation in place the matrix $K$. Having established that the regularization via decomposition components of a reproducing kernel Krein space is effective, we perform a series of experiments on real-world datasets with different structured representations (i.e., strings, graphs, shapes). More specifically, we evaluate the effectiveness of our approach with respect to the state-of-the-art baselines for learning in reproducing kernel Krein spaces: i) Krein support vector machine (Loosli et al., 2016), and ii) linear ridge regression with similarities as features (Alabdulmohsin et al., 2015; Chen et al., 2009). In addition to this, we perform a series of experiments with variants of standard indefinite kernels on vectorial data (described in Appendix D) and demonstrate that on some problems indefinite kernels can be more effective than the positive definite ones. A detailed description of the experimental setup can be found in Appendix C.
Table 3. This table presents the results of experiments on real-world datasets in which the proposed risk minimization problem is used to evaluate the effectiveness of indefinite kernels on classification and regression tasks. For classification tasks, we measure the effectiveness of a kernel using the average percentage of misclassified examples, computed after performing 10 fold cross-validation. The effectiveness on regression tasks is measured using the root mean squared error, which is also computed after performing 10 fold cross-validation.

<table>
<thead>
<tr>
<th>DATASET</th>
<th>SIGMOID e</th>
<th>RL-SIGMOID e</th>
<th>DELTA-GAUSS e</th>
<th>EFRANGELINHOV e</th>
<th>GAUSS e</th>
<th>RL-GAUSS e</th>
</tr>
</thead>
<tbody>
<tr>
<td>RABEN (n = 306)</td>
<td>29.99 (5.76) 0.11</td>
<td>30.76 (5.85) 0.21</td>
<td>30.31 (5.63) 0.60</td>
<td>32.25 (5.78) 0.02</td>
<td>30.61 (5.80) 0.00</td>
<td>29.69 (5.80) 0.00</td>
</tr>
<tr>
<td>INOSOPHIE (n = 351)</td>
<td>9.95 (4.26) 0.34</td>
<td>7.96 (5.22) 0.40</td>
<td>6.20 (4.92) 0.06</td>
<td>7.45 (5.07) 0.02</td>
<td>6.20 (4.92) 0.00</td>
<td>8.25 (4.42) 0.00</td>
</tr>
<tr>
<td>BREASTCANCER (n = 683)</td>
<td>2.63 (1.71) 0.29</td>
<td>3.15 (2.91) 0.26</td>
<td>2.93 (1.86) 0.40</td>
<td>3.36 (2.79) 0.03</td>
<td>3.21 (2.68) 0.00</td>
<td>2.63 (1.94) 0.00</td>
</tr>
<tr>
<td>AUSTRALIAN (n = 690)</td>
<td>14.32 (4.89) 0.14</td>
<td>15.89 (4.02) 0.38</td>
<td>14.18 (4.80) 0.60</td>
<td>13.76 (4.80) 0.01</td>
<td>14.18 (4.58) 0.00</td>
<td>13.74 (4.16) 0.00</td>
</tr>
<tr>
<td>AIRFOIL (n = 1563)</td>
<td>8.31 (1.62) 0.07</td>
<td>7.59 (1.03) 0.25</td>
<td>6.12 (0.53) 0.49</td>
<td>8.84 (0.77) 0.04</td>
<td>8.54 (1.89) 0.00</td>
<td>9.21 (1.74) 0.00</td>
</tr>
</tbody>
</table>

Conclusion

We have proposed a novel regularized risk minimization problem for learning in reproducing kernel Krein spaces and showed that the strong representor theorem applies to it. The approach is consistent and guaranteed to find an optimal solution in time cubic in the number of training examples. Moreover, we have provided means for efficient hyperparameter tuning by deriving the gradient of the solution with respect to its hyperparameters. Our empirical results demonstrate the effectiveness of regularizing via decomposition components of a reproducing kernel Krein space compared to learning with different spectrum transformations, as well as the state-of-the-art competing approaches. The results obtained on real-world vectorial datasets show that on some problems variants of the well-known indefinite kernels can outperform the frequently used positive definite ones.
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