ANALYSIS OF REGULARIZED NYSTRÖM SUBSAMPLING FOR
REGRESSION FUNCTIONS OF LOW SMOOTHNESS

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Abstract. This paper studies a Nyström type subsampling approach to large kernel learning methods in the misspecified case, where the target function is not assumed to belong to the reproducing kernel Hilbert space generated by the underlying kernel. This case is less understood, in spite of its practical importance. To model such a case, the smoothness of target functions is described in terms of general source conditions. It is surprising that almost for the whole range of the source conditions, describing the misspecified case, the corresponding learning rate bounds can be achieved with just one value of the regularization parameter. This observation allows a formulation of mild conditions under which the plain Nyström subsampling can be realized with subquadratic cost maintaining the guaranteed learning rates.

1. Introduction

The supervised learning can often be formalized as the problem of minimizing the expected squared loss

$$\mathcal{E}(f) = \int_{X \times Y} (f(x) - y)^2 d\rho(x,y),$$

given a training set $z = \{z_i, i = 1, 2, ..., |z|\}$ of samples $z_i = (x_i, y_i)$ drawn independently from a fixed but unknown (joint) probability distribution $\rho$ on $Z = X \times Y$, where $X$ is a set of $d$-dimensional input vectors $x$, and $Y$ is a set of corresponding outputs labeled by real numbers $y$. Here we denote $|z|$ be the number of the observations. The primary objective is the regression function $f_\rho$ that minimizes $\mathcal{E}(f)$ and can be written as

$$f_\rho(x) = \int_Y y d\rho(y|x), \quad x \in X,$$

where $\rho(y|x)$ is the conditional distribution at $x$ induced by $\rho$ such that $\rho(x, y) = \rho(y|x) \rho_X(x)$, and $\rho_X$ is the marginal probability measure on $X$.

Since the conditional distribution $\rho(y|x)$ is unknown, the above integral representation for $f_\rho$ is of no help in practice, and the goal is to find an estimator $\hat{f}_z$, on
the base of the given training data $z$, that approximates the unknown regression function $f_\rho$ well with high probability.

Ideally, a good estimator $\hat{f}_z$ should have small excess loss $\mathcal{E}(\hat{f}_z) - \mathcal{E}(f_\rho)$. Due to a version of Fubini’s theorem we have

$$\mathcal{E}(\hat{f}_z) - \mathcal{E}(f_\rho) = \| \hat{f}_z - f_\rho \|_\rho^2,$$

where $\| \cdot \|_\rho := \| \cdot \|_{L^2(X, \rho_X)}$ is the norm in the space $L^2(X, \rho_X)$ of square integrable functions with respect to the marginal probability measure. Therefore, the standard way of measuring the performance of the estimator $\hat{f}_z$ is by studying its convergence to $f_\rho$ in $\| \cdot \|_\rho$-norm.

In kernel machine learning the estimator $\hat{f}_z$ is sought within some hypothesis space, often taken to be a reproducing kernel Hilbert space $H_K$ associated with a Mercer kernel $K : X \times X \to \mathbb{R}$. The space $H_K$ is then defined to be the closure of the linear span of the set of functions $K_x = K(\cdot, x)$, $x \in X$, with the inner product satisfying

$$\langle K_x, K_y \rangle_{H_K} := K(x, y), \quad x, y \in X.$$

One of the main drawbacks of kernel learning machines is that the storing and manipulating the kernel Gram matrix $K_{|z|} = \{ K(x_i, x_j) \}_{i,j=1}^{|z|}$ require $O(|z|^2)$ space, and the amount of computations required to find $\hat{f}_z \in H_K$ scales as $O(|z|^3)$, that can become intractable in the case of the so-called Big Data, when $|z|$ grows. The Nyström type subsampling [20, 16] is a popular tool for overcoming these limitations.

Up to now, the theoretical analysis of the Nyström approach has been carried out extensively in the well-specified case, when the regression function $f_\rho \in H_K$ [1, 6, 9, 11, 13, 14]. In the present paper we concentrate ourselves on the misspecified case such that $f_\rho \in L^2(X, \rho_X) \setminus H_K$, which is much less understood, in spite of its practical importance.

The quality of the approximation $\hat{f}_z$ depends on smoothness properties of the underlying regression function $f_\rho$, often given in terms of source conditions and the canonical inclusion operator $J_K : H_K \hookrightarrow L^2(X, \rho_X)$.

We highlight that the misspecified case yields the fact that the (unknown) target function $f_\rho$ does not belong to $H_K$, and hence that for the regularized empirical risk functional $T_\lambda^z$ from (2.1) below, we will have that $T_\lambda^z(f_\rho) = +\infty$. Such an oversmoothing penalty term is not standard in classic regularization theory, see e.g. [1], but it has gained attention in numerical differentiation [19, 18] and regularization in Hilbert scales [12, 5]. In the present setting the convergence analysis shall be carried out in the norm in the space $L^2(X, \rho_X)$ instead of the norm in the reproducing kernel Hilbert space $H_K$.

Due to [13] the Nyström approach can be seen as a combination of random projections with a regularization scheme, and the regularization theory tells us that such a scheme should have enough qualification to utilize the whole smoothness of $f_\rho$. On the other hand, from this perspective it follows that, because of low smoothness of $f_\rho$, even a scheme with a modest qualification, such as the standard Tikhonov regularization, is sufficient for the misspecified case. For this reason, in the present study we restrict ourselves to the Nyström subsampling for Tikhonov regularization known also as the kernel ridge regression (KRR).
The learning rate (i.e., the convergence rate of the approximant to the target function \( f_\rho \) in \( \| \cdot \|_\rho \)-norm) of KRR in the misspecified case was first studied in [15]. As one may see from that study, for \( f_\rho \in L_2(X, \rho_X) \setminus \mathcal{H}_K \) the learning rate of KRR cannot be in general described by the same formula as in the well-specified case \( f_\rho \in \mathcal{H}_K \). A uniform description for both cases was obtained in [17] under additional assumptions on the inclusion operator \( J_K \), which may not be always satisfied. To the best of our knowledge, the best known learning rates, that are valid for KRR with arbitrary Mercer kernel functions \( K \), have been recently given in [7]. In the present research we study conditions under which the above mentioned rates can be achieved at a subquadratic cost (with respect to the number of observations \( |z| \)) by KRR combined with the Nyström approach.

The paper is organized as follows. In the next section we recall KRR setting. Then we follow [13] and consider the Nyström approach to KRR as a projection method regularized by Tikhonov regularization. In Section 3 we estimate the learning rate of KRR combined with the plain Nyström subsampling in the misspecified case. The technical proofs are given separately in Section 4.

In contrast to previous studies, we employ general source conditions to measure the smoothness \( f_\rho \in L_2(X, \rho_X) \setminus \mathcal{H}_K \). One important and interesting observation here is that almost for the whole range of source conditions describing the misspecified case the corresponding learning rate bounds can be achieved with the same value of Tikhonov regularization parameter that can be chosen a priori and without any knowledge of the smoothness of \( f_\rho \). This observation allows us to formulate simple conditions under which the plain Nyström subsampling can be realized with subquadratic cost, still maintaining guaranteed learning rates.

2. KRR with Nyström subsampling

Recall that in KRR the goal is to approximate \( f_\rho \) by the minimizer \( f^\lambda_z \) of the regularized empirical risk functional

\[
T^\lambda_z(f) := |z|^{-1} \sum_{i=1}^{|z|} (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}_K}^2, \quad f \in \mathcal{H}_K.
\]

For the subsequent analysis we shall use the identical operator \( I: \mathcal{H}_K \to \mathcal{H}_K \), the canonical inclusion \( J_K: \mathcal{H}_K \to L_2(X, \rho_X) \), and the sampling operators \( S_x: \mathcal{H}_K \to \mathbb{R}^{|z|} \), given as \( S_x f = (f(x_i))_{i=1}^{|z|} \), and its adjoint \( S^*_x: \mathbb{R}^{|z|} \to \mathcal{H}_K \). It is known, cf. [7], that the product of the inclusion operator \( J_K \) and its adjoint is the integral operator defined by

\[
(J_K J^*_K) f(x) = \int_X K(x,t) f(t) d\rho_X(t), \quad f \in L_2(X, \rho_X), \quad x \in X.
\]

The celebrated representer theorem of G. S. Kimeldorf and G. Wahba tells us that the minimizer of (2.1) has the form

\[
f_z^\lambda = \sum_{i=1}^{|z|} c_i \cdot K(\cdot, x_i), \quad c = (c_i)_{i=1}^{|z|} = (\mathbb{K}_{|z|} + \lambda \mathbb{I})^{-1} \mathbb{Y},
\]

where \( \mathbb{I} \) is the \( |z| \times |z| \) diagonal identity matrix and \( \mathbb{Y} = (y_i)_{i=1}^{|z|} \).
It is clear that KRR has at least quadratic computational cost $\mathcal{O}(|z|^2)$, as this is the cost of computing the kernel Gram matrix $K_{[z]} = \{K(x_i, x_j)\}_{i,j=1}^{|z|}$. Therefore, in the setting, where $|z|$ is large, one tries to avoid the computation of the minimizer $f_z^\lambda$.

2.1. Plain Nyström subsampling. In the Nyström algorithms this is done by replacing $K_{[z]}$ with a smaller low-rank matrix obtained by random subsampling of columns of $K_{[z]}$. In the forthcoming analysis, we restrict attention to the so-called plain Nyström subsampling approach, where the points $(x_i, y_i)$ forming the subsample $z''$ are sampled uniformly at random without replacement from the training set $z$.

An important observation made in [13] is that the Nyström subsampling can be interpreted as a restriction of the minimization of $T_z^\lambda(f)$ to the (randomly chosen) space

$$\mathcal{H}_K^{z''} := \{f : f = \sum_{x_i, (y_i, y_j) \in z''} c_i K(\cdot, x_i), c_i \in \mathbb{R}\} \subset \mathcal{H}_K,$$

where $z''$ is a randomly selected subset of $z$ with the cardinality $|z''| \ll |z|$.

We let $P_{z''} : \mathcal{H}_K \to \mathcal{H}_K^{z''}$ be the orthogonal projection operator in $\mathcal{H}_K$ with the range $\mathcal{H}_K^{z''}$. It is clear that $P_{z''}$ has a probabilistic character and depends on the way we perform the subsampling $z''$.

In the analysis the composition $B_{z''} := S_x P_{z''} : \mathcal{H}_K \to \mathbb{R}^{|z|}$ will be relevant. Then the minimizer $f_{z'',z''}^\lambda$ of $T_{z''}^\lambda(f)$ over $\mathcal{H}_K^{z''}$ is given as

$$f_{z'',z''}^\lambda = (\lambda I + P_{z''} S_x^* S_x P_{z''})^{-1} P_{z''} S_x^* Y,$$

where the latter follows because $f_{z'',z''}^\lambda \in \mathcal{H}_K^{z''}$. Note that $f_{z'',z''}^\lambda$ can be computed with a computational cost

$$\text{cost}(f_{z'',z''}^\lambda) = \mathcal{O}(|z| \cdot |z''|^2), \quad \text{as } |z| \geq |z''| \to \infty.$$ (see, e.g., [13]).

2.2. Assumptions. The answer to the learning rate depends on additional assumptions. The first two assumptions, concerning properties of the underlying kernel and the noise moments, will not be referenced explicitly throughout the study.

**Assumption 1** (kernel properties). The kernel $K : X \times X \to \mathbb{R}$ is continuous, symmetric, positive definite and

$$\sup_{x \in X} K(x, x) = \kappa < \infty.$$ Then it is clear that

$$\sup_{x \in X} \|K_x\|_{L_2(X, \rho_X)} \leq \sup_{x \in X} \|K_x\|_{C(X)} \leq \sup_{x \in X} \|K_x\|_{\mathcal{H}_K}^2 = \kappa.$$

Under Assumption [13] the operator $J_K J_K^*$ from (2.2) has a finite trace. Specifically, for each $\lambda > 0$ it holds that

$$\mathcal{N}_x(\lambda) := \langle K(\cdot, x), (\lambda I + J_K J_K^*)^{-1} K(\cdot, x) \rangle_{\mathcal{H}_K} = \|(\lambda + J_K^* J_K)^{-1/2} K_x\|^2 < \infty.$$
We highlight the related quantities

\[(2.4) \quad \mathcal{N}_\infty(\lambda) := \sup_{x \in \mathcal{X}} \mathcal{N}_\varepsilon(\lambda) \quad (\leq \kappa/\lambda), \]

and

\[(2.5) \quad \mathcal{N}(\lambda) := \int_{\mathcal{X}} \mathcal{N}_\varepsilon(\lambda) d\rho_X(x) = \text{trace}\{ (\lambda I + J_K^* J_K)^{-1} J_K^* J_K \}. \]

The function \( \mathcal{N} \) measures the capacity of the RKHS \( \mathcal{H}_K \) in the space \( L_2(X, \rho_X) \), and it is called the effective dimension. It is well known that this is a decreasing function of \( \lambda \) with \( \lim_{\lambda \to 0+} \mathcal{N}(\lambda) = \infty \), provided that the RKHS \( \mathcal{H}_K \) is infinite dimensional, c.f. [8]. Extended discussion on properties of the effective dimension for general operators can be found in [8].

For the efficiency of the Nyström subsampling we shall need an additional assumption on the kernel, specified in Assumption 4 below.

**Assumption 2** (noise moments). The family of random variables \( \varepsilon_x := y - f_\rho(x) \), \( x \in \mathcal{X} \) has all moments \( p \geq 2 \), which satisfy

\[ E|\varepsilon_x|^p \leq \frac{1}{2} p! M^{p-2} \sigma^2, \quad x \in \mathcal{X}, \text{ a.e.}, \]

for some positive constants \( M \) and \( \sigma \).

Next, an assumption is made on the underlying smoothness of the regression function \( f_\rho \).

**Assumption 3** (source condition). There is an operator concave index function \( \varphi : [0, d] \to [0, \infty) \), for some \( d > \| J_K J_K^* \| \), such that

\[ f = \varphi(J_K J_K^*) v_f, \quad \| v_f \|_\rho \leq 1. \]

The function \( t \to \sqrt{t}/\varphi(t) \) is nondecreasing.

**Remark 1.** First, from [10] we know that for every \( f \in L_2(X, \rho_X) \) and \( \varepsilon > 0 \) there exists an index function \( \varphi : [0, \| J_K J_K^* \|] \to [0, \infty) \) such that

\[(2.6) \quad f = \varphi(J_K J_K^*) v_f, \quad \| v_f \|_\rho \leq (1 + \varepsilon) \| f \|_\rho, \]

In the context of learning it is used starting from the paper [15], where \( f = f_\rho \) was assumed to satisfy \( 2.6 \) with \( \varphi(t) = t^r, r \in (0, 1] \).

Secondly, the following is known. If the function \( t \to \sqrt{t}/\varphi(t) \) is nonincreasing, then the image of \( \varphi(J_K J_K^*) \) is contained in \( \mathcal{H}_K \). Therefore, in order to treat the low-smoothness case we assume that \( t \to \sqrt{t}/\varphi(t) \) is nondecreasing. Thus, the misspecified case studied here corresponds to \( 2.6 \) with \( \varphi(t) \) increasing not faster than \( \sqrt{t} \).

Moreover, as in [8], in order to control the effect of subsampling, we assume that \( \varphi \) is operator concave on \( [0, d] \), \( d > \| J_K J_K^* \| \). Note that previously considered Hölder-type index functions \( \varphi(t) = t^r, r \in (0, \frac{1}{2}] \), as well as logarithmic functions \( \varphi(t) = \log^{-r} \frac{1}{t}, \quad 0 < r \leq 1 \), are operator monotone, and hence operator concave. An important implication of operator monotonicity is that there is a number \( d_\varphi \)

\[ 1 \quad \text{A function } \varphi : [0, d] \to [0, \infty) \text{ is called an index function if it is continuous, strictly increasing, obeying } \varphi(0) = 0. \text{ It is called operator concave if for self-adjoint operator } C, C_1 : L_2(X, \rho_X) \to L_2(X, \rho_X) \text{ we have that } \varphi \left( \frac{1}{2} (C + C_1) \right) \geq \frac{1}{2} (\varphi(C) + \varphi(C_1)). \]
depending only on \( \varphi \) such that for any self-adjoint operators \( C, C_1 : L_2(X, \rho_X) \to L_2(X, \rho_X) \) with spectra in \([0, d]\) it holds

\[
\| \varphi(C) - \varphi(C_1) \|_{L_2(X, \rho_X) \to L_2(X, \rho_X)} \leq d \varphi \left( \| C - C_1 \|_{L_2(X, \rho_X) \to L_2(X, \rho_X)} \right).
\]

3. Main results

3.1. Error bound for Nyström subsampling in the misspecified case. We formulate the main result below. For this to hold we must obey the following relations for the parameter \( \lambda > 0 \), the overall sample size \(|z|\), and the subsample size \(|z^\nu|\). Given, for \( 0 < \delta < 1 \), a confidence level \( 1 - \delta \), we require that

\[
|z^\nu| \geq cN_\infty(\lambda) \log \frac{1}{\lambda} \log \frac{1}{\delta},
\]

and

\[
\lambda \in \left[ c|z|^{-1} \log \frac{|z|}{\delta}, \|J_K^*J_K\|_{\mathcal{H}_K \to \mathcal{H}_K} \right].
\]

Concerning the choice of the size \(|z^\nu|\) of the subsample, two competing goals are relevant. First, it should be large enough to maintain the learning rate as this was obtained by using the full sample \( z \). On the other hand, it should be as small as possible to reduce the computational burden. Here this choice in (3.1) is analyzed in the low smoothness situation.

Here and in the sequel, we adopt the convention that \( c \) denotes a generic positive coefficient, which can vary from estimation to estimation and may only depend on basic parameters, such as \( K, \rho \). Also, for functions \( a, b \) depending on \( \lambda \) or \(|z|\), respectively, the relation \( a \asymp b \) means that \( a = O(b) \) and \( b = O(a) \) as \( \lambda \to 0 \), or \(|z| \to \infty \).

Note that the Nyström approximant from (2.3) represents an element of \( \mathcal{H}_K \), and to estimate \( \mathcal{E}(f^\lambda_{z^\nu}) \) we need to embed \( f^\lambda_{z^\nu} \) in \( L_2(X, \rho_X) \). Then the error decomposes as

\[
\|J_K f^\lambda_{z^\nu} - f_\rho\|_\rho \leq \|f_\rho - J_K(\lambda I + B^*_\nu B_\nu)^{-1}P_{z^\nu} J_K^* J_K^* J_K f_\rho\|_\rho \\
+ \|J_K(\lambda I + B^*_\nu B_\nu)^{-1}P_{z^\nu}(J_K^* f_\rho - S^*_x \mathcal{Y})\|_\rho,
\]

which can be regarded as decomposition into approximation error and the sample error, respectively. By estimating both terms in the right-hand side of (3.3), we establish the main error estimate.

**Theorem 1.** Assume that in the plain Nyström subsampling the values \(|z^\nu|\) and \( \lambda \) satisfy (3.1) and (3.2). If \( f_\rho \) obeys Assumption 3 for the index function \( \varphi \), then with probability at least \( 1 - \delta \) we have

\[
\|f_\rho - J_K(\lambda I + B^*_\nu B_\nu)^{-1}P_{z^\nu} J_K^* J_K^* J_K f_\rho\|_\rho \leq c\varphi(\lambda) \log \frac{1}{\delta} \left( 1 + \sqrt{\frac{N(\lambda)}{\lambda|z|}} \right);
\]

\[
\|J_K(\lambda I + B^*_\nu B_\nu)^{-1}P_{z^\nu}(J_K^* f_\rho - S^*_x \mathcal{Y})\|_\rho \leq c\sqrt{\lambda} \log \frac{1}{\delta} \left( 1 + \sqrt{\frac{N(\lambda)}{\lambda|z|}} \right);
\]
and the total error estimate

\[ \| J_K f_{\lambda,z,z'} - f_\rho \|_\rho \leq c \varphi(\lambda) \log \frac{1}{\delta} \left( 1 + \sqrt{\frac{\mathcal{N}(\lambda)}{|z|}} \right). \]

It is interesting to observe that the approximation error dominates the sample error, which is not standard in regularization theory. This is a consequence of the misspecified source condition, Assumption 3, for a function \( \varphi(\lambda) \geq c \sqrt{\lambda} \). We will provide more explanation in Remark 5 after the proof of the above theorem, which has been postponed in Section 4.

3.2. Parameter choice. A somewhat surprising message of the above theorem is that the \( \lambda \)-dependent term

\[ \theta_\varphi(\lambda) = \varphi(\lambda) \left( 1 + \sqrt{\frac{\mathcal{N}(\lambda)}{|z|}} \right), \quad \lambda > 0. \]

bounding (the square root of) the excess loss \( \mathcal{E}(f_{\lambda,z,z'}) - \mathcal{E}(f_\rho) \) attains its minimum (up to a constant factor) at a value of the regularization parameter \( \lambda = \lambda_0 \), which can be chosen a priori and does not require the knowledge of the index function \( \varphi \). Precisely, let \( \lambda_0 = \lambda_0(|z|) \) solve the equation

\[ \mathcal{N}(\lambda) = \lambda |z|. \] (3.4)

Notice that this equation always has a unique solution, and that it does not depend on the underlying smoothness, as expressed in the function \( \varphi \). Also, as \( |z| \to \infty \) we have that \( \lambda_0(|z|) \to 0 \).

Corollary 1. For any index function \( \varphi \) in Assumption 3 we have

\[ \varphi(\lambda_0) \leq \min_\lambda \theta_\varphi(\lambda) \leq 2 \varphi(\lambda_0), \] (3.5)

where \( \lambda_0 \) is chosen in (3.4).

Consequently, under the conditions of Theorem 1 and if \( \lambda_0 \) obeys (3.2) then we have that

\[ \| J_K f_{\lambda,z,z'} - f_\rho \|_\rho = \mathcal{O}(\varphi(\lambda_0(|z|))), \quad \text{as} \quad |z| \to \infty. \]

Remark 2. The effective dimension \( \mathcal{N}(\lambda) \) can be rather accurately estimated from the data (see, e.g., [13, Prop. 1]) that makes the parameter choice \( \lambda = \lambda_0 \) practically feasible.

Remark 3. We comment when the above choice of \( \lambda_0 \) obeys the condition from (3.2). We claim that this holds true whenever the effective dimension grows at least as \( \log(1/\lambda) \), as \( \lambda \to 0 \). Indeed, we have that \( |z|\lambda_0 \leq 1 \), and hence that \( \log(|z|) \leq \log(1/\lambda_0) \), such that in this case we find that

\[ |z|\lambda_0 = \mathcal{N}(\lambda_0) \geq \log(1/\lambda_0) \geq \frac{1}{2} \log \left( \frac{|z|}{\delta} \right), \]

provided that for given confidence level \( 1 - \delta \), the sample size \( |z| \) is large enough. This condition on the effective dimension is fulfilled for all types of the behavior of the effective dimension discussed in the literature, (see, e.g., the discussion with power type behavior in Section 3.4 below).
3.3. Full data. Note that in the case when \(|z'v| = |zv|\), the inequality \([3.1]\) is satisfied because in view of \([2.4]\) and \([3.2]\), \(\mathcal{N}\infty(\lambda) \log(1/\lambda)\) is of lower order than \(|z'v| = |zv|\), i.e. \(\mathcal{N}\infty(\lambda) \log(1/\lambda) = \mathcal{O}(|z|^{-1} \cdot \log |z|)\). Therefore, Theorem 1 has the following corollary.

Corollary 2. If \(z'v = z\), then under the conditions of Theorem 1 we have

\[
\|f_{\lambda}^z - f_{\rho}\|_{\rho} = \mathcal{O}\left(\varphi(\lambda_0) \log \frac{1}{\delta}\right) \quad \text{as} \quad |z| \to \infty. \tag{3.6}
\]

The error of Nyström subsampling that follows from Theorem 1 and Corollary 1, coincides with the best learning rate known in the misspecified case for KRR with general Mercer kernels and full data, i.e \(z'v = z\).

Example. We discuss the previously considered Hölder-type index functions \(\varphi(t) = t^r, r \in (0, 1/2]\), and under the usual assumption on the effective dimension \(\mathcal{N}(\lambda) = \mathcal{O}(\lambda^{-s}), s \in (0, 1]\). Then the bound \(3.6\) is of order \(\mathcal{O}\left(|z|^{-r/(s+1)}\right)\). For KRR with full data, this result is in accordance with [7].

3.4. Efficiency of Subsampling. Now we are in position to discuss conditions under which the plain Nyström subsampling achieves \(3.6\) with subquadratic cost \(\mathcal{O}(|z|^2)\).

In order to actually establish the superiority of the subsampling an additional assumption is made, borrowed from [3].

Assumption 4 (source condition for kernel). There exist \(\gamma \in (0, 1]\) and \(c_\gamma > 0\) such that for all \(x \in X\) the kernel sections \(K(\cdot, x) \in \mathcal{H}_K\) satisfy the source condition

\[
K(\cdot, x) = (J_K^* J_K)^{\gamma/2} v_x, \quad \|v_x\|_{\mathcal{H}_K} \leq c_\gamma. \tag{3.7}
\]

Remark 4. As discussed in Remark 1 there is always an index function, say \(\psi\), which guarantees that

\[
K(\cdot, x) = \psi(J_K^* J_K) v_x, \quad \|v_x\|_{\mathcal{H}_K} \leq (1 + \varepsilon) \|K_x\|_{\mathcal{H}_K} \leq (1 + \varepsilon) \sqrt{\kappa}.
\]

Thus, Assumption 4 requires this index function to be of at least power type.

We mention the following consequence of Assumption 4.

Lemma 1. Under Assumption 4 we have that

\[
\mathcal{N}\infty(\lambda) \leq c_\gamma^2 \lambda^{\gamma-1}.
\]

Proof. This simply follows from

\[
\mathcal{N}\infty(\lambda) = \sup_{x \in X} \left\| (\lambda I + J_K^* J_K)^{-1/2} K(\cdot, x) \right\|_{\mathcal{H}_K}^2
\]

\[
\leq \sup_{x \in X} \|v_x\|_{\mathcal{H}_K}^2 \sup_{t > 0} \left(\lambda + t\right)^{-1/2} t^{\gamma/2}
\]

\[
\leq c_\gamma^2 \sup_{t > 0} (\lambda + t)^{-1} t^\gamma \leq c_\gamma^2 \lambda^{\gamma-1},
\]

which completes the proof. \(\square\)

Recall that \(f_{\lambda}^z\) can be computed with a computational cost \(\mathcal{O}(|z| \cdot |z'v|^2)\), and note that \([3.1]\) is the only condition on the subsampling size \(|z''v|\) that is needed.
in Theorem \ref{thm:subquadratic}. Then from Corollary \ref{cor:subquadratic} it follows that the Nyström approximation \( f_{z,\nu}^{\lambda_0} \) realizing the order \((3.6)\) can be computed with a computational cost

\[
\text{cost} \left( f_{z,\nu}^{\lambda_0} \right) = O \left( |z| \cdot \left( \mathcal{N}_\infty(\lambda_0) \log \frac{1}{\gamma_0} \right)^2 \right).
\]

If we stay with the standard assumption that \( \mathcal{N}(\lambda) \propto \lambda^{-s} \), then from the very definition and Lemma \ref{lem:gamma} it follows that

\[
\mathcal{N}(\lambda) \leq \mathcal{N}_\infty(\lambda) \Rightarrow s + \gamma \leq 1.
\]

In the considered scenario, from \((3.4)\) and \((3.8)\), we have \( \lambda_0 \propto |z|^{-1/(s+1)} \), and the cost can be bounded as

\[
\text{cost} \left( f_{z,\nu}^{\lambda_0} \right) = O \left( |z| \cdot |z|^{2(1-\gamma)/(s+1)} \log^2 |z| \right) = O \left( |z|^{(3+s-2\gamma)/(1+s)} \log^2 |z| \right),
\]

which is subquadratic whenever \( 2\gamma + s > 1 \). We summarize this as

**Proposition 1.** Assume that Assumption \ref{assumption} holds true and \( \mathcal{N}(\lambda) \propto \lambda^{-s} \), \( s \in (0,1-\gamma] \). If \( 2\gamma + s > 1 \), then the plain Nyström approximation \( f_{z,\nu}^{\lambda_0} \) can be computed at a subquadratic computational cost, and it preserves the learning rate \((3.6)\) guaranteed for the full amount of data.

In particular, if Assumption \ref{assumption} is satisfied with \( \gamma > 1/2 \), then the plain Nyström approximation can always be computed at a subquadratic cost still maintaining guaranteed learning rates.

### 4. Proofs

**4.1. A regularization perspective to KRR.** Here we briefly emphasize the aspects of regularization theory which will be relevant in the subsequent proofs. We recall the structure of the estimator \( f_{z,\nu}^{\lambda} \) from \((2.3)\) as

\[
f_{z,\nu}^{\lambda} = (\lambda I + B^* P_\nu B)^{-1} B^* Y,
\]

with \( B_\nu = S_x P_\nu \). We can write this as \( f_{z,\nu}^{\lambda} = g_\lambda(B^* B_\nu)B^* Y \), where we introduced the KRR filter function \( g_\lambda(t) := 1/(t + \lambda) \), \( t, \lambda > 0 \), applied to the non-negative self-adjoint operator \( B^* B_\nu \) via spectral calculus. We shall also employ the fact that for any linear bounded operator, say \( B \) acting between Hilbert spaces, and for any bounded function \( g \) it holds \( g(B^* B)B^* = B^* g(BB^*) \). The corresponding residual function is given as \( r_\lambda(t) := 1 - g_\lambda(t) = \lambda/(t + \lambda) \), \( t, \lambda > 0 \). In particular we have that \( 0 < r_\lambda(t) \leq 1 \). The impact of the residual function on the given solution smoothness is measured by its qualification, and we mention the well known result that

\[
\sup_{t > 0} |r_\lambda(t)\varphi(t)| \leq \varphi(\lambda), \quad \lambda > 0,
\]

provided that the index function \( \varphi \) is such that \( \varphi(t)/t \) is non-decreasing, as this is the case for the functions \( \varphi \) which obey Assumption \ref{assumption}. Applying this for the index function \( t \mapsto t^q \varphi(t) \), with \( 0 \leq q \leq 1/2 \), we find that this still obeys the assumption for \((4.1)\), and hence, (see, e.g., (16) in \cite{6}), we have that

\[
\sup_{t > 0} |r_\lambda(t) t^q \varphi(t)| \leq c\lambda^q \varphi(\lambda), \quad \text{when } q \in [0,\frac{1}{2}],
\]
Finally, by the specific structure we see that 

\[ g_\lambda(t) = \frac{r_\lambda(t)}{\lambda}, \]

such that (4.2) yields with \( q := 1/2 \) that

\[
|g_\lambda(t)\sqrt{t}\varphi(t)| \leq \varphi(\lambda)\lambda^{-1/2}, \quad \lambda > 0. 
\]

4.2. Probabilistic bounds. We shall also use probabilistic bounds. From [13 Lem. 6] and [11 Cor. 1] it follows that if \( z^{\nu} \) is subsampled according to the plain Nyström approach, then with probability at least \( 1 - \delta \) we have

\[
\| J_K(I - P_{z^{\nu}}) \|^2_{\mathcal{H}_K \rightarrow L^2(X, \rho_X)} \leq 3\lambda, \quad (4.4)
\]

provided that (3.1) holds.

We also recourse to the following inequality from [13 Lem. 5], which asserts

\[
\| (\lambda I + J^*_KJ_K)^{1/2}(\lambda I + S_x^*S_x)^{1/2} \|_{\mathcal{H}_K \rightarrow \mathcal{H}_K} \leq 2, \quad (4.5)
\]

the latter one is satisfied with probability at least \( 1 - \delta \) if (3.2) holds.

Moreover, from Lemma 5.1 [2] it follows that for \( \lambda \) satisfying (3.2) with probability at least \( 1 - \delta \) we have

\[
\| (\lambda I + J^*_KJ_K)^{-1/2}(J^*_Kf_\rho - S_x^*Y) \|_{\mathcal{H}_K} \leq c \log \frac{1}{\delta} \sqrt{\frac{N(\lambda)}{|z|}}, \quad (4.6)
\]

\[
\| (\lambda I + J^*_KJ_K)^{-1/2}(J^*_KJ_K - S_x^*S_x) \|_{\mathcal{H}_K \rightarrow \mathcal{H}_K} \leq c \log \frac{1}{\delta} \sqrt{\frac{N(\lambda)}{|z|}}, \quad (4.7)
\]

4.3. Proof of Theorem [1] We first mention the following well known bound, using spectral calculus.

\[
\| J_K(\lambda I + J^*_KJ_K)^{-1/2} \|_{\mathcal{H}_K \rightarrow L^2(X, \rho_X)} = \| (J^*_KJ_K)^{1/2}(\lambda I + J^*_KJ_K)^{-1/2} \|_{\mathcal{H}_K \rightarrow \mathcal{H}_K} \leq \sup_{t>0} (t/(\lambda + t))^{1/2} \leq 1. \quad (4.8)
\]

Furthermore, the following result will be used, and we refer to [13 Lem. 2&8]. For every choice \( z^{\nu} \) from the sample \( z \) we have that

\[
\| (\lambda I + S_x^*S_x)^{1/2}P_{z^{\nu}}(\lambda I + P_{z^{\nu}}S_x^*S_xP_{z^{\nu}})^{-1}P_{z^{\nu}}(\lambda I + S_x^*S_x)^{1/2} \|_{\mathcal{H}_K \rightarrow \mathcal{H}_K} \leq 1. \quad (4.9)
\]

Recall the error decomposition

\[
\| J_Kf^\lambda_{z^{\nu}} - f_\rho \|_\rho \leq \| f_\rho - J_K(\lambda I + B_x^*B_\rho)^{-1}P_{z^{\nu}}J^*_Kf_\rho \|_\rho \\
+ \| J_K(\lambda I + B_x^*B_\rho)^{-1}P_{z^{\nu}}(J^*_Kf_\rho - S_x^*Y) \|_\rho.
\]
The sample error, i.e. the second term on the right hand side of above inequality, can be estimated with the use of \((4.8), (4.9), (4.5)\) and \((4.7)\) as follows
\[
\|J_K(\lambda I + B^*_v B_v)^{-1}P_{z^*}(J_K^* f_\rho - S^*_z Y)\|_{\rho} \\
\leq \|J_K(\lambda I + J_K^* J_K)^{-1/2}\|_{\mathcal{H}_K \to L_2(X,\rho_X)} \times \|\lambda I + J_K^* J_K)^{1/2}(\lambda I + S^*_z S_z)^{-1/2}\|_{\mathcal{H}_K \to \mathcal{H}_K} \\
\times \|J_K(2.6)\|_{\mathcal{H}_K \to \mathcal{H}_K} \times \|P_{z^*}(\lambda I + J_K^* J_K)^{1/2}\|_{\mathcal{H}_K \to \mathcal{H}_K} \\
\times \|J_K(\lambda I + J_K^* J_K)^{-1/2}(J_K^* f_\rho - S^*_z Y)\|_{\mathcal{H}_K}.
\]
(4.10) \[
\leq 4c \log \frac{1}{\delta} \sqrt{\frac{N(\lambda)}{|z|}} \leq 4c \sqrt{\lambda} \log \left(1 + \sqrt{\frac{N(\lambda)}{\lambda |z|}}\right).
\]

The rest of the proof is to estimate the approximation error, i.e. the first term on the right hand side of \((3.3)\). This can further be decomposed as
\[
\|f_\rho - J_K(\lambda I + B^*_v B_v)^{-1}P_{z^*}P_{z^*} f_\rho\| \leq I_1 + I_2,
\]
where
\[
I_1 = \|f_\rho - J_K(\lambda I + P_{z^*}J_K^* J_K P_{z^*})^{-1}P_{z^*}J_K^* f_\rho\|, \\
I_2 = \|J_K[(\lambda I + P_{z^*}J_K^* J_K P_{z^*})^{-1} - (\lambda I + B^*_v B_v)^{-1}]P_{z^*}J_K^* f_\rho\|_{\rho} \\
= \|J_K(\lambda I + B^*_v B_v)^{-1}P_{z^*}(J_K^* J_K - S^*_z S_z) \\
\times (\lambda I + P_{z^*}J_K^* J_K P_{z^*})^{-1}P_{z^*}J_K^* f_\rho\|_{\rho}.
\]

To estimate \(I_1\) we recall \((4.2)\). Moreover, from \((2.7), (4.4)\) it follows that under the condition \((3.1)\) we have
\[
\|\varphi(J_K^* J_K^*) - \varphi(J_K^* P_{z^*} J_K^*)\|_{L_2(X,\rho_X) \to L_2(X,\rho_X)}(\lambda I + P_{z^*}J_K^* J_K P_{z^*})^{-1}) \leq c\varphi(\lambda).
\]
Then, using the source condition \((2.6)\) with \(f = f_\rho\), and the qualification of KRR as in \((4.1)\), we can estimate \(I_1\), by using \(r_\lambda(t) := \lambda/(\lambda + t)\), \(t, \lambda > 0\), as follows
\[
I_1 = \|J_K^* J_K^* (\lambda I + J_K^* J_K P_{z^*} J_K^*)^{-1}f_\rho\|_{\rho} \\
\leq \|r_\lambda(J_K^* J_K^* (\lambda I + J_K^* J_K P_{z^*} J_K^*)^{-1})f_\rho\|_{\rho} \\
+ \|r_\lambda(J_K^* J_K^* f_\rho) - \varphi(J_K^* f_\rho)\|_{\rho} \\
\leq c\varphi(\lambda).
\]

To estimate \(I_2\) we observe that \(I_2 \leq I_{2.1} \cdot I_{2.2}\), where
\[
I_{2.1} = \|J_K(\lambda I + B^*_v B_v)^{-1}P_{z^*}J_K^* J_K - S^*_z S_z\|_{\mathcal{H}_K \to \mathcal{H}_K}, \\
I_{2.2} = \|\lambda I + P_{z^*}J_K^* J_K P_{z^*})^{-1}P_{z^*}J_K^* f_\rho\|_{\mathcal{H}_K}.
\]
By the same chain of arguments as in (4.10) we obtain that
\[ I_{2,1} \leq c \log \frac{1}{\delta} \sqrt{\frac{N(\lambda)}{|z|}}, \]
where the only difference is that one needs to use (4.6) instead of (4.7).

Observing that \( I_{2,2} \leq I_{2,2,1} + I_{2,2,2} \), we then have
\[
I_{2,2,1} = \| Pv^* J_K^* (\lambda I + J_K Pz^* J_K^*)^{-1} \varphi (J_K Pz^* J_K^*) \|_{\mathcal{H}_K},
\]
\[
I_{2,2,2} = \| Pv^* J_K^* (\lambda I + J_K Pz^* J_K^*)^{-1} (\varphi (J_K J_K^*) - \varphi (J_K Pz^* J_K^*)) \|_{\mathcal{H}_K}.
\]

Using (4.3) we derive
\[
I_{2,2,1} = \| g_{\lambda} (J_K Pz^* J_K^*) (J_K Pz^* J_K^*)^{1/2} \varphi (J_K Pz^* J_K^*) \| \| v_{f_r} \|_\rho
\leq \| v_{f_r} \|_\rho \sup_{t > 0} |g_{\lambda}(t)| t^{1/2} \varphi(t) \leq c \varphi(\lambda) \lambda^{-1/2}.
\]

Moreover, similarly to (4.8) and (4.12) there holds
\[
I_{2,2,2} \leq c \| v_{f_r} \|_\rho \varphi(\lambda) \sup_{t > 0} |g_{\lambda}(t)| t^{1/2} \leq c \varphi(\lambda) \lambda^{-1/2}.
\]

Thus, we have that \( I_{2,2} \leq c \varphi(\lambda) \lambda^{-1/2} \), and hence overall
\[
I_2 \leq c \log \frac{1}{\delta} \varphi(\lambda) \sqrt{\frac{N(\lambda)}{\lambda |z|}}, \quad \lambda > 0.
\]

Combining this with (3.3), (4.10), (4.11) and (4.9) we obtain the statement of the theorem, and the proof is complete.

**Remark 5.** We shall emphasize that in Theorem 1 the total error estimate is dominated by the approximation error which is actually induced by the estimate of the term \( I_{2,2,2} \) in (4.13). The misspecified source condition Assumption 3 then yields an increasing function \( \varphi(\lambda) \lambda^{-1/2} \) which blows up as \( \lambda \to 0 \). As a consequence, the estimate of \( I_2 \) in (4.14) dominates the sample error.

4.4. **Proof of Corollary 1.** The right inequality in (3.5) is obvious by the choice of \( \lambda_0 \) from (3.4). To prove the left inequality we distinguish two cases. First, if \( \lambda > \lambda_0 \) then \( \theta_\varphi(\lambda) > \varphi(\lambda) > \varphi(\lambda_0) \). Otherwise, if \( \lambda \leq \lambda_0 \), then we use that by assumption the function \( \lambda \to \varphi(\lambda)/\sqrt{\lambda} \) is decreasing, and hence
\[
\theta_\varphi(\lambda) = \frac{\varphi(\lambda)}{\sqrt{\lambda}} \left( \sqrt{\lambda} + \sqrt{\frac{N(\lambda)}{|z|}} \right) \geq \frac{\varphi(\lambda)}{\sqrt{\lambda}} \sqrt{\frac{N(\lambda)}{|z|}} \geq \frac{\varphi(\lambda_0)}{\sqrt{\lambda_0}} \sqrt{\frac{N(\lambda_0)}{|z|}} = \varphi(\lambda_0).
\]
This proves the left hand side bound and completes the proof of the first assertion. The second one is an immediate application of the theorem, and the proof is complete.

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