Connections and Equivalences between the Nyström Method and Sparse Variational Gaussian Processes

Veit Wild
Department of Statistics, University of Oxford, UK

Motonobu Kanagawa
Data Science Department, EURECOM, France

Dino Sejdinovic
School of Computer and Mathematical Sciences, University of Adelaide, Australia

Abstract

We investigate the connections between sparse approximation methods for making kernel methods and Gaussian processes (GPs) scalable to large-scale data, focusing on the Nyström method and the Sparse Variational Gaussian Processes (SVGP). While sparse approximation methods for GPs and kernel methods share some algebraic similarities, the literature lacks a deep understanding of how and why they are related. This may pose an obstacle to the communications between the GP and kernel communities, making it difficult to transfer results from one side to the other. Our motivation is to remove this obstacle, by clarifying the connections between the sparse approximations for GPs and kernel methods. In this work, we study the two popular approaches, the Nyström and SVGP approximations, in the context of a regression problem, and establish various connections and equivalences between them. In particular, we provide an RKHS interpretation of the SVGP approximation, and show that the Evidence Lower Bound of the SVGP contains the objective function of the Nyström approximation, revealing the origin of the algebraic equivalence between the two approaches. We also study recently established convergence results for the SVGP and how they are related to the approximation quality of the Nyström method.

Keywords: Gaussian Processes, Kernel Methods, Sparse Approximation, Nyström Method, Sparse Variational Gaussian Processes

Contents

1 Introduction 2
  1.1 Notation . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 5

2 Kernels and Gaussian Processes for Regression 5
  2.1 Kernel Ridge Regression (KRR) . . . . . . . . . . . . . . . . . . . . . . . . . . 5
    2.1.1 Kernels and RKHSs . . . . . . . . . . . . . . . . . . . . . . . . . . . . 5
    2.1.2 Regression Approach . . . . . . . . . . . . . . . . . . . . . . . . . . . 6
  2.2 Gaussian Process Regression (GPR) . . . . . . . . . . . . . . . . . . . . . . 7
    2.2.1 Gaussian Processes . . . . . . . . . . . . . . . . . . . . . . . . . . . . 7
    2.2.2 Regression Approach . . . . . . . . . . . . . . . . . . . . . . . . . . . 7
Gaussian processes (GPs) and kernel methods are the two principled learning approaches that make use of positive definite kernels, and have been studied extensively in statistics and machine learning. On one hand, GP-based approaches (Rasmussen and Williams 2006) employ a kernel to induce the corresponding GP, in order to define a prior distribution of the ground-truth latent function of interest. Given data, Bayes’ rule is then applied to obtain the posterior distribution of the latent function. On the other hand, kernel methods (Schölkopf and Smola 2002) make use of a kernel to induce the corresponding Reproducing Kernel Hilbert Space (RKHS) as a “hypothesis space.” Given data, empirical risk minimization is then performed in the RKHS to estimate the ground-truth function of interest. Although the GP and kernel approaches have different modeling philosophies, there are indeed deep connections and equivalences between them, which extend beyond a superficial similarity.
Connections between the Nyström and Sparse Variational Gaussian Processes

(Parzen, 1961; Kimeldorf and Wahba, 1970; Berlinet and Thomas-Agnan, 2004; Kanagawa et al., 2018).

The elegance of the GP and kernel approaches is that the infinite-dimensional learning problems can be reduced to the corresponding finite-dimensional problems. However, this comes with a cost: a naive implementation for supervised learning usually leads to the computational complexity that is cubic in the data size. This unfavorable scaling property has motivated the developments of several approximation methods to make the GP and kernel approaches scalable. Sparse approximation methods, which approximate the solution of interest using a set of input points smaller than training data, are among the most popular and successful approximation approaches. These approaches have been studied since the earliest developments of the GP and kernel approaches (e.g., Williams and Seeger, 2001; Csató and Opper, 2002; Smola and Schölkopf, 2000; Seeger et al., 2003).

As the GP and kernel communities grow, sparse approximation methods for either approach tend to be developed independently to those for the other approach. For instance, consider the Sparse Variational Gaussian Process (SVGP) approach of Titsias (2009a,b), which is one of the most successful and widely used sparse approximation methods for GPs. The SVGP is derived in the framework of variational Bayesian inference, so that the sparse approximation is to be chosen to minimize the KL divergence to the exact GP posterior. As such, the developments in SVGP (e.g., Hensman et al., 2013, 2015a; Matthews et al., 2016; Burt et al., 2019; Rossi et al., 2021) have proceeded almost independently of the corresponding literature on sparse approximations for kernel methods. Similarly, the recent advances in using and understanding the Nyström method (Williams and Seeger, 2001), which is one of the most popular sparse approximations in kernel methods, have been made independently to those of sparse GP approximations. The majority of these advances focus on an efficient approximation of the kernel matrix (e.g., Drineas and Mahoney, 2005; Belabbas and Wolfe, 2009; Gittens and Mahoney, 2016; Derezinski et al., 2020) or empirical risk minimization in the RKHS with a reduced basis (e.g, Bach, 2013; El Alaoui and Mahoney, 2015; Rudi et al., 2015, 2017; Meanti et al., 2020). This separation of two lines of research is arguably due to the difference in the notations and modelling philosophies of GPs and kernel methods. The separation makes it difficult to transfer useful and interesting results from one side to the other, and the communities might have missed an important advance that may have been obtained otherwise. The motivation of the current work is to overcome this potential difficulty by bridging the two lines of research.

This work investigates connections between sparse approximation methods for GPs and kernel methods, focusing on two fundamental methods: the SVGP and Nyström approximations. We consider the regression setting, where the exact solutions of Gaussian process regression (GPR) and kernel ridge regression (KRR) are to be approximated. Both the SVGP and Nyström approximations use \( m \) input locations for approximating the exact solutions, where \( m \) is one’s choice and smaller than the training data size \( n \). They can be computed in the \( O(m^2 n + m^3) \) complexity and thus can be much faster than the naive implementations requiring the \( O(n^3) \) complexity.

The SVGP defines a class of GPs (the variational family used for approximation), parameterized by \( m \) input locations called inducing points and by other parameters defining the means and covariances of the function values at the inducing points. For fixed inducing inputs, the mean and covariance parameters are obtained by minimizing the Kullback-
Leibler (KL) divergence between the thus parametrized GP and the exact posterior of GPR, or equivalently by maximizing the Evidence Lower Bound (ELBO); the resulting optimal parametrized GP is the SVGP approximation. On the other hand, the Nyström method uses $m$ inducing points (or landmark points) to define a $m$-dimensional subspace of the RKHS, and solves the regularized least-squares problem of KRR in this subspace; the resulting solution is the Nyström approximation.

We first show that the ELBO objective for the parametric mean function of the SVGP is equivalent to the objective function for the Nyström KRR (Section 4.1). Consequently, the optimized mean function of the SVGP approximation is identical to the Nyström KRR estimator. This equivalence shows that the SVGP mean function solves a regularized least-squares problem on the subspace in the RKHS spanned by inducing points. It is parallel to the well-known equivalence between GPR and KRR (Kimeldorf and Wahba, 1970; Kanagawa et al., 2018), which the SVGP and Nyström respectively approximate.

RKHS interpretations are also provided for the covariance function of the SVGP (Section 4.3). The ELBO objective for the parametric covariance function of the SVGP is analyzed in terms of the RKHS geometry. The analysis elucidates how the covariance function of the SVGP approximates the posterior covariance function of the exact GPR. Moreover, the variance function of the SVGP is shown to be equal to the sum of the worst-case error of the Nyström KRR in the RKHS and that of a kernel interpolant on inducing points. This equivalence enables understanding how SVGP quantifies uncertainties from a function-space viewpoint and how the choice of the kernel impacts uncertainty estimates.

Lastly, connections are established for the approximation quality of the SVGP and Nyström approximations. It is shown that the approximation error of the SVGP (as measured by the KL divergence) is closely related to the approximation error of the Nyström (as measured by the regularized empirical risk). By leveraging this connection, we demonstrate how upper and lower bounds for the SVGP approximation error by Burt et al. (2020) can be translated into the corresponding bounds for the Nyström approximation error (Sections 5.2 and 5.4). Similarly, we show how an approximation error bound for the Nyström as measured by the RKHS distance, which is novel and may be of independent interest, can be translated into an approximation error bound for the derivatives of the mean function of the SVGP (Section 5.3).

To summarize, our contributions are in providing novel interpretations for the SVGP and Nyström approximations by establishing their connections and equivalences. These interpretations will help understand either approach from the perspective of the other approach, enable translating results from one side to the other, and encourage new algorithmic developments.

This paper is organized as follows. We provide relevant background on Gaussian processes and kernel methods in Section 2, and on the SVGP and Nyström approximations in Section 3. We investigate the equivalences between the SVGP and Nyström approximations in Section 4, and study the connections between their approximation properties in Section 5. We conclude in Section 6. The appendix provides proofs for the main theoretical results, and a derivation of the optimal variational parameters of the SVGP based on Khan and Rue (2021) on the Bayesian learning rule.
1.1 Notation

We use the following notation in this paper. Let $\mathbb{N}$ be the set of natural numbers, $\mathbb{R}$ be the real line, and $\mathbb{R}^d$ for $d \in \mathbb{N}$ be the $d$-dimensional Euclidean space. For any $v \in \mathbb{R}^d$, $\|v\|$ denotes the Euclidean norm.

Let $\mathcal{X}$ be a nonempty set. For a function $f : \mathcal{X} \to \mathbb{R}$ and $X := (x_1, \ldots, x_n) \in \mathcal{X}^n$ with $n \in \mathbb{N}$, denote by $f_X$ the $n$-vector consisting of function values evaluated at points in $X$: $f_X := (f(x_1), \ldots, f(x_n))^\top \in \mathbb{R}^n$. Similarly, for a function with two arguments $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, and $X := (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $Z := (z_1, \ldots, z_m) \in \mathcal{X}^m$ with $n, m \in \mathbb{N}$, define $k_{XZ} \in \mathbb{R}^{n \times m}$ by $(k_{XZ})_{i,j} = k(x_i, z_j)$ for $i = 1, \ldots, n$, $j = 1, \ldots, m$. For a matrix $X := (x_1, \ldots, x_n) \in \mathcal{X}^n$, let $k_X(x) := (k(x_1, x), \ldots, k(x_n, x))^\top \in \mathbb{R}^n$ for any $x \in \mathcal{X}$ and denote by $k_X(\cdot)$ the vector-valued function $x \in \mathcal{X} \mapsto k_X(x) \in \mathbb{R}^n$.

For a symmetric matrix $\Sigma$, denote by $\Sigma > 0$ and $\Sigma \succeq 0$ that $\Sigma$ is positive definite and positive semi-definite, respectively. For $\mu \in \mathbb{R}^n$ and $\Sigma \in \mathbb{R}^{n \times n}$ with $\Sigma \succeq 0$, denote by $\mathcal{N}(\mu, \Sigma)$ the Gaussian distribution on $\mathbb{R}^n$ with mean vector $\mu$ and covariance matrix $\Sigma$. Let $\mathcal{N}(\cdot \mid \mu, \Sigma)$ be its probability density function. For a matrix $A \in \mathbb{R}^{n \times n}$, tr$(A)$ and det$(A)$ denote its trace and determinant, respectively.

Let $\mathcal{Y}$ be a measurable space, $Y \in \mathcal{Y}$ be a random variable, and $\mathbb{P}$ be a probability measure on $\mathcal{Y}$. We write $Y \sim \mathbb{P}$ to mean that $Y$ follows $\mathbb{P}$. For a measurable function $g : \mathcal{Y} \to \mathbb{R}$, denote by $\int g(y) d\mathbb{P}(y)$ its integral with respect to $\mathbb{P}$ and by $\mathbb{E}[g(Y)]$ the expectation of $g(Y)$. When $\mathbb{P}$ has a density function $p : \mathcal{Y} \to \mathbb{R}$ with respect to a reference measure $\lambda$ on $\mathcal{Y}$ (e.g., the Lebesgue measure when $\mathcal{Y} = \mathbb{R}^n$), the integral is denoted by $\int g(y) p(y) d\lambda(y)$.

2. Kernels and Gaussian Processes for Regression

This section briefly reviews reproducing kernel Hilbert spaces (RKHS) and Gaussian processes (GP). In particular, we focus on the respective approaches to regression, namely kernel ridge regression (KRR) and Gaussian process regression (GPR), which are reviewed in Sections 2.1 and 2.2, respectively. We review their connections in Section 2.3.

We first describe the regression problem. Let $\mathcal{X}$ be a non-empty set. Suppose we are given $n \in \mathbb{N}$ paired observations

$$(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathbb{R}. $$

We assume that there exists a function $f_0 : \mathcal{X} \to \mathbb{R}$ such that

$$y_i = f_0(x_i) + \epsilon_i, \quad i = 1, \ldots, n. $$

where $\epsilon_1, \ldots, \epsilon_n \in \mathbb{R}$ are independent, zero-mean, noise variables. This $f_0$ is called regression function. The task of regression is to estimate (or learn) $f_0$ from the training data $(x_i, y_i)_{i=1}^n$.

We will often write $X := (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $y := (y_1, \ldots, y_n) \in \mathbb{R}^n$.

2.1 Kernel Ridge Regression (KRR)

2.1.1 Kernels and RKHSs

We review here basics of kernels and RKHSs. For details, we refer to Schölkopf and Smola (2002); Hofmann et al. (2008); Steinwart and Christmann (2008).
Let $\mathcal{X}$ be an arbitrary non-empty set. A symmetric function $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called positive definite kernel, if for every $n \in \mathbb{N}$ and every $X = (x_1, \ldots, x_n) \in \mathcal{X}^n$, the induced kernel matrix $k_{XX} = (k(x_i, x_j))_{i,j=1}^n \in \mathbb{R}^{n \times n}$ is positive semi-definite. We may simply call such $k$ kernel. Examples of kernels on $\mathcal{X} \subset \mathbb{R}^d$ include the Gaussian or square-exponential kernel $k(x, x') = \exp(-\frac{||x-x'||^2}{2\gamma})$ for $\gamma > 0$, and polynomial kernels $k(x, x') = (x^\top x' + c)^m$ for $m \in \mathbb{N}$ and $c \geq 0$.

By the Moore-Aronszajn theorem (Aronszajn, 1950), any positive definite kernel $k$ is uniquely associated with a Hilbert space $\mathcal{H}_k$ of real-valued functions $f: \mathcal{X} \to \mathbb{R}$ called reproducing kernel Hilbert space (RKHS) that satisfies

1. $k(\cdot, x) \in \mathcal{H}_k$ for every $x \in \mathcal{X}$ and
2. $f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}_k}$ for every $f \in \mathcal{H}_k$ and $x \in \mathcal{X}$ (reproducing property),

where $\langle f, g \rangle_{\mathcal{H}_k}$ for $f, g \in \mathcal{H}_k$ denotes the inner product in $\mathcal{H}_k$, and $k(\cdot, x)$ denotes the function of the first argument with $x$ being fixed: $x' \mapsto k(x', x)$, for $x' \in \mathcal{X}$. This $k(\cdot, x)$ is interpreted as a feature vector of $x$, and the kernel $k(x, x') = \langle k(\cdot, x), k(\cdot, x') \rangle_{\mathcal{H}_k}$ as a similarity of inputs $x$ and $x'$. The kernel $k$ is called reproducing kernel of $\mathcal{H}_k$.

The RKHS $\mathcal{H}_k$ consists of functions that can be approximated arbitrarily well by a linear combination of feature vectors of the form $\sum_{i=1}^n c_i k(\cdot, x_i)$ for some $c_1, \ldots, c_n \in \mathbb{R}$ and $x_1, \ldots, x_n \in \mathcal{X}$. In other words, the set of functions

$$\mathcal{H}_0 := \left\{ \sum_{i=1}^n \alpha_i k(\cdot, x_i) \mid n \in \mathbb{N}, \alpha_1, \ldots, \alpha_n \in \mathbb{R}, x_1, \ldots, x_n \in \mathcal{X} \right\}.$$ 

is a dense subset of $\mathcal{H}_k$ (e.g., Hofmann et al., 2008, Section 2.2.1).

2.1.2 Regression Approach

Kernel ridge regression (KRR) is an approach to regression using a kernel $k$ and its RKHS $\mathcal{H}_k$. The KRR estimator $\hat{f}$ of the regression function $f_0$ in (1) is defined as the solution of the following regularized least-squares problem

$$\hat{f} = \arg\min_{f \in \mathcal{H}_k} \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|^2_{\mathcal{H}_k}, \quad (2)$$

where $\lambda > 0$ is a regularization constant. Since the RKHS norm $\|f\|_{\mathcal{H}_k}$ quantifies the smoothness of $f$ and becomes large for non-smooth $f$, the regularization term in (2) makes the optimal solution $\hat{f}$ smooth; the constant $\lambda$ determines the strength of this smoothing effect.

Let $X := (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $y := (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$. By the representer theorem (Schölkopf et al., 2001), the solution $\hat{f}$ is given as a linear combination of $k(\cdot, x_1), \ldots, k(\cdot, x_n)$. Hence, the optimization problem (2) reduces to that of the coefficients of the linear combination. As a result, the estimator is given by

$$\hat{f} = \sum_{i=1}^n \alpha_i k(\cdot, x_i), \quad \text{with} \quad \alpha := (\alpha_1, \ldots, \alpha_n)^\top := (k_{XX} + n\lambda I_n)^{-1} y \in \mathbb{R}^n, \quad (3)$$

Wild, Kanagawa and Sejdinovic
where $I_n \in \mathbb{R}^{n \times n}$ is the identity matrix. The prediction of KRR at any $x \in \mathcal{X}$ is compactly written as
\[
\hat{f}(x) = k_X(x)^	op \alpha = k_X(x)^	op (k_{XX} + n\lambda I_n)^{-1} y,
\] where $k_X(x) = (k(x_1, x), \ldots, k(x_n, x))^	op \in \mathbb{R}^n$.

### 2.2 Gaussian Process Regression (GPR)

#### 2.2.1 Gaussian Processes

Gaussian processes (GPs) are one of the main workhorses of Bayesian nonparametric statistics and machine learning, as they can be used to place a prior distribution over functions. See Rasmussen and Williams (2006) for more details.

Let $\mathcal{X}$ be a non-empty set, $m : \mathcal{X} \rightarrow \mathbb{R}$ a function and $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ a positive definite kernel. A random function $F : \mathcal{X} \rightarrow \mathbb{R}$ is called Gaussian process (GP) with mean function $m$ and covariance kernel $k$, if for all $n \in \mathbb{N}$ and all $X = (x_1, \ldots, x_n) \in \mathcal{X}^n$, the random vector $F_X := (F(x_1), \ldots, F(x_n))^	op \in \mathbb{R}^n$ satisfies $F_X \sim \mathcal{N}(m_X, k_{XX})$, i.e., $F_X$ follows the Gaussian distribution with mean vector $m_X = (m(x_1), \ldots, m(x_n))^	op \in \mathbb{R}^n$ and covariance matrix $k_{XX} = (k(x_i, x_j))_{i,j=1}^n \in \mathbb{R}^{n \times n}$. In this case, we write $F \sim GP(m, k)$.

For any function $m : \mathcal{X} \rightarrow \mathbb{R}$ and kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, there exists a GP whose mean function is $m$ and covariance function is $k$. Therefore, by choosing $m$ and $k$, one can implicitly define the corresponding GP, $F \sim GP(m, k)$. This is how a GP is used to define a prior distribution in Bayesian nonparametrics.

#### 2.2.2 Regression Approach

Gaussian process regression (GPR) is a Bayesian nonparametric approach to the regression problem. In GPR, the regression function $f_0$ in Eq. (1) is the quantity of interest and modeled as a random function $F$. The prior distribution is given by a GP
\[
F \sim GP(m, k),
\] where the mean function $m$ and covariance function $k$ are chosen to encode one’s prior knowledge/assumption about the regression function $f_0$. The observation model of $F$ for the observations $y = (y_1, \ldots, y_n)^	op$ is given by
\[
y_i = F(x_i) + \varepsilon_i, \quad i = 1, \ldots, n,
\] where $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ is an independent Gaussian noise with variance $\sigma^2 > 0$.

By Bayes’ rule, the posterior distribution of $F$ given $y$, under the prior (5), is given by another GP (e.g., Rasmussen and Williams, 2006):
\[
F \mid y \sim GP(\bar{m}, \bar{k}),
\]
where $\bar{k} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ and $\bar{m} : \mathcal{X} \rightarrow \mathbb{R}$ are defined as
\[
\bar{m}(x) := m(x) + k_X(x)^	op (k_{XX} + \sigma^2 I_n)^{-1} (y - m_X),
\] (7)
\[
\bar{k}(x, x') := k(x, x') - k_X(x)^	op (k_{XX} + \sigma^2 I_n)^{-1} k_X(x'),
\] (8)
where \(k_X(x) = (k(x_1, x), \ldots, k(x_n, x))^\top \in \mathbb{R}^n\). We call \(GP(\bar{m}, \bar{k})\) the posterior GP, \(\bar{m}\) the posterior mean function and \(\bar{k}\) the posterior covariance function. We use the following notation for the probability measure of the posterior GP:

\[
P_{\mathcal{F}|y} := GP(\bar{m}, \bar{k}).
\]  

(9)

The posterior mean \(\bar{m}(x)\) serves as a predictor of the ground-truth function value \(f_0(x)\), while the posterior variance \(\bar{k}(x, x)\) quantifies its uncertainty.

2.3 Connections between the Exact Solutions for KRR and GPR

It is well-known that there are connections between KRR and GPR (Kimeldorf and Wahba, 1970; Kanagawa et al., 2018), which are briefly summarized here.

First, there is an equivalence between the predictors of KRR and GPR. Suppose that the same kernel \(k\) is used in KRR and GPR, and that the prior mean function of GPR is zero, \(m(x) = 0\). Then the posterior mean function \(\bar{m}(x)\) of GPR in (7) is identical to the KRR estimator \(\hat{f}(x)\) in (4), provided that the regularization constant \(\lambda\) in KRR satisfies \(\sigma^2 = n\lambda\). This equivalence provides a Bayesian interpretation of the KRR estimator, and a least-squares interpretation of the GPR posterior mean function.

Second, the posterior variance \(\bar{k}(x, x)\) of GPR can be interpreted as a worst case error of KRR predictions in the RKHS of a certain augmented kernel defined from the GP covariance kernel \(k\) and the noise variance \(\sigma^2\) (Kanagawa et al., 2018, Section 3.4). This interpretation enables discussing how the RKHS is related to the uncertainty estimates of GPR. Further connections between the two approaches can be found in Kanagawa et al. (2018).

This paper investigates whether these parallels between KRR and GPR extend to their sparse approximations, which are reviewed in the next section.

3. Sparse Approximation Methods

This section reviews sparse approximation methods for KRR and GPR, specifically the Nyström method in Section 3.1 and Sparse Variational Gaussian Processes (SVGP) in Section 3.2. While closed-form expressions are available for KRR and GPR, their computations require the \(O(n^3)\) complexity for training data size \(n\), which is challenging when \(n\) is large. A sparse approximation method reduces this computational complexity by approximating the exact solution based on a smaller set of input points \(z_1, \ldots, z_m \in \mathcal{X}\), where \(m < n\). The Nyström and SVGP approximations are commonly used sparse approximation methods for kernel methods and GPs, respectively. We review them here as a preliminary for our investigation of their connections in the subsequent sections.

3.1 Nyström Approximation

The Nyström method was first proposed by Williams and Seeger (2001) for scaling up kernel-based learning algorithms. It has been successfully used in a variety of applications including manifold leaning (Talwalkar et al., 2008, 2013), computer vision (Fowlkes et al., 2004; Belabbas and Wolfe, 2009), and approximate sampling (Affandi et al., 2013), to name a few. Recent studies make use of the Nyström method to enable KRR to handle millions to billions of data points (e.g., Rudi et al., 2017; Meanti et al. 2020).
We describe here the use of the Nyström approximation in KRR. In particular, we consider a popular version classically known as the subset of regressors (Wahba, 1990, Chapter 7), which has been widely used both in practice and theory (e.g., Smola and Schölkopf, 2000; Rudi et al., 2015, 2017; Meanti et al., 2020). As before, let \((x_i, y_i)_{i=1}^n \subset \mathcal{X} \times \mathbb{R}\) be training data, and let \(X := (x_1, \ldots, x_n) \in \mathcal{X}^n\) and \(y := (y_1, \ldots, y_n)^\top \in \mathbb{R}^n\).

For \(m \in \mathbb{N}\), let \(z_1, \ldots, z_m \in \mathcal{X}\) be a set of input points based on which we approximate the KRR solution. These points \(z_1, \ldots, z_m\) are usually a subset of training input points \(x_1, \ldots, x_n\) in the kernel literature, but we allow for \(z_1, \ldots, z_m\) to be generic points in \(\mathcal{X}\) for a later comparison with the GP counterpart. Write \(Z = (z_1, \ldots, z_m) \in \mathcal{X}^m\). Suppose that the kernel matrix \(k_{ZZ} = (k(z_i, z_j))_{i,j=1}^m \in \mathbb{R}^{m \times m}\) is invertible.

Let \(M \subset \mathcal{H}_k\) be the finite dimensional subspace spanned by \(k(\cdot, z_1), \ldots, k(\cdot, z_m)\):

\[
M := \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m)) := \left\{ \sum_{j=1}^m \alpha_j k(\cdot, z_j) \mid \alpha_1, \ldots, \alpha_m \in \mathbb{R} \right\}. \tag{10}
\]

We replace the hypothesis space \(\mathcal{H}_k\) in the KRR objective function (2) by this subspace \(M\), and define its solution \(\hat{f}\) as the Nyström approximation of the KRR solution \(\hat{f}\):

\[
\hat{f} := \arg \min_{f \in M} \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|^2_{\mathcal{H}_k}. \tag{11}
\]

In other words, we approximately solve the minimization problem of KRR by searching for the solution of the form

\[
f = \sum_{i=1}^m \beta_i k(\cdot, z_i) = k_Z(\cdot)\top \beta
\]

for some coefficients \(\beta := (\beta_1, \ldots, \beta_m)\top \in \mathbb{R}^m\), where \(k_Z(\cdot) := (k(\cdot, z_1), \ldots, k(\cdot, z_m))\top\). Inserting this expression in (11), the optimization problem now becomes

\[
\min_{\beta \in \mathbb{R}^m} \frac{1}{n} \|y - k_{XZ} \beta\|^2 + \lambda \beta\top k_{ZZ} \beta,
\]

where \(k_{XZ} \in \mathbb{R}^{n \times m}\) with \((k_{XZ})_{i,j} = k(x_i, z_j)\) and \(k_{ZZ} \in \mathbb{R}^{m \times m}\) with \((k_{ZZ})_{i,j} = k(z_i, z_j)\). Taking the first order derivative with respect to \(\beta\) leads to the condition

\[
-\frac{2}{n} k_{ZX} y + \frac{2}{n} k_{XX} k_{XZ} \beta + 2\lambda k_{ZZ} \beta = 0,
\]

which is satisfied for

\[
\beta = (k_{XX} k_{XZ} + n \lambda k_{ZZ})^{-1} k_{XY}.
\]

This leads to the following expression of the Nyström approximation:

\[
\hat{f}(x) = k_Z(x)\top (n \lambda k_{ZZ} + k_{XX} k_{XZ})^{-1} k_{ZY}.
\tag{12}
\]

This approximation can be computed with the complexity of \(\mathcal{O}(nm^2 + m^3)\) instead of \(\mathcal{O}(n^3)\), since the inversion of an \(n \times n\) matrix is replaced by that of an \(m \times m\) matrix. (The complexity \(\mathcal{O}(nm^2)\) is that of the matrix multiplication \(k_{XX} k_{XZ}\), which is the dominating part as \(m < n\).) This grants significant computational gains, if \(m\) is much smaller than \(n\) and hence allows KRR to be applied to large data sets. Of course, how to choose \(m\) and the input points \(z_1, \ldots, z_m\) depends not only on the computational budget but also on how accurately \(\hat{f}\) approximates the KRR solution \(\hat{f}\). We discuss this issue in Section 5.
3.2 Sparse Variational Gaussian Processes

We review here the Sparse Variational Gaussian Process (SVGP) approach by Titsias (2009a) based on a measure-theoretic formulation suggested by Matthews et al. (2016). There have been many works on sparse approximations for scaling up GP-based methods. In a nutshell, there are two common approaches: either the generative model is approximated and inference is performed exactly (Seeger et al., 2003; Snelson and Ghahramani, 2006, 2007) or the generative model is left unaltered and inference is done approximately (Csató and Opper, 2002; Titsias, 2009a). In this work, we mainly focus on the SVGP approximation by Titsias (2009a), which is the latter approach. We refer to Bauer et al. (2016) and Bauer (2020, Part I) for a systematic comparison of the two approaches.

Since we focus on the basic framework of Titsias (2009a) and its comparison to the kernel counterpart in a regression setting, we do not discuss sparse variational GP approaches to the classification problem (Hensman et al., 2015a) and other (more recent) developments (e.g., Hensman et al., 2015b, 2018; Dutordoir et al., 2020; Adam et al., 2020; Shi et al., 2020; Rossi et al., 2021; Tran et al., 2021). See e.g., Leibfried et al. (2020) for an overview over variational GP approaches.

We first recall the setting of GPR using a measure-theoretic notation. As before, let \((x_i, y_i)_{i=1}^n \subset \mathcal{X} \times \mathbb{R}^n\) be training data and let \(X = (x_1, \ldots, x_n) \in \mathcal{X}^n\) and \(y = (y_1, \ldots, y_n) \in \mathbb{R}^n\). For simplicity, we assume the zero prior mean function, \(m(x) = 0\). We denote by \(\mathbb{P}\) the probability measure of a Gaussian process \(F \sim \text{GP}(0, k)\). For any finite set of points \(D := (d_1, \ldots, d_\ell) \in \mathcal{X}^\ell\) with \(\ell \in \mathbb{N}\), let \(\mathbb{P}_D\) be the corresponding distribution of \(F_D := (F(d_1), \ldots, F(d_\ell))^\top\) on \(\mathbb{R}^\ell\), which is \(\mathbb{P}_D = \mathcal{N}(0, k_{DD})\) by definition.

3.2.1 Variational Family

We first introduce a variational family of probability measures of functions on \(\mathcal{X}\), from which we search for a computationally tractable approximation of the GP posterior \(\mathbb{P}^{F|y} = \text{GP}(\bar{m}, \bar{k})\) in (9). Let \(m \in \mathbb{N}\) be fixed, and \(\Gamma\) be a set of variational parameters defined by

\[
\Gamma := \{ \nu := (Z, \mu, \Sigma) \mid Z := (z_1, \ldots, z_m) \in \mathcal{X}^m, k_{ZZ} \text{ is invertible,}
\mu \in \mathbb{R}^m, \Sigma \in \mathbb{R}^{m \times m}_{>0}\}
\]

where \(\mathbb{R}^{m \times m}_{>0}\) stands for symmetric and positive definite matrices in \(\mathbb{R}^{m \times m}\). The points \(Z = (z_1, \ldots, z_m)\) are the so-called inducing inputs, based on which we approximate the posterior GP. On the other hand, \(\mu\) and \(\Sigma\) are parameters for the distribution of function values at \(z_1, \ldots, z_m\).

---

1. The main reason for presenting in the measure-theoretic formulation is to treat the variational mean \(m^*(x)\) and covariance \(k^*(x, x')\) introduced below as functions; this is needed for establishing the equivalences and connections to the RKHS counterparts, which are also functions.
We then define a variational family \( Q_\Gamma := \{ Q^\nu \mid \nu \in \Gamma \} \) as a set of Gaussian processes parametrized by the triplet\(^2 \nu = (Z, \mu, \Sigma) \) defined as follows:

\[
Q^\nu := GP(m^\nu, k^\nu), \\
m^\nu(x) := k_Z(x)^\top k_Z^{-1} \mu, \\
k^\nu(x, x') := k(x, x') - k_Z(x)^\top k_Z^{-1} k_Z(x') + k_Z(x)^\top k_Z^{-1} \Sigma k_Z^{-1} k_Z(x').
\]

Each variational distribution (13) is defined so as to satisfy the following properties, where \( F^\nu \sim GP(m^\nu, k^\nu) \) denotes the corresponding GP sample function:

1. The function values\(^3 \) \( F^\nu := (F^\nu(z_1), \ldots, F^\nu(z_m))^{\top} \in \mathbb{R}^m \) at the inducing inputs \( z_1, \ldots, z_m \) follow the Gaussian distribution with mean vector \( \mu \in \mathbb{R}^m \) and covariance matrix \( \Sigma \in \mathbb{R}^{m \times m} \), i.e., \( F^\nu_Z \sim \mathcal{N}(\mu, \Sigma) \). We denote by \( Q^\nu_Z \) by the distribution of \( F^\nu_Z \), i.e., \( Q^\nu_Z = \mathcal{N}(\mu, \Sigma) \).

2. The conditional distribution of the process \( F^\nu \) given \( (z_i, F^\nu(z_i))_{i=1}^m \) is identical to the conditional distribution of \( F \sim GP(m, k) \) given \( (z_i, F(z_i))_{i=1}^m \):

\[
F^\nu \mid (z_i, F^\nu(z_i))_{i=1}^m \xrightarrow{d} F \mid (z_i, F(z_i))_{i=1}^m.
\]

### 3.2.2 Evidence Lower Bound and Optimal Variational Parameters

The aim of variational inference is to obtain a distribution \( Q^{\nu^*} \) from the variational family \( Q_\Gamma \) that best approximates the posterior measure \( P^{F \mid y} \) in terms of the Kullback-Leibler (KL) divergence, without explicitly computing the posterior. That is, we want to compute \( \nu^* \in \Gamma \) such that

\[
\nu^* = \arg \min_{\nu \in \Gamma} \text{KL}(Q^\nu \| P^{F \mid y}).
\]

where \( \text{KL}(Q^\nu \| P^{F \mid y}) \) is the KL divergence between \( Q^\nu \) and \( P^{F \mid y} \) defined by

\[
\text{KL}(Q^\nu \| P^{F \mid y}) := \int \log \left( \frac{dQ^\nu}{dP^{F \mid y}}(f) \right) dQ^\nu(f).
\]

with \( \frac{dQ^\nu}{dP^{F \mid y}} \) being the Radon-Nikodym derivative of \( Q^\nu \) with respect to \( P^{F \mid y} \), which exists by the construction of \( Q^\nu \) (Matthews et al., 2016, Section 3.3).

Matthews et al. (2016, Eq. 15) show that this KL divergence can be written as

\[
\text{KL}(Q^\nu \| P^{F \mid y}) = \log p(y) - \mathcal{L}(\nu),
\]

where \( p(y) \) is the marginal likelihood, or the Evidence, of observing \( y = (y_1, \ldots, y_n)^\top \) under the prior \( F \sim GP(m, k) \) and the observation model \( y_i \sim \mathcal{N}(F(x_i), \sigma^2) \), while \( \mathcal{L}(\nu) \) is the Evidence Lower Bound (ELBO) defined as

\[
\mathcal{L}(\nu) := -\text{KL}(Q^\nu_Z \| P_Z) + \mathbb{E}_{F^\nu \sim Q^\nu} \left[ \log p(y | F^\nu_Z) \right],
\]

where

\(^2\) Note that we assume that the kernel \( k \) is fixed, and hence the variational family is parametrized by this triplet. If we consider the learning of the parameters of the kernel \( k \) as well, then they may be included as parameters of the variational family.

\(^3\) Note that \( F^\nu_Z \) is usually called inducing variables and is denoted with symbol \( u \) in the literature.
• $KL(Q^\nu_Z \parallel P_Z)$ is the standard KL divergence between $Q^\nu_Z = \mathcal{N}(\mu, \Sigma)$, which is the marginal distribution of $F^\nu_Z \in \mathbb{R}^m$ of the parameterized Gaussian process $F^\nu \sim Q^\nu = GP(m^\nu, k^\nu)$ in (13), and $P_Z = \mathcal{N}(0, k_{ZZ})$, which is the marginal distribution of $F_Z \in \mathbb{R}^m$ of the prior Gaussian process $F \sim P = GP(0, k)$:

$$KL(Q^\nu_Z \parallel P_Z) = \int_{\mathbb{R}^m} \log \left( \frac{dQ^\nu_Z}{dP_Z}(f_Z) \right) dQ^\nu_Z(f_Z)$$

$$= \frac{1}{2} \left( \text{tr}(k_{ZZ}^{-1} \Sigma) + \mu^\top k_{ZZ}^{-1} \mu - m + \log \left( \frac{\det(k_{ZZ})}{\det(\Sigma)} \right) \right),$$

(20)

where the last identity is the well-known expression of the KL divergence between multivariate Gaussian densities (see, e.g., Appendix A.5 of Rasmussen and Williams 2006).

• $E_{F^\nu \sim Q^\nu}[\log p(y|F^\nu_X)]$ is the marginal log likelihood of observing $y = (y_1, \ldots, y_n)^\top$ under the observation model $y_i = F^\nu(x_i) + \varepsilon_i$ with independent $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ and the parametrized process $F^\nu \sim Q^\nu$:

$$E_{F^\nu \sim Q^\nu}[\log p(y|F^\nu_X)] = -\frac{n}{2} \log \left( \overline{2\pi \sigma^2} \right) - \frac{n}{2} \sum_{i=1}^{n} \frac{(y_i - F^\nu(x_i))^2}{2\sigma^2}$$

(21)

where $p(y|F^\nu_X) := \mathcal{N}(y; F^\nu_X, \sigma^2 I_n)$ is the Gaussian density of the likelihood function (6).

Since the marginal likelihood $p(y)$ under the original GP prior does not depend on the variational parameters $\nu$, the minimization of the KL divergence (18) is equivalent to the maximization of the ELBO $L(\nu)$ in (19). Titsias (2009a, Eq.(10)) show that, for fixed inducing points $Z$, the optimal parameters $\mu^*$ and $\Sigma^*$ that maximize the ELBO are given analytically as

$$\mu^* := k_{ZZ}(\sigma^2 k_{ZZ} + k_{XX}k_{XZ})^{-1}k_{XX}y$$

(22)

$$\Sigma^* := k_{ZZ}(k_{ZZ} + \sigma^{-2}k_{XX}k_{XZ})^{-1}k_{ZZ}$$

(23)

and the resulting ELBO, denoted by $L^*$, is

$$L^* = -\frac{1}{2} \log \det(q_{XX} + \sigma^2 I_n) - \frac{1}{2}y^\top(q_{XX} + \sigma^2 I)^{-1}y$$

$$- \frac{n}{2} \log 2\pi - \frac{1}{2\sigma^2} \text{tr}(k_{XX} - q_{XX}),$$

(24)

where $q$ is the approximate kernel in (34). Inserting these expressions in the definition of the variational distribution (13), the optimal variational approximation (for fixed inducing
connections between the Nyström and Sparse Variational Gaussian Processes

points \( Z \) is given by \( GP(m^*, k^*) \) with \(^5\)

\[
m^*(x) := k_Z(x)^	op \left( \sigma^2 k_{ZZ} + k_{XX} k_{XZ} \right)^{-1} k_{XY}
\]

\[
k^*(x, x') := k(x, x') - k_Z(x)^	op k_{ZZ}^{-1} k_Z(x)
+ k_Z(x)^	op (k_{ZZ} + \sigma^{-2} k_{XX} k_{XZ})^{-1} k_Z(x').
\]

The computational complexity of obtaining the mean function \( m^* \) and the covariance function \( k^* \) is \( O(nm^2 + m^3) \), which can be much smaller than the complexity \( O(n^3) \) of the exact posterior as long as the number of inducing points \( m \) is much smaller than the training data size \( n \).

The ELBO (24) with optimal \( \mu^* \) and \( \Sigma^* \) is a key quantity, as it can be used i) as a criterion for optimizing the inducing inputs \( z_1, \ldots, z_m \) and ii) for theoretically analyzing the quality of variational approximation.

We have seen that the Nyström and SVGP approximations are derived from quite different principles; the former approximately solves KRR by replacing the RKHS by its subspace spanned by the inducing points, while the latter variationally approximates the GP posterior using variational GPs defined with the inducing points. How are these two approximations related? This is the question we investigate in the rest of the paper.

4. Connections between the SVGP and Nyström Approximations

This section studies how the Nyström and SVGP approximations are related. We first analyze the equivalence between the Nyström KRR and the optimized mean function of the SVGP in Section 4.1. We then introduce orthogonal projections on the RKHS subspace in Section 4.2, and investigate RKHS interpretations of the SVGP covariance function in Section 4.3.

4.1 Equivalence between the Nyström KRR and the SVGP Posterior Mean

We first study how the Nyström KRR (12) is related to the optimized mean function (25) of the SVGP. Their equivalence immediately follows from their forms, as summarized below.

Theorem 1 Let \( k \) be a kernel, and suppose that data \((x_i, y_i)_{i=1}^n \subset \mathcal{X} \times \mathbb{R} \) are given. Let \( Z = (z_1, \ldots, z_m) \in \mathcal{X}^m \) be fixed inducing inputs such that the kernel matrix \( k_{ZZ} = (k(z_i, z_j))_{i,j=1}^m \in \mathbb{R}^{m\times m} \) is invertible.

- Let \( m^* \) be the optimized mean function (25) of the SVGP approximation using \( Z \) as inducing points for defining the variational family (13).

- Let \( \bar{f} \) be the Nyström approximation (12) using \( Z \) as landmark points for defining the subspace \( \mathcal{M} = \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m)) \).

5. Note that these \( m^* \) and \( k^* \) are also equal to the predictive mean and covariance functions of the so-called Deterministic Training Conditional (DTC) approximation (Seeger et al. 2003) (Quiñonero-Candela and Rasmussen 2005, Section 5); see Bauer (2020 Sections 2.3 and 2.4). Therefore, RKHS interpretations for these functions also apply to the DTC approximation. However, the DTC’s objective function for hyperparameter optimization is different from that of the SVGP, i.e., the ELBO in (24). Therefore RKHS interpretations for the ELBO (24) is only valid for the SVGP.
Then we have $m^* = \bar{f}$, provided $\sigma^2 = n\lambda$ for the noise variance $\sigma^2$ in (6) and the regularization constant $\lambda$ in (11).

The condition $\sigma^2 = n\lambda$ in Theorem 1 is the same as that required for the equivalence between KRR and GPR, as mentioned in Section 2.3.

Now the question is why the equivalence in Theorem 1 holds, even though the Nyström and SVGP approximations are the solutions to seemingly unrelated optimization problems. To investigate this question, we closely inspect the ELBO in (19), the objective function of the SVGP, as summarized in Theorem 2 below. The proof can be found in Appendix B.2.

**Theorem 2** Let $\nu = (Z, \mu, \Sigma) \in \mathcal{X}^m \times \mathbb{R}^m \times \mathbb{R}_{>0}^{m \times m}$ be such that the kernel matrix $k_{ZZ} \in \mathbb{R}^{m \times m}$ is invertible, and let $\mathcal{L}(\nu)$ be the ELBO in (19). Then we have

$$-2\sigma^2 \mathcal{L}(\nu) = \sum_{i=1}^{n} \left( y_i - k_{Z}(x_i)^\top k_{ZZ}^{-1}\mu \right)^2 + \sigma^2 \mu k_{ZZ}^{-1}\mu \quad (27)$$

$$+ \sum_{i=1}^{n} k_{Z}(x_i)^\top k_{ZZ}^{-1}\Sigma k_{ZZ}^{-1}k_{Z}(x_i) \quad (28)$$

$$+ \sigma^2 \left( \text{tr}(k_{ZZ}^{-1}\Sigma) + \log \left( \frac{\det(k_{ZZ})}{\det(\Sigma)} \right) - m \right) \quad (29)$$

$$+ \sum_{i=1}^{n} \left( k(x_i, x_i) - k_{Z}(x_i)^\top k_{ZZ}^{-1}k_{Z}(x_i) \right). \quad (30)$$

Theorem 2 disentangles the ELBO (19) into i) the part (27) that depends only on the mean parameter $\mu$ and the inducing inputs $Z$, ii) the part (28) (29) that depends only on the covariance parameter $\Sigma$ and $Z$, and iii) the part (30) that depends only on $Z$. We focus here on the part i) to understand the equivalence in Theorem 1. The other parts are analyzed later.

As a preliminary, notice that the SVGP mean function $m^\nu = k_{Z}(\cdot)^\top k_{ZZ}^{-1}\mu$ in (14) lies in the subspace $M = \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m))$, because it can be written $m^\nu =
\[ \sum_{i=1}^{m} \alpha_i k(\cdot, z_i) \text{ for } \alpha := (\alpha_1, \ldots, \alpha_m)^\top := k^{-1}_{ZZ} \mu. \] Define then a map \( \psi : \mathbb{R}^m \mapsto M \) that maps the mean vector \( \mu \in \mathbb{R}^m \) to the mean function \( m^\nu \):

\[ \psi(\mu) := k_Z(\cdot)^\top k^{-1}_{ZZ} \mu \in M, \quad \mu \in \mathbb{R}^m. \] (31)

This map is one-to-one, because each \( f \in M \) can be written \( f = \sum_{i=1}^{m} \alpha_i k(\cdot, z_i) \) for uniquely associated \( \alpha := (\alpha_1, \ldots, \alpha_m)^\top \in \mathbb{R}^m \) and we have \( f = \psi(\mu) \) for \( \mu = k_{ZZ} \alpha = f_Z \in \mathbb{R}^m \), which is the evaluations of \( f \) at the inducing points \( Z = (z_1, \ldots, z_m) \) (see Figure 1 for an illustration.). Therefore, the inverse map \( \psi^{-1} : M \mapsto \mathbb{R}^m \) is given by:

\[ \psi^{-1}(f) = f_Z \in \mathbb{R}^m, \quad f \in M. \]

With this preparation, and letting \( f := \psi(\mu) \in M \), the part (27) can be written

\[ \sum_{i=1}^{n} \left( y_i - k_Z(x_i)^\top k^{-1}_{ZZ} \mu \right)^2 + \sigma^2 \mu^\top k_{ZZ} \mu = \sum_{i=1}^{n} (y_i - f(x_i))^2 + \sigma^2 \|f\|_{\mathcal{H}_k}^2. \] (32)

The right expression of (32) is exactly the objective function (11) of the Nyström KRR if \( \sigma^2 = n \lambda \). Hence, the negative ELBO as an objective function of \( \mu \in \mathbb{R}^m \) is equivalent to the Nyström KRR objective as a function \( f = \psi(\mu) \in M \). Consequently, they lead to the identical solution in Theorem 1. These findings are summarized below.

**Corollary 3** Let \( \nu = (Z, \mu, \Sigma) \in \mathcal{X}^m \times \mathbb{R}^m \times \mathbb{R}^{m \times m} \) be such that the kernel matrix \( k_{ZZ} \in \mathbb{R}^{m \times m} \) is invertible, \( M = \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m)) \subset \mathcal{H}_k \) be the subspace, and let \( \mathcal{L}(\nu) \) be the ELBO in (19). Let \( \psi : \mathbb{R}^m \mapsto M \) be the one-to-one map in (31). Then we have for \( f = \psi(\mu) \in M \)

\[ -2\sigma^2 \mathcal{L}(\nu) = \sum_{i=1}^{n} (y_i - f(x_i))^2 + \sigma^2 \|f\|_{\mathcal{H}_k}^2 + L(Z, \Sigma), \]

where \( L(Z, \Sigma) \in \mathbb{R} \) is a constant not depending on \( \mu \). In particular, we have \( \psi(\mu^*) = f^* \), where

\[ \mu^* := \arg \max_{\mu \in \mathbb{R}^m} \mathcal{L}(\nu), \quad f^* := \arg \min_{f \in M} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \sigma^2 \|f\|_{\mathcal{H}_k}^2. \]

It has been shown that the equivalence between the optimized SVGP mean function and the Nyström KRR in Theorem 1 stems from the equivalence between their objective functions. Specifically, the optimized SVGP mean function is interpreted as minimizing the KRR objective on the subspace \( M = \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m)) \).

We now turn our attention to the SVGP covariance function (26) and investigate its connection to the Nyström approximation. To this end, we need the notion of **orthogonal projections** onto the subspace \( M \), which is defined next.
4.2 Orthogonal Projections onto the Subspace

As a preliminary for analyzing the SVGP covariance function, we introduce orthogonal projections onto the RKHS subspace $M = \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m))$. We show that such projections define an approximate kernel whose RKHS is identical to $M$, and the use of this kernel in KRR leads to the Nyström KRR. These points are summarized here, as they will be useful later.

Define $P_M : \mathcal{H}_k \mapsto M$ as the orthogonal projection operator that maps a given $f \in \mathcal{H}_k$ to its best approximation $P_M(f)$ in the subspace $M$. That is, $P_M(f)$ is the element in $M$ having the minimum RKHS distance to $f$ (see Figure 2):

$$
\|f - P_M(f)\|_{\mathcal{H}_k} = \min_{g \in M} \|f - g\|_{\mathcal{H}_k} = \min_{\alpha_1, \ldots, \alpha_m \in \mathbb{R}} \left\| f - \sum_{i=1}^{m} \alpha_i k(\cdot, z_i) \right\|_{\mathcal{H}_k}.
$$

If the feature maps $k(\cdot, z_1), \ldots, k(\cdot, z_m)$ are linearly independent, which is equivalent to the kernel matrix $k_{ZZ} \in \mathbb{R}^{m \times m}$ being invertible, it can be shown that the minimizer $\alpha_1, \ldots, \alpha_m$ for the right expression is unique and given by $\alpha := (\alpha_1, \ldots, \alpha_m)^\top = k_{ZZ}^{-1}f_Z$ with $f_Z = (f(z_1), \ldots, f(z_m))^\top$. Thus the orthogonal projection is given as

$$
P_M(f) = k_Z(\cdot)^\top k_{ZZ}^{-1}f_Z. \quad (33)
$$

One can use the orthogonal projection operator $P_M$ to define an approximate kernel. Note that the kernel $k(x, x')$ can be written as the inner product between the feature maps $k(\cdot, x)$ and $k(\cdot, x')$:

$$
k(x, x') = \langle k(\cdot, x), k(\cdot, x') \rangle_{\mathcal{H}_k}, \quad x, x' \in \mathcal{X}.
$$

---

6. By the reproducing property, we have $\|f - \sum_{i=1}^{m} \alpha_i k(\cdot, z_i)\|_{\mathcal{H}_k}^2 = \|f\|_{\mathcal{H}_k}^2 - 2f_Z^\top k_{ZZ}\alpha + \alpha^\top k_{ZZ}\alpha$, where $\alpha = (\alpha_1, \ldots, \alpha_m)$. Taking the derivative with respect to $\alpha$ and equating it to 0 yields the expression.
By replacing \( k(\cdot, x) \) and \( k(\cdot, x') \) by their best approximations \( P_M(k(\cdot, x)) \) and \( P_M(k(\cdot, x')) \), we can define an approximation \( q(x, x') \) of \( k(x, x') \) as

\[
q(x, x') := \langle P_M(k(\cdot, x)), P_M(k(\cdot, x')) \rangle_{\mathcal{H}_k}
\]

\[
= \langle k_Z(x)^\top k_{ZZ}^{-1} k_Z(\cdot), k_Z(x')^\top k_{ZZ}^{-1} k_Z(\cdot) \rangle_{\mathcal{H}_k}
\]

\[
= k_Z(x)^\top k_{ZZ}^{-1} k_Z(x'), \quad x, x' \in \mathcal{X},
\]

(34)

where the second line follows from (33), and the third uses the reproducing property.

Since \( q(x, x') \) in (34) is a positive definite kernel, it induces its own RKHS \( \mathcal{H}_q \). As the following lemma shows, this RKHS \( \mathcal{H}_q \) is nothing but the subspace \( M \), and the inner product \( \langle \cdot, \cdot \rangle_{\mathcal{H}_q} \) of \( \mathcal{H}_q \) is the same as that of the original RKHS \( \mathcal{H}_k \). The proof can be found in Appendix B.1.

**Lemma 4** Let \( Z = (z_1, \ldots, z_m) \in \mathcal{X}^m \) be such that the kernel matrix \( k_{ZZ} \) is invertible. Let \( M = \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m)) \) be the subspace of \( \mathcal{H}_k \) in (10), and \( \mathcal{H}_q \) be the RKHS of the approximate kernel \( q \) in (34). Then we have \( M = \mathcal{H}_q \) as a set of functions, and

\[
\langle f, g \rangle_{\mathcal{H}_q} = \langle f, g \rangle_{\mathcal{H}_k}, \quad \forall f, g \in M = \mathcal{H}_q.
\]

In particular, we have

\[
\|f\|_{\mathcal{H}_q} = \|f\|_{\mathcal{H}_k}, \quad \forall f \in M = \mathcal{H}_q.
\]

By using Lemma 4, the Nyström KRR in (11) can be rewritten as KRR using the approximate kernel \( q \) in (34) as summarized as follows.

**Theorem 5** Let \( X := (x_1, \ldots, x_n) \in \mathcal{X}^n \) and \( y := (y_1, \ldots, y_n)^\top \in \mathbb{R}^n \) be given. Let \( Z = (z_1, \ldots, z_m) \in \mathcal{X}^m \) be such that the kernel matrix \( k_{ZZ} \) is invertible, and \( \bar{f} \) be the Nyström approximation \( \bar{f} \) of KRR in (11). Then we have

\[
\bar{f} = \arg\min_{f \in \mathcal{H}_q} \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{H}_q}^2
\]

where \( q \) is the approximate kernel defined in (34).

Theorem 5 shows that the Nyström KRR can be interpreted as KRR using the approximate kernel (34).

Consider now GPR using the approximate kernel \( q \) in (34) as the prior, \( F \sim GP(0, q) \), instead of the original kernel \( k \) (Quiñonero-Candela and Rasmussen, 2005, Section 4). The resulting posterior mean function \( \tilde{m}(x) \) and covariance function \( \bar{q}(x, x') \) are given by

\[
\tilde{m}(x) = q_X(x)^\top (q_{XX} + \sigma^2 I_n)^{-1} y
\]

\[
= k_Z(x)^\top (\sigma^2 k_{ZZ} + k_{ZX} k_{XZ})^{-1} k_{ZX} y,
\]

(35)

\[
\bar{q}(x, x') = q(x, x') - q_X(x) (q_{XX} + \sigma^2 I_n)^{-1} q_X(x')
\]

\[
= k_Z(x)^\top (k_{ZZ} + \sigma^2 k_{ZX} k_{XZ})^{-1} k_Z(x').
\]

The posterior mean function (35) is identical to the the Nyström approximation (12), if \( \sigma^2 = n\lambda \). This equivalence follows from the equivalence between the KRR and GPR and Theorem 5.
4.3 RKHS Interpretations of the SVGP Covariance Function

Given the above preliminaries, we now analyze the optimized SVGP covariance function (26), which is given as

\[
\begin{aligned}
k^*(x, x') &= k(x, x') - k_Z(x) k_Z(x')^{-1} k_Z(x') + k_Z(x) (k_{ZZ} + \sigma^{-2} k_{XX} k_{XZ})^{-1} k_Z(x'). \\
&= (a) - (b).
\end{aligned}
\]

The term \((a)\) is the posterior covariance function of GPR using the prior \(F \sim GP(0, k)\) given noise-free observations at the inducing inputs \(Z = (z_1, \ldots, z_m)\), as can be seen from (8) with \(X = Z\) and \(\sigma^2 = 0\). The term \((b)\) is the posterior covariance function (36) of GPR using the prior \(F \sim GP(0, q)\) with the approximate kernel in (34) given noisy observations at training inputs \(X = (x_1, \ldots, x_m)\). Therefore the optimized SVGP covariance function is the sum of two posterior covariance functions.

The optimized SVGP covariance function is an approximation to the exact GP posterior covariance function \(k(x, x')\) in (8). To understand how this approximation is done, consider the optimized SVGP variance, i.e., \(x = x'\) in (37), which approximates the exact GP posterior variance \(k(x, x)\). Intuitively, the term \((a)\) represents the uncertainty arising from approximating the GP prior \(F \sim GP(0, k)\) using the approximate prior \(F \sim GP(0, q)\), as it can be written as \(k(x, x) - q(x, x)\). The term \((b)\) represents the posterior uncertainty using the approximate prior \(F \sim GP(0, q)\).

We provide two RKHS interpretations of the SVGP posterior covariance, one geometric and one based on a function-space viewpoint. They supplement the understanding of how the SVGP covariance approximates the exact GP posterior covariance.

4.3.1 Geometric Interpretation

We describe a geometric interpretation of the optimized SVGP covariance function (37). To this end, we first analyze the SVGP covariance function \(k'\) in (15) parametrized by \(\Sigma \in \mathbb{R}^{m \times m}_{>0}\):

\[
k'(x, x') = k(x, x') - k_Z(x) k_Z(x')^{-1} k_Z(x') + k_Z(x) (k_{ZZ} + \Sigma^{-1} k_{XX} k_{XZ})^{-1} k_Z(x').
\]

The first term \((a')\) in (38) is the same as the first term \((a)\) in (37). It can be written as

\[
k(x, x') - q(x, x') = \langle k(\cdot, x) - P_M(k(\cdot, x)), k(\cdot, x') - P_M(k(\cdot, x')) \rangle_{\mathcal{H}_k},
\]

where \(q(x, x')\) is the approximate kernel in (34) and \(P_M(k(\cdot, x)) \in \mathcal{M}\) is the orthogonal projection of the feature map \(k(\cdot, x)\) onto the subspace \(\mathcal{M} = \text{span}(k(\cdot, z_1), \ldots, k(\cdot, z_m))\); see Section 4.2. The difference \(k(\cdot, x) - P_M(k(\cdot, x))\) is thus the residual of the approximation of \(k(\cdot, x)\) by \(P_M(k(\cdot, x))\) (imagine Figure 2 with \(f = k(\cdot, x)\)). Therefore, the term \((a')\) is the inner product between two such residuals. In particular, for \(x = x'\) the term \((a')\) is equal to the squared length of the residual of approximation:

\[
\| k(\cdot, x) - P_M(k(\cdot, x)) \|_{\mathcal{H}_k}^2.
\]
This quantifies how closely \( k(\cdot, x) \) can be approximated by a linear combination of the feature maps \( k(\cdot, z_1), \ldots, k(\cdot, z_m) \) of the inducing inputs \( Z = (z_1, \ldots, z_m) \).

The second term \((b')\) is interpreted as a kernel defined as

\[
k^\Sigma(x, x') := \langle \phi^\Sigma(x), \phi^\Sigma(x') \rangle_{\mathbb{R}^m}, \tag{39}\]

where \( \phi^\Sigma : \mathcal{X} \rightarrow \mathbb{R}^m \) is a finite-dimensional feature map parametrized by \( \Sigma \) and \( Z \):

\[
\phi^\Sigma(x) := \Sigma^{1/2} k_{ZZ}^{-1} k_Z(x) \in \mathbb{R}^m. \tag{40}
\]

The parameter matrix \( \Sigma \) specifies the covariance matrix at the inducing variables \( Z = (z_1, \ldots, z_m) \): we have \( k_{ZZ}^\Sigma = \Sigma \).

The term \((b)\) of the optimized SVGP covariance in (37) is the kernel (39) with \( \Sigma = \Sigma^* \) being the optimal covariance matrix (23) that maximizes the ELBO. By Theorem 2, this optimal \( \Sigma^* \) is the minimizer of the sum of (28) and (29), which can be written as

\[
\sum_{i=1}^n k^\Sigma(x_i, x_i) + \sigma^2 KL(\mathcal{N}(0, \Sigma) \parallel \mathcal{N}(0, k_{ZZ})), \tag{41}
\]

As an objective function of \( \Sigma \), this is interpreted as a regularized empirical risk. The first term, interpreted as an empirical risk, is the sum of uncertainties (variances) \( k^\Sigma(x_i, x_i) \) of the latent function at the training inputs \( x_1, \ldots, x_n \); lower uncertainties are encouraged because observations \( y_1, \ldots, y_n \) are given. The second term is a regularizer that encourages the covariance matrix \( k_{ZZ}^\Sigma = \Sigma \) at the inducing inputs \( Z = (z_1, \ldots, z_m) \) to be similar to the covariance matrix \( k_{ZZ} \) of the prior GP for the latent function. If the noise variance \( \sigma^2 \) is smaller (larger), the observations \( y_1, \ldots, y_n \) contain more (less) information about the latent function, and thus \( \Sigma \) should make the uncertainties \( k^\Sigma(x_i, x_i) \) smaller (larger).

Dividing (41) by \( n \), defining \( \lambda = \sigma^2/n \), and using the feature map (40), the objective function of \( \Sigma \) can be written as

\[
\frac{1}{n} \sum_{i=1}^n \| \phi^\Sigma(x_i) \|_{\mathbb{R}^m}^2 + \lambda KL(\mathcal{N}(0, \Sigma) \parallel \mathcal{N}(0, k_{ZZ})). \tag{42}
\]

Geometrically, \( \Sigma \) is optimized to minimize the average lengths of the feature vectors \( \phi^\Sigma(x_i) \) at the training input points \( x_1, \ldots, x_n \), with a constraint to that \( \Sigma \) does not too deviate from \( k_{ZZ} \). In the limit \( n \rightarrow \infty \) and for fixed \( Z \), the second term vanishes (since \( \lambda = \sigma^2/n \)), while the first term converges to

\[
\int \| \phi^\Sigma(x) \|_{\mathbb{R}^m}^2 dP(x),
\]

assuming that training inputs \( x_1, \ldots, x_n \) are i.i.d. with a probability distribution \( P \). The optimal \( \Sigma^* \) in this limit thus minimizes this population average of the length of the feature vector \( \phi^\Sigma(x) \).
4.3.2 Worst Case Error Interpretation

We next provide a worst case error interpretation of the optimized SVGP variance function. In general, the posterior variance function of GPR can be written as a worst case error of KRR in the unit ball of the RKHS (Kanagawa et al., 2018, Section 3.4). Therefore, the optimized SVGP variance function, $k^*(x, x)$, can be written as the sum of two worst case errors: one is that of KRR with noise-free observations at $Z = (z_1, \ldots, z_m)$, and the other is that of Nyström KRR given training observations at $X = (x_1, \ldots, x_n)$. Formally, the following RKHS interpretation holds for the optimized SVGP variance function.

**Theorem 6** Suppose that data $(x_i, y_i)_{i=1}^n \subset \mathcal{X} \times \mathbb{R}$ are given, and that $Z = (z_1, \ldots, z_m) \in \mathcal{X}^m$ are fixed inducing inputs such that the kernel matrix $k_{ZZ} = (k(z_i, z_j))_{i,j=1}^m \in \mathbb{R}^{m \times m}$ is invertible. For the approximate kernel $q$ in (34), define $q^\sigma$ as

$$q^\sigma(x, x') = q(x, x') + \sigma^2 \delta(x, x'),$$

(43)

where $\delta(x, x') = 1$ if $x = x'$ and $\delta(x, x') = 0$ otherwise, and let $\mathcal{H}_{q^\sigma}$ be the RKHS of $q^\sigma$. Let $k^*$ be the optimized SVGP covariance function (26). Then, for $x \notin \{x_1, \ldots, x_n\}$, we have

$$k^*(x, x) + \sigma^2 = \left( \sup \{ f(x) - k_Z(x)^\top k_{ZZ}^{-1} k_{ZZ} f_Z \} \right)^2 \quad \text{Kernel Interpolation}$$

$$+ \left( \sup \{ h(x) - k_Z(x)^\top (\sigma^2 k_{ZZ} + k_{ZX} k_{XZ})^{-1} k_{ZX} h_X \} \right)^2. \quad \text{Nyström KRR}$$

(44)

(45)

**Proof** The assertion follows from Theorem 5, (36), and Kanagawa et al. (2018, Propositions 3.8 and 3.10).

Theorem 6 shows that the optimized SVGP variance $k^*(x, x)$ plus the noise variance $\sigma^2$ is equal to the sum of two terms in (44) and (45). The first term (44) is the worst case error of kernel-based interpolation $k_Z(x)^\top k_{ZZ}^{-1} f_Z$, where each $f \in \mathcal{H}_k$ with $\|f\|_{\mathcal{H}_k} \leq 1$ represents an unknown ground-truth whose output $f(x)$ at test input $x$ is to be interpolated from noise-free observations $f_Z = (f(z_1), \ldots, f(z_m))^\top$ at the inducing inputs $Z = (z_1, \ldots, z_m)$.

The second term (45) is the worst case error of the Nyström KRR prediction (see (12))

$$k_Z(x)^\top (\sigma^2 k_{ZZ} + k_{ZX} k_{XZ})^{-1} k_{ZX} h_X$$

of the output $h(x)$ based on observations $h_X = (h(x_1), \ldots, h(x_n))^\top$ at training inputs $X = (x_1, \ldots, x_n)$, where each $h \in \mathcal{H}_{q^\sigma}$ with $\|h\|_{\mathcal{H}_{q^\sigma}} \leq 1$ represents an unknown ground-truth function plus a noise function: it can be written as $h = f + \xi$ for some $f \in \mathcal{H}_q$ and $\xi \in \mathcal{H}_{q^\sigma}$, where $\mathcal{H}_{q^\sigma}$ is the RKHS of the Kronecker delta kernel $\sigma^2 \delta(x, x')$ and $\xi$ is interpreted as a noise function; see Kanagawa et al. (2018, Section 3.4); the $\sigma^2$ in the left hand side of (44) corresponds to the prediction error of this noise component.

We have discussed the equivalences and connections between the Nyström and SVGP approximations. In the next section, we focus on their theoretical properties, focusing on the quality of approximation.
5. Connections in Theoretical Properties of Sparse Approximations

We investigate here connections between the theoretical properties of the Nyström and SVGP approximations. The Nyström method provides an approximation to the exact KRR solution, and the SVGP approximates the exact GP posterior. The quality of approximation of either approach depends on the choice of inducing inputs $Z = (z_1, \ldots, z_m)$. We focus here on theoretical error bounds for the approximation quality of either approach, and investigate how they are related.

For the Nyström approximation, researchers have studied various approaches for subsampling inducing inputs $z_1, \ldots, z_m$ from training inputs $x_1, \ldots, x_n$ and their theoretical properties. These range from uniform subsampling to subsampling methods based on leverage scores (Rudi et al., 2015; Musco and Musco, 2017; Chen and Yang, 2021), determinantal point processes (DPPs) (Li et al., 2016), and to ensemble methods (Kumar et al., 2009, 2012). Theoretical works either quantify a (relative) deviation of the approximate kernel matrix from the exact one and its impact on downstream tasks (e.g., Cortes et al., 2010; Musco and Musco, 2017), or more directly bound the expected loss of the resulting approximate KRR estimator (e.g., Bach, 2013; El Alaoui and Mahoney, 2015; Rudi et al., 2015). On the other hand, for the SVGP approach, Burt et al. (2019, 2020) provided the first theoretical analysis of its approximation quality. Subsequently, Nieman et al. (2022) extended this analysis to the Frequentist analysis of the contraction of the SVGP posterior to the regression function. Vakili et al. (2022) conducted an asymptotic analysis of confidence intervals obtained from the SVGP approximation.

In Section 5.1, we first discuss a fundamental bound of Burt et al. (2020) on the KL divergence between the approximate and exact GP posteriors. Section 5.2 then discusses a connection between the KL divergence for the SVGP approximation and the excess risk of the Nyström KRR over the exact KRR. Specifically, we show how an upper bound on the KL divergence leads to an upper bound on the excess risk. Section 5.3 establishes an upper bound on the approximation error of the Nyström KRR as measured by the RKHS distance. We then describe how this bound leads to upper bounds on the approximation errors of the SVGP posterior mean function and its derivatives. Lastly, Section 5.4 describes how a lower bound for the approximation error of the SVGP leads to a lower bound for the approximation error of the Nyström KRR.

5.1 A Fundamental Result of Burt et al. (2020)

We first consider the approximation quality of the SVGP approach. In particular, we study a fundamental result of Burt (Lemma 3), from which many other results in Burt et al. (2020) are derived. As before, let $\mu^*$ and $\Sigma^*$ be the optimal variational parameters in (22) and (23), respectively, and let $Z = (z_1, \ldots, z_m) \in \mathcal{X}^m$ be $m$ inducing inputs such that the kernel matrix $k_{ZZ}$ is invertible. Let $\nu^* := (Z, \mu^*, \Sigma^*)$ and $Q^{\nu^*} = GP(m^*, k^*)$ be the resulting variational GP posterior with mean function $m^*$ and covariance function $k^*$ in (14) and (15), respectively.

A natural metric of quantifying the approximation quality of $Q^{\nu^*}$ is the KL divergence to the exact GP posterior $\mathbb{P}^F|y$, which is given by (18) with $\nu^* = (Z, \mu^*, \Sigma^*)$

$$KL(Q^{\nu^*} \parallel \mathbb{P}^F|y) = \log p(y) - L^*,$$
where \(p(y)\) is the marginal likelihood and \(\mathcal{L}^*\) is the ELBO in (24). We know that (e.g., Rasmussen and Williams, 2006, Eq. (5.8))

\[
\log p(y) = -\frac{1}{2} \log \det(k_{XX} + \sigma^2 I_n) - \frac{1}{2} y^\top (k_{XX} + \sigma^2 I_n)^{-1} y - \frac{n}{2} \log 2\pi
\]

Therefore,

\[
2KL(Q^{\nu^*} \parallel \mathbb{P}^F|y) = 2 \log p(y) - 2\mathcal{L}^*
\]

\[
\begin{align*}
&= -\log \det(k_{XX} + \sigma^2 I_n) + \log \det(q_{XX} + \sigma^2 I_n) \\
&\quad - y^\top (k_{XX} + \sigma^2 I_n)^{-1} y + y^\top (q_{XX} + \sigma^2 I_n)^{-1} y + \frac{1}{\sigma^2} \text{tr}(k_{XX} - q_{XX}) \\
&\leq -y^\top (k_{XX} + \sigma^2 I_n)^{-1} y + y^\top (q_{XX} + \sigma^2 I_n)^{-1} y + \frac{1}{\sigma^2} \text{tr}(k_{XX} - q_{XX}),
\end{align*}
\]

(46)

where the inequality follows from \(k_{XX} - q_{XX}\) being positive semi-definite.

Burt et al. (2020, Proof of Lemma 3) proceed to bound the first two terms in (47) as

\[
- y^\top (k_{XX} + \sigma^2 I_n)^{-1} y + y^\top (q_{XX} + \sigma^2 I_n)^{-1} y \\
\leq \|y\|^2 \|k_{XX} - q_{XX}\|_{\text{op}} \leq \|y\|^2 \text{tr}(k_{XX} - q_{XX}) + \sigma^2\),
\]

(48)

where \(\|A\|_{\text{op}} := \sup_{\|v\|\leq 1} \|Av\|\) denotes the operator norm for any \(A \in \mathbb{R}^{n \times n}\). Thus, we arrive at the following bound (Burt et al., 2020, Lemma 3):

\[
2KL(Q^{\nu^*} \parallel \mathbb{P}^F|y) \leq \frac{\text{tr}(k_{XX} - q_{XX})}{\sigma^2} \left(\frac{\|y\|^2}{\text{tr}(k_{XX} - q_{XX}) + \sigma^2} + 1\right).
\]

\[
\leq \frac{\text{tr}(k_{XX} - q_{XX})}{\sigma^2} \left(\frac{\|y\|^2}{\sigma^2} + 1\right).
\]

(49)

This result shows that the KL divergence becomes small if \(\text{tr}(k_{XX} - q_{XX})\) is small. The latter quantity becomes small if, intuitively, the approximate kernel matrix \(q_{XX} = k_{XX}k_{XX}^{-1}k_{XX}\) is close to the exact one \(k_{XX}\).

Burt et al. (2020) then establish various results on the KL divergence for the SVGP approximation by i) relating \(\text{tr}(k_{XX} - q_{XX})\) to the eigenvalues of \(k_{XX}\) by considering a specific sampling scheme for \(Z\), such as DPPs and leverage score sampling, ii) relating the eigenvalues of \(k_{XX}\) to those of the corresponding kernel integral operator, and iii) bounding the eigenvalue decays of the integral operator by considering specific choices of the kernel \(k\) and the probability distribution of training input points \(x_1, \ldots, x_n\).

### 5.2 Connection to the Nyström KRR

We now investigate how the bounds on the KL divergence for the SVGP approach are related to the Nyström KRR. The key is the following lemma, which provides an RKHS interpretation of \(y^\top (k_{XX} + \sigma^2 I)^{-1} y\) (and \(y^\top (q_{XX} + \sigma^2 I)^{-1} y\)) appearing in the bound (47).

**Lemma 7** Let \(k\) be a kernel with RKHS \(\mathcal{H}_k\). Let \(X = (x_1, \ldots, x_n) \in \mathcal{X}^n\) and \(y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n\) be given. Then for any \(\sigma^2 > 0\), we have

\[
y^\top (k_{XX} + \sigma^2 I_n)^{-1} y = \min_{f \in \mathcal{H}_k} \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - f(x_i))^2 + \|f\|_{\mathcal{H}_k}^2.
\]
Connections between the Nyström and Sparse Variational Gaussian Processes

**Proof** The proof can be found in Appendix B.3.

Lemma 7 shows that $y^\top (k_{XX} + \sigma^2 I_n)^{-1} y$ is the minimum of a scaled version of the KRR objective function (2) with $\sigma^2 = n\lambda$. Since the minimum is attained by the KRR solution $\hat{f} = k_X(\cdot)^\top (k_{XX} + \sigma^2 I_n)^{-1} y$, Lemma 7 thus implies that, for $\sigma^2 = n\lambda$,

$$ y^\top (k_{XX} + \sigma^2 I_n)^{-1} y = \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \hat{f}(x_i))^2 + \|\hat{f}\|^2_{\mathcal{H}_k} = n R_n(\hat{f}; y), $$

where we define $R_n(f; y)$ for any $f : \mathcal{X} \mapsto \mathbb{R}$ as the regularized empirical risk of KRR:

$$ R_n(f; y) := \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|^2_{\mathcal{H}_k} $$

Similarly, Lemma 7, Theorem 5 and Lemma 4 imply that $y^\top (q_{XX} + \sigma^2 I_n) y$ is proportional to the KRR objective value of the Nyström KRR solution $\hat{f} = k_Z(\cdot)^\top (\sigma^2 k_{ZZ} + k_{ZX} k_{XX})^{-1} k_{ZX} y$:

$$ y^\top (q_{XX} + \sigma^2 I_n)^{-1} y = \min_{f \in \mathcal{H}_q} \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \bar{f}(x_i))^2 + \|\bar{f}\|^2_{\mathcal{H}_q} = \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \bar{f}(x_i))^2 + \|\bar{f}\|^2_{\mathcal{H}_k} = n R(\bar{f}; y). $$

Therefore the quantity $y^\top (q_{XX} + \sigma^2 I_n)^{-1} y - y^\top (k_{XX} + \sigma^2 I_n)^{-1} y$ appearing in the KL divergence (46) can be written as the difference between the KRR objectives for the Nyström and exact solutions:

$$ y^\top (q_{XX} + \sigma^2 I_n)^{-1} y - y^\top (k_{XX} + \sigma^2 I_n)^{-1} y = n \left( R_n(\hat{f}; y) - R_n(\bar{f}; y) \right) = n \left( \min_{f \in M} R_n(f, y) - \min_{f \in \mathcal{H}_k} R_n(f; y) \right) \geq 0, $$

where the last identity follows from (2) and (11) and the inequality from $M \subset \mathcal{H}_k$. Thus, one can understand the difference (50) as the “excess risk” of the Nyström KRR estimator $\hat{f}$ over the exact KRR estimator $\bar{f}$. In this sense, it measures the approximation quality of the Nyström KRR.

Now, combining the bounds in (48) and the expression (50), we immediately have the corresponding bounds on the “excess risk” of the Nyström KRR.

**Corollary 8** Let $k$ be a kernel with RKHS $\mathcal{H}_k$. Let $X = (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$ be given, and let $Z = (z_1, \ldots, z_m) \in \mathcal{X}^m$ be such that the kernel matrix $k_{ZZ} \in \mathbb{R}^{m \times m}$ is invertible. Let $\hat{f}$ and $\bar{f}$ be the Nyström and exact KRR estimators in (12) and (4), respectively, with a regularization constant $\lambda > 0$. Then we have

$$ R_n(\hat{f}; y) - R_n(\bar{f}; y) \leq \frac{n}{\sigma^2} \|k_{XX} - q_{XX}\|_{\text{op}} \leq \frac{n}{\sigma^2} \text{tr}(k_{XX} - q_{XX}) + n\lambda \|\bar{f}\|^2_{\mathcal{H}_k}, $$

where $R_n(f; y) := \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|^2_{\mathcal{H}_k}$.
Proof Using (48) and (50) and setting $\sigma^2 = n\lambda$, we have

$$n \left( R_n(f, y) - R_n(\hat{f}, y) \right) = -y^\top (k_{XX} + n\lambda I_n)^{-1} y + y^\top (q_{XX} + n\lambda I_n)^{-1} y$$

$$\leq \frac{\|y\|^2 \|k_{XX} - q_{XX}\|_{op}}{n\lambda(\|k_{XX} - q_{XX}\|_{op} + n\lambda)} \leq \frac{\|y\|^2 \text{tr}(k_{XX} - q_{XX})}{n\lambda(\text{tr}(k_{XX} - q_{XX}) + n\lambda)}.$$

The assertion follows immediately. \(\square\)

We have shown that the KL divergence (46) for the SVGP approximation contains the excess risk of the Nyström KRR (50). Using this connection and bounds for the KL divergence from Burt et al. (2020), we have derived corresponding bounds for the excess risk of the Nyström KRR. This demonstrates how one can translate results on GPs to RKHS-based methods.

On the other hand, since we now know that there exist KRR objective functions in the expression (46) of the KL divergence, it may be possible to use more sophisticated theoretical arguments for the Nyström KRR (e.g. Bach, 2013; El Alaoui and Mahoney, 2015; Rudi et al., 2015; Chen and Yang, 2021) to obtain sharper bounds on the KL divergence for the SVGP approximation. This investigation is reserved for future research.

5.3 RKHS Error Bound for Nyström KRR and its Implications to SVGP

We present here an upper bound on the RKHS distance between the Nyström and exact KRR estimators, which is novel to the best of our knowledge. We will apply this bound to obtain error bounds for the SVGP posterior mean function and its derivatives. The bound is summarized below, whose proof can be found in Appendix B.4.

**Theorem 9** Let $k$ be a kernel with RKHS $\mathcal{H}_k$. Let $X = (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$ be given, and let $Z = (z_1, \ldots, z_m) \in \mathcal{X}^m$ be such that the kernel matrix $k_{ZZ} \in \mathbb{R}^{m \times m}$ is invertible. Let $\bar{f}$ and $\hat{f}$ be the Nyström and exact KRR estimators in (12) and (4), respectively, with a regularization constant $\lambda > 0$. Then we have

$$\|\hat{f} - \bar{f}\|_{\mathcal{H}_k}^2 \leq \frac{2 \text{tr}(k_{XX} - q_{XX}) \|y\|^2}{(n\lambda)^2}.$$

The upper-bound takes a similar form as the bound (49) on KL divergence for the SVGP approximation in terms of the dependence on $\text{tr}(k_{XX} - q_{XX})$, $\|y\|^2$ and $\sigma^2 = n\lambda$.

By the equivalence between the KRR estimator $\hat{f}$ and the GP posterior mean function $m^*$, and that of the Nyström KRR estimator $\bar{f}$ and the SVGP posterior mean function $\bar{m}$ in Theorem 1, Theorem 9 directly leads to the corresponding bound for the SVGP posterior mean function, as summarize as follows.

**Corollary 10** Let $k$ be a kernel with RKHS $\mathcal{H}_k$. Let $X = (x_1, \ldots, x_n) \in \mathcal{X}^n$ and $y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$ be given, and let $Z = (z_1, \ldots, z_m) \in \mathcal{X}^m$ be such that the kernel matrix $k_{ZZ} \in \mathbb{R}^{m \times m}$ is invertible. Let $m^*$ and $\bar{m}$ be the SVGP and exact GP posterior mean functions, respectively.
functions in (25) and (7), respectively, with prior $F \sim \text{GP}(0, k)$ and likelihood model (6) with noise variance $\sigma^2 > 0$. Then we have

$$\|\bar{m} - m^*\|_{H_k}^2 \leq \frac{2 \text{tr}(k_{XX} - q_{XX})\|y\|^2}{\sigma^4}. $$

Note that the RKHS distance is stronger than the supremum norm between two functions. In fact, by the reproducing property, it can be shown that

$$(\bar{f}(x) - \hat{f}(x))^2 \leq \|\bar{f} - \hat{f}\|_{H_k}^2 k(x, x), \quad \forall x \in \mathcal{X}. $$

Moreover, if the kernel $k$ is smooth, then the RKHS distance upper-bounds the derivatives of the RKHS functions. To describe this, let $\mathcal{X} \subset \mathbb{R}^d$ be an open set. Suppose that the kernel $k$ is continuously differentiable\(^7\) on $\mathcal{X}$ in the sense that, for any $j = 1, \ldots, d$, the partial derivative $\partial_j \partial_j' k(x, x')$ exists and is continuous on $\mathcal{X}$, where $\partial_j$ and $\partial_j'$ denote the partial derivatives with respect to the $j$-th coordinate of the first and second arguments of $k(x, x')$, respectively. Then Steinwart and Christmann (2008, Corollary 4.36) implies that, for all $j = 1, \ldots, d$ and all $x \in \mathcal{X}$,

$$(\partial_j \bar{f}(x) - \partial_j \hat{f}(x))^2 \leq \|\bar{f} - \hat{f}\|_{H_k}^2 \partial_j \partial_j' k(x, x),$$

Thus, the bound in Theorem 9 implies that, if $\text{tr}(k_{XX} - q_{XX})$ is small, then the partial derivatives (and thus the gradients) of the Nyström KRR approximate well those of the exact KRR. By the same argument and Corollary 10, we immediately obtain the following corollary on the equivalent result for the SVGP approximation.

**Corollary 11** Suppose the same notation and assumptions in Corollary 10. Let $\mathcal{X} \subset \mathbb{R}^d$ be an open set and assume that $k$ is continuously differentiable on $\mathcal{X}$. Then we have for all $j = 1, \ldots, d$ and all $x \in \mathcal{X}$,

$$(\partial_j m^*(x) - \partial_j \bar{m}(x))^2 \leq \frac{2 \text{tr}(k_{XX} - q_{XX})\|y\|^2 \partial_j \partial_j' k(x, x)}{\sigma^4}. $$

This shows that the SVGP can approximate not only the exact posterior mean function but also its derivatives, if $\text{tr}(k_{XX} - q_{XX})$ is small. In applications where the derivative estimates are used (e.g., see Wu et al. 2017), this result provides a support for using the SVGP approximation in place of the exact GP posterior means of derivatives.

### 5.4 Lower Bounds for Approximation Errors

Lastly, we describe how lower bounds for the SVGP approximation lead to lower bounds for the Nyström approximation. We discuss lower bounds for the average case errors of sparse approximations, by assuming a probabilistic model for training outputs $y = (y_1, \ldots, y_n)^\top$. As before, we fix training inputs $X = (x_1, \ldots, x_n)$ and inducing inputs $Z = (z_1, \ldots, z_m)$. Following Burt et al. (2020), we consider the following model for $y$:

$$y | X \sim \mathcal{N}(0, k_{XX} + \sigma^2 I_n) \quad (51)$$

\(^7\) Many commonly used kernels, such as the Gaussian kernel, satisfy this requirement.
which is given by the likelihood model (6) and by marginalizing the latent prior GP, \( F \sim GP(0, k) \). Burt et al. (2020, Lemma 4) shows the following lower and upper bounds for the averaged KL divergence between the SVGP and exact GP posteriors:

\[
\frac{\text{tr}(k_{XX} - q_{XX})}{2\sigma^2} \leq \mathbb{E}_y \left[ KL(\mathcal{Q}^{\nu^*} \| \mathbb{P}^F|y) \right] \leq \frac{\text{tr}(k_{XX} - q_{XX})}{\sigma^2},
\]

where \( \mathbb{E}_y \) denotes the expectation with respect to \( y \) generated according to (51).

These lower and upper bounds are \textit{a priori} bounds in the sense that they hold for the average with respect to the prior model and thus are informative before observing the actual training outputs \( y_1, \ldots, y_n \). While this performance measure (the averaged KL divergence) is less informative for the approximation accuracy after one has observed actual training outputs \( y_1, \ldots, y_n \) (the \textit{a posteori} setting), the lower bound still provides a useful insight. Specifically, the lower bound (52) is proportional to \( \text{tr}(k_{XX} - q_{XX}) \). Thus if \( \text{tr}(k_{XX} - q_{XX}) \) is large, then the SVGP posterior \( \mathcal{Q}^{\nu^*} \) cannot accurately approximate the exact posterior \( \mathbb{P}^F|y \) on average. This is intuitively the case where the inducing inputs \( Z = (z_1, \ldots, z_m) \) do not effectively “cover” the training inputs \( X = (x_1, \ldots, x_n) \). Since \( \text{tr}(k_{XX} - q_{XX}) \) appears both in the upper and lower bounds, the above result shows that \( \text{tr}(k_{XX} - q_{XX}) \) can serve as an average performance metric for the SVGP approximation.

Now, based on the interpretation that the KL divergence (46) contains the excess risk (50) of the Nyström KRR, the lower bound (52) for the KL divergence leads to a lower bound for the excess risk of the Nyström KRR.

**Corollary 12** Let \( k \) be a kernel with RKHS \( \mathcal{H}_k \). Let \( X = (x_1, \ldots, x_n) \in \mathcal{X}^n \) and let \( Z = (z_1, \ldots, z_m) \in \mathcal{X}^m \) be such that the kernel matrix \( k_{ZZ} \in \mathbb{R}^{m \times m} \) is invertible. Suppose \( y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n \) are generated as (51). Let \( \bar{f} \) and \( \hat{f} \) be the Nyström and exact KRR estimators in (12) and (4), respectively, with a regularization constant \( \lambda > 0 \). Then we have

\[
\frac{1}{n} \log \frac{\det(k_{XX} + n\lambda I_n)}{\det(q_{XX} + n\lambda I_n)} \leq \mathbb{E}_y \left[ R_n(\bar{f}; y) - R_n(\hat{f}; y) \right]
\]

where \( R_n(f; y) := \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \| f \|_{\mathcal{H}_k}^2 \).

**Proof** By (46), (50) and (52) with \( \sigma^2 = n\lambda \), we have

\[
\frac{\text{tr}(k_{XX} - q_{XX})}{n\lambda} \leq 2\mathbb{E}_y \left[ KL(\mathcal{Q}^{\nu^*} \| \mathbb{P}^F|y) \right] = -\log \frac{\det(k_{XX} + n\lambda I_n)}{\det(q_{XX} + n\lambda I_n)} + \mathbb{E}_y \left[ n \left( R_n(\bar{f}; y) - R_n(\hat{f}; y) \right) \right] + \frac{\text{tr}(k_{XX} - q_{XX})}{n\lambda}.
\]

The assertion immediately follows. \( \blacksquare \)

In the left hand side of Corollary 12, \( \log \det(k_{XX} + n\lambda I) \) and \( \log \det(q_{XX} + n\lambda I) \) can intuitively be interpreted as the complexities of the models associated with the kernels \( k \).
and $q$, respectively. Thus, Corollary shows that, if the complexity for $q$ is much smaller than that for $k$, then the difference of the KRR objectives cannot be small on average. This suggests that the left hand side of Corollary 12 may be useful as a quality metric for the Nyström approximation in the \textit{a priori} setting.

6. Conclusions

We have established various connections and equivalences between sparse approximation methods for GPR and KRR, namely the SVGP and Nyström approximations. We hope these contributions will help the two fields grow closer together and allow researchers to readily translate results from one field to another. In general, equivalent characterizations of the same problem enable one to look at the problem from a new angle and ultimately lead to new approaches. For example, the equivalent formulation of Bayesian posterior inference as an optimization problem (Csiszár, 1975; Donsker and Varadhan, 1975) has led to a whole new class of inference algorithms (e.g., Jordan et al., 1999; Knoblauch et al., 2019; Khan and Rue, 2021). Similarly, we hope our contributions will stimulate new research in both GP and RKHS communities by leveraging and extending the equivalences and connections in the paper.

Acknowledgements

We express our gratitude to the Action Editor and the anonymous reviewers for their time and thoughtful comments that helped improve the paper. This work in part has been supported by the French Government, through the 3IA Cote d’Azur Investment in the Future Project managed by the National Research Agency (ANR) with the reference number ANR-19-P3IA-0002.

Appendix A. Derivations of the Optimal Variational Mean and Covariance Parameters

We present derivations of the optimal variational mean $\mu^*$ and covariance matrix $\Sigma^*$ in (22) and (23) based on the formulation of Khan and Rue (2021). To this end, let us rewrite the ELBO in (19) as

$$
\mathcal{L}(\nu) = \mathbb{E}_{F^\nu \sim Q^\nu} \left[ \log p(y|F^\nu_X) \right] - KL(Q^\nu_Z \parallel P_Z)
$$

\begin{equation}
= \mathbb{E}_{F^\nu_{Z} \sim Q^\nu} \left[ \mathbb{E}_{F^\nu \sim Q^\nu} \left[ \log p(y|F^\nu_X) \right] F^\nu_{Z} \right] - KL(Q^\nu_Z \parallel P_Z)
\end{equation}

\begin{equation}
= \mathbb{E}_{F^\nu_{Z} \sim Q^\nu} \left[ \mathbb{E}_{F^\nu \sim Q^\nu} \left[ \log p(y|F^\nu_X) \right] F^\nu_{Z} \right] - \mathbb{E}_{F^\nu_{Z} \sim Q^\nu} \left[ \log Q^\nu_Z(F^\nu_{Z}) \right]
\end{equation}

\begin{equation}
= -\mathbb{E}_{F^\nu_{Z} \sim Q^\nu} \left[ \bar{\ell}(F^\nu_{Z}) \right] + H(Q^\nu_Z),
\end{equation}

(53)
where (A) follows from the law of total expectation, (B) from the definition of the KL divergence, and we defined

\[ \bar{\ell}(u) := -E_{F^u \sim Q^u} [\log p(y|F^u_X) | F^u_Z = u] - \log P_Z(u), \]

\[ = -E_{F^u \sim Q^u} [\log N(\mu) | \sigma^2 I_n) | F^u_Z = u] - \log P_Z(u), \quad u \in \mathbb{R}^m, \]

\[ H(Q^u_Z) := -E_{F^u \sim Q^u} [\log Q^u_Z(F^u_Z)] = \frac{1}{2} \log \det(2\pi e \Sigma). \]

The \( H(Q^u_Z) \) is the entropy of the distribution \( Q^u_Z = N(\mu, \Sigma). \)

The optimality conditions for the variational parameters \( \mu \in \mathbb{R}^m \) and \( \Sigma \in \mathbb{R}^{m \times m} \) are thus given by setting the gradients of (53) to zero (Khan and Rue, 2021, Eq.(5)); this leads to

\[ \nabla_\mu E_{F^u \sim Q^u} [\bar{\ell}(F^u_Z)] = \nabla_\mu H(Q^u_Z) = 0, \]  

(54)

\[ \nabla_\Sigma E_{F^u \sim Q^u} [\bar{\ell}(F^u_Z)] = \nabla_\Sigma H(Q^u_Z) = \frac{1}{2} \Sigma^{-1}. \]  

(55)

To use these conditions to derive optimal \( \mu \) and \( \Sigma \), we first analyze the function \( \bar{\ell}(u) \).

Note that we have \( F^u_X|F^u_Z = u \sim N(\mu_u, \Sigma_u) \), where

\[ \mu_u := k_{XX}^{-1}k_{ZZ}^{-1}u \in \mathbb{R}^m, \quad \Sigma_u := k_{XX} - k_{XX}k_{ZZ}^{-1}k_{ZZ} = k_{XX} - \dot{q}_{XX} \in \mathbb{R}^{m \times m}. \]

From this, one can show that

\[ E_{F^u \sim Q^u} [\log N(y|F^u_X, \sigma^2 I_n) | F^u_Z = u] = \log N(y | \mu_u, \sigma^2 I_n) - \frac{1}{2\sigma^2} \text{tr}(k_{XX} - \dot{q}_{XX}), \]

and therefore we obtain

\[ \bar{\ell}(u) = -\log N(y | \mu_u, \sigma^2 I_n) + \frac{1}{2\sigma^2} \text{tr}(k_{XX} - \dot{q}_{XX}) - \log P_Z(f_Z) \]

\[ = \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - k_Z(x_i)^T k_{ZZ}^{-1} u)^2 + \frac{1}{2} u^T k_{ZZ}^{-1} u + C \]

\[ = \frac{1}{2\sigma^2} \|y - \mu_u\|_2^2 + \frac{1}{2} u^T k_{ZZ}^{-1} u + C, \]

where we absorb everything that does not depend on \( u \) in \( C \). Thus, the gradient and the Hessian matrix of \( \bar{\ell}(u) \) with respect to \( u \) are given by

\[ \nabla_u \bar{\ell}(u) = -\frac{1}{\sigma^2} k_{ZZ}^{-1} k_{ZX}(y - \mu_u) + k_{ZZ}^{-1} u \]

\[ = -\frac{1}{\sigma^2} k_{ZZ}^{-1} k_{ZX} y + \frac{1}{\sigma^2} k_{ZZ}^{-1} k_{ZX} \mu_u + k_{ZZ}^{-1} u, \]

\[ \nabla_u^2 \bar{\ell}(u) = \frac{1}{\sigma^2} k_{ZZ}^{-1} k_{ZX} k_{XX} k_{ZZ}^{-1} + k_{ZZ}^{-1}. \]
We are ready to derive optimal \( \mu \) and \( \Sigma \). We first use (54) to derive optimal \( \mu \), following the derivation in Khan and Rue (2021, Eq.(25)). We have

\[
\nabla_\mu \mathbb{E}_{F_Z^x \sim Q_Z^x} [\tilde{\ell}(F_Z^x)] \overset{(A)}{=} \mathbb{E}_{F_Z^x \sim Q_Z^x} \left[ \nabla_u \tilde{\ell}(u) \bigg|_{u=F_Z^x} \right] \\
= \mathbb{E}_{F_Z^x \sim Q_Z^x} \left[ -\frac{1}{\sigma^2} k_{Zx} k_{Zx} y + \frac{1}{\sigma^2} k_{ZZ} k_{Zx} x z + k_{Zx}^\top \Sigma + k_{Zx} \mu \right] \\
= \frac{1}{\sigma^2} k_{Zx} k_{Zx} y + \frac{1}{\sigma^2} k_{ZZ} k_{Zx} x z + k_{Zx} \mu.
\]

where (A) follows Bonnet’s theorem. Therefore (54) leads to

\[
\mu = k_{ZZ} (\sigma^2 k_{ZZ} + k_{Zx} k_{Zx})^{-1} k_{Zx} y,
\]

which recovers the optimal \( \mu^* \) in (22).

We next use (55) to derive optimal \( \Sigma \), following the derivation in Khan and Rue (2021, Eq.(26)). We have

\[
\nabla_\Sigma \mathbb{E}_{F_Z^x \sim Q_Z^x} [\tilde{\ell}(F_Z^x)] \overset{(A)}{=} \frac{1}{2} \mathbb{E}_{F_Z^x \sim Q_Z^x} \left[ \nabla_u^2 \tilde{\ell}(u) \bigg|_{u=F_Z^x} \right] = \frac{1}{\sigma^2} k_{Zx} k_{Zx} k_{Zx} k_{Zx} + k_{Zx}^{-1} k_{Zx}.
\]

where (A) holds from Opper and Archambeau (2009, Eq.(A.3)). Thus (55) leads to

\[
\Sigma = \left( \frac{1}{\sigma^2} k_{Zx} k_{Zx} k_{Zx} k_{Zx} + k_{Zx}^{-1} \right)^{-1} = k_{ZZ} \left( \frac{1}{\sigma^2} k_{Zx} k_{Zx} + k_{Zx} \right)^{-1} k_{Zx},
\]

recovering the optimal \( \Sigma^* \) in (23).

Appendix B. Proofs

B.1 Proof of Lemma 4

Proof We first show \( \mathcal{H}_q = M \) as a set of functions. First note that

\[
q(\cdot, x) = k_Z(\cdot)^\top k_{ZZ}^{-1} k_Z(x) = P_M(k(\cdot, x)), \quad \forall x \in \mathcal{X}.
\]

Define \( \mathcal{H}_{0,q} \) as the vector space

\[
\mathcal{H}_{0,q} := \left\{ f = \sum_{i=1}^n \alpha_i q(\cdot, d_i) \mid n \in \mathbb{N}, \ \alpha = (\alpha_1, \ldots, \alpha_n)^\top \in \mathbb{R}^n, \ D = (d_1, \ldots, d_n) \in \mathcal{X}^n \right\}.
\]

Let \( f := \sum_{i=1}^n \alpha_i q(\cdot, d_i) \in \mathcal{H}_{0,q} \) be arbitrary. Since \( q(\cdot, d_i) = P_M(k(\cdot, d_i)) \in M \), we have \( f = \sum_{i=1}^n \alpha_i q(\cdot, d_i) \in M \) by the linearity of \( M \). Therefore \( \mathcal{H}_{0,q} \subset M \). On the other hand, for any \( f = \sum_{j=1}^m \beta_j k(\cdot, z_j) \in M \) with some \( \beta_1, \ldots, \beta_m \in \mathbb{R} \), we have \( f = \sum_{j=1}^m \beta_j P_M(k(\cdot, z_j)) = \sum_{j=1}^m \beta_j q(\cdot, z_j) \in \mathcal{H}_{0,0} \). Therefore \( M \subset \mathcal{H}_{0,0} \). Thus we have shown \( \mathcal{H}_{0,q} = M \) as a set.
Note that the RKHS $\mathcal{H}_q$ is by definition the closure\textsuperscript{8} of $\mathcal{H}_{0,q}$ with respect to the norm
\[
\left\| \sum_{i=1}^{n} \alpha_i q(\cdot, d_i) \right\|^2_{\mathcal{H}_q} = \alpha^\top q_{DD} \alpha = \alpha^\top k_{DZ} k_{ZZ}^{-1} k_{ZD} \alpha = \alpha^\top k_{DZ} k_{ZZ}^{-1} k_{ZD} \alpha
\]

which coincides with the norm of $\mathcal{H}_k$. As $\mathcal{H}_q = M$ is a finite-dimensional subspace of $\mathcal{H}_k$, it is closed and therefore
\[
\mathcal{H}_q = \overline{\mathcal{H}_{0,q}} = \overline{M} = M.
\]
where the closure is with respect to the norm $\| \cdot \|_{\mathcal{H}_q} = \| \cdot \|_{\mathcal{H}_q}$.

Next we show that the scalar products on $M$ and $\mathcal{H}_q$ also coincide. Take arbitrary $f$ and $g$ from $\mathcal{H}_q$. As $\mathcal{H}_q = \mathcal{H}_{0,q}$, we find a representation of the form
\[
f = q_D(\cdot)^\top \alpha = k_Z(\cdot)^\top k_{ZZ}^{-1} k_{ZD} \alpha = k_Z(\cdot)^\top \tilde{\alpha}
g = q_E(\cdot)^\top \beta = k_Z(\cdot)^\top k_{ZZ}^{-1} k_{ZE} \beta = k_Z(\cdot)^\top \tilde{\beta},
\]
where $D = (d_1, ..., d_n) \in \mathcal{X}^n$, $E = (e_1, ..., e_\ell) \in \mathcal{X}^\ell$, $\alpha \in \mathbb{R}^n$, $\beta \in \mathbb{R}^\ell$, $\tilde{\alpha} := k_{ZZ}^{-1} k_{ZD} \alpha$ and $\tilde{\beta} := k_{ZZ}^{-1} k_{ZE} \beta$. This leads to
\[
\langle f, g \rangle_{\mathcal{H}_q} = \alpha^\top q_{DE} \beta = \alpha^\top k_{DZ} k_{ZZ}^{-1} k_{ZE} \beta
\]
and
\[
\langle f, g \rangle_{\mathcal{H}_k} = \tilde{\alpha}^\top k_{ZZ} \tilde{\beta} = \alpha^\top k_{DZ} k_{ZZ}^{-1} k_{ZE} \beta,
\]
which shows that the scalar products are the same.

\textbf{B.2 Proof of Theorem 2}

\textbf{Proof} Recall that the ELBO, which we defined in (19) is given as
\[
\mathcal{L}(\nu) = -KL(Q_\nu^\nu \| P_\nu) + E_{F^\nu \sim Q^\nu} \left[ \log p(y | F^\nu_X) \right]. \quad (56)
\]
The KL-term in $\mathcal{L}$ is tractable as KL-divergence between the two Gaussians $\mathcal{N}(\mu, \Sigma)$ and $\mathcal{N}(0, k(Z, Z))$ and given as
\[
KL(Q_\nu^\nu \| P_\nu) = \frac{1}{2} \left( \text{tr}(k^{-1}_Z \Sigma) + \mu^\top k^{-1}_Z \mu - m + \log \left( \frac{\det k_Z}{\det \Sigma} \right) \right). \quad (57)
\]
We now focus on the expected log-likelihood-term. Let $f_Z \in \mathbb{R}^m$ be an arbitrary vector in the support of $Q_\nu^\nu$. Define a notation for the conditional expectation
\[
F_m(x) := E[F(x) | F_Z = f_Z] = E[F^\nu(x) | F^\nu_Z = f_Z].
\]
\textsuperscript{8} The closure of a subset $A$ in a Hilbert space $\mathcal{H}$ is defined as $\overline{A} := \{ h \in \mathcal{H} \mid \text{there exists a sequence } \{a_n\}_{n=1}^\infty \subset A \text{ such that } \lim_{n \to \infty} \|a_n - h\|_n = 0 \}$. 

30
where the identity follows from the definition of $F^\nu \sim Q^\nu$. Then, from the standard bias-variance decomposition argument, we have

$$\sum_{i=1}^{n} \mathbb{E} [(y_i - F^\nu(x_i))^2 \mid F_Z = f_Z] = \sum_{i=1}^{n} \mathbb{E} [(y_i - F(x_i))^2 \mid F_Z = f_Z]$$

$$= \sum_{i=1}^{n} \mathbb{E} [(y_i - F_m(x_i))^2 \mid F_Z = f_Z] + \sum_{i=1}^{n} \mathbb{E} [(F_m(x_i) - F(x_i))^2 \mid F_Z = f_Z]$$

$$= \sum_{i=1}^{n} (y_i - F_m(x_i))^2 + \sum_{i=1}^{n} \mathbb{E} [(F_m(x_i) - F(x_i))^2 \mid F_Z = f_Z].$$  (58)

Note that, because $F_m(x)$ is the conditional expectation of $F(x)$ given $F_Z = f_Z$, it is equivalent to the kernel interpolator with training data $(z_i, F(z_i))_{i=1}^{n}$ and can be written as

$$F_m(x) = k_Z(x)^\top k_Z^{-1} f_Z.$$  

Therefore

$$\int (y_i - F_m(x_i))^2 dQ_Z^\nu(f_Z) = \int (y_i - k_Z(x_i)^\top k_Z^{-1} f_Z)^2 dQ_Z^\nu(f_Z)$$

$$= \int (y_i - k_Z(x_i)^\top k_Z^{-1} \mu)^2 dQ_Z^\nu(f_Z) + \int (k_Z(x_i)^\top k_Z^{-1} \mu - k_Z(x_i)^\top k_Z^{-1} f_Z)^2 dQ_Z^\nu(f_Z)$$

$$= (y_i - k_Z(x_i)^\top k_Z^{-1} \mu)^2 + k_Z(x_i)^\top k_Z^{-1} \Sigma k_Z^{-1} k_Z(x_i),$$

where the last identity follows from $Q^\nu_Z = \mathcal{N}(\mu, \Sigma)$ by definition.

On the other hand, the second term in (58) is the conditional variance of $F(x_i)$ given $F_Z = f_Z$, and thus given by

$$\mathbb{E} [(F_m(x_i) - F(x_i))^2 \mid F_Z = f_Z] = k(x_i, x_i) - k_Z(x_i)^\top k_Z^{-1} k_Z(x_i),$$

which is independent to the “observations” $f_Z$. Therefore

$$\int \mathbb{E} [(F_m(x_i) - F(x_i))^2 \mid F_Z = f_Z] dQ_Z^\nu(f_Z) = k(x_i, x_i) - k_Z(x_i)^\top k_Z^{-1} k_Z(x_i).$$

Using these identities, we have

$$\int \left( \sum_{i=1}^{n} \mathbb{E} [(y_i - F^\nu(x_i))^2 \mid F_Z = f_Z] \right) dQ_Z^\nu(f_Z)$$

$$= \sum_{i=1}^{n} (y_i - k_Z(x_i)^\top k_Z^{-1} \mu)^2 + \sum_{i=1}^{n} k_Z(x_i)^\top k_Z^{-1} \Sigma k_Z^{-1} k_Z(x_i)$$

$$+ \sum_{i=1}^{n} \left( k(x_i, x_i) - k_Z(x_i)^\top k_Z^{-1} k_Z(x_i) \right).$$

The assertion follows from these derived expressions.
symmetric, we have
\[ \|B\| = \|B\|_{op} \]
where we used the formula \( A(A + \sigma^2 I_n)^{-1} = I_n - \sigma^2 (A + \sigma^2 I_n)^{-1} \) that holds for any positive semidefinite matrix \( A \). Now we have
\[
\min_{f \in \mathcal{H}_k} \sum_{i=1}^n (y_i - f(x_i))^2 + \sigma^2 \|f\|_{\mathcal{H}_k}^2 = \|y - \hat{f}_X\|_2^2 + \sigma^2 \|\hat{f}\|_{\mathcal{H}_k}^2
\]
The first term can be expanded as
\[
\|y - \hat{f}_X\|_2^2 = \|y\|_2^2 - 2y^\top \hat{f}_X + \|\hat{f}_X\|_2^2
\]
\[
= \|y\|_2^2 - 2y^\top (I_n - \sigma^2 (k_{XX} + \sigma^2 I_n)^{-1})y + y^\top (I_n - \sigma^2 (k_{XX} + \sigma^2 I_n)^{-1})^2 y
\]
\[
= \|y\|_2^2 - 2y^\top (I_n - \sigma^2 (k_{XX} + \sigma^2 I_n)^{-1})y
\]
\[
+ y^\top (I_n - 2\sigma^2 (k_{XX} + \sigma^2 I_n)^{-1} + \sigma^4 (k_{XX} + \sigma^2 I_n)^{-2}) y
\]
\[
= \sigma^4 y^\top (k_{XX} + \sigma^2 I_n)^{-2} y.
\]
The second term is
\[
\sigma^2 \|\hat{f}\|_{\mathcal{H}_k}^2 = \sigma^2 y^\top (k_{XX} + \sigma^2 I_n)^{-1} k_{XX} (k_{XX} + \sigma^2 I_n)^{-1} y
\]
\[
= \sigma^2 y^\top (k_{XX} + \sigma^2 I_n)^{-1} (I_n - \sigma^2 (k_{XX} + \sigma^2 I_n)^{-1}) y
\]
\[
= \sigma^2 y^\top (k_{XX} + \sigma^2 I_n)^{-1} y - \sigma^4 y^\top (k_{XX} + \sigma^2 I_n)^{-2} y.
\]
Therefore,
\[
\|y - \hat{f}_X\|_2^2 + \sigma^2 \|\hat{f}\|_{\mathcal{H}_k}^2 = \sigma^2 y^\top (k_{XX} + \sigma^2 I_n)^{-1} y.
\]

### B.4 Proof of Theorem 9

**Proof** We first make preliminaries for proving the theorem. For a symmetric matrix \( B \in \mathbb{R}^{n \times n} \) with \( n \in \mathbb{N} \), denote by \( \lambda_1(B) \geq \cdots \geq \lambda_n(B) \) its eigenvalues with multiplicities in the decreasing order. For any symmetric and positive semi-definite (SPSD) matrix \( A \in \mathbb{R}^{n \times n} \) and any \( B \in \mathbb{R}^{n \times n} \), we have (see Saniuk and Rhodes, 1987)
\[
\text{tr}(AB) \leq \text{tr}(A)\|B\|_{op},
\]
where \( \|B\|_{op} := \sup_{\|v\| \leq 1} \|Bv\| \) denotes the operator norm (or spectral norm). If \( B \) is symmetric, we have \( \|B\|_{op} = \max(|\lambda_1(B)|, |\lambda_n(B)|) \).
For any SPSD matrix \( A \in \mathbb{R}^{n \times n} \) and any symmetric and negative semi-definite (SNSD) matrix \( B \in \mathbb{R}^{n \times n} \), we have
\[
\text{tr}(AB) = \text{tr}(BA) = \text{tr}(A^{1/2}BA^{1/2}) = \sum_{i=1}^n \lambda_i(A^{1/2}BA^{1/2}) \leq 0,
\]
where the inequality follows from the fact that $A^{1/2}BA^{1/2}$ is SNSD and hence all its eigenvalues are non-positive.

We also use the following short hand notation

$$K := k_{XX}, \quad Q := q_{XX}, \quad \tilde{K} := K + n\lambda I_n, \quad \tilde{Q} := Q + n\lambda I_n,$$

$$\alpha = \tilde{K}^{-1}y, \quad \beta = \tilde{Q}^{-1}y, \quad \tilde{\beta} = (n\lambda k_{ZZ} + k_{XX}k_{XZ})^{-1}k_{ZXY}.$$

Note that the matrices $K, Q, \tilde{K}, \tilde{Q}$ are SPSD. It holds that

$$\|\tilde{K}^{-1}\|_{op} \leq \frac{1}{n\lambda}, \quad \|\tilde{Q}^{-1}\|_{op} \leq \frac{1}{n\lambda}, \quad \|K\tilde{K}^{-1}\|_{op} \leq 1, \quad \|Q\tilde{Q}^{-1}\|_{op} \leq 1.$$

Using the above notation, the KRR estimator $\hat{f}$ and the Nyström approximation $\tilde{f}$ can be written for any $x \in \mathcal{X}$ as

$$\hat{f}(x) = k_X(x)^\top \tilde{K}^{-1}y,$$

$$\tilde{f}(x) = k_Z(x)^\top (n\lambda k_{ZZ} + k_{XX}k_{XZ})^{-1}k_{ZXY} = k_Z(x)^\top \tilde{\beta}.$$

We will use the following identity:

$$k_{XZ}\tilde{\beta} = \hat{f}_X = q_{XX}\tilde{Q}^{-1}y = Q\tilde{Q}^{-1}y.$$

With these preparations, we now prove the assertion. First we have

$$\|\hat{f} - \tilde{f}\|_{\tilde{H}_k}^2 = \|\hat{f}\|_{\tilde{H}_k}^2 - 2\langle \hat{f}, \tilde{f} \rangle_{\tilde{H}_k} + \|\tilde{f}\|_{\tilde{H}_k}^2$$

$$= \|\hat{f}\|_{\tilde{H}_k}^2 - 2\langle \hat{f}, \tilde{f} \rangle_{\tilde{H}_k} + \|\tilde{f}\|_{\tilde{H}_k}^2,$$

where we used $\|\hat{f}\|_{\tilde{H}_k}^2 = \|\tilde{f}\|_{\tilde{H}_q}^2$, which holds from $\tilde{f} \in M$ and Lemma 4. The expression is equal to

$$= \alpha^\top K\alpha - 2\alpha^\top k_{XZ}\tilde{\beta} + \tilde{\beta}^\top Q\tilde{\beta}$$

$$= \text{tr}(K\alpha\alpha^\top) - 2\text{tr}(k_{XZ}\tilde{\beta}\alpha^\top) + \text{tr}(Q\tilde{\beta}\tilde{\beta}^\top)$$

$$= \text{tr}(K\tilde{K}^{-1}yy^\top\tilde{K}^{-1}) - \text{tr}(QQ^{-1}yy^\top\tilde{K}^{-1}) + \text{tr}(QQ^{-1}yy^\top\tilde{Q}^{-1}) - \text{tr}(QQ^{-1}yy^\top\tilde{K}^{-1})$$

$$= \text{tr}((K\tilde{K}^{-1} - QQ^{-1})yy^\top\tilde{K}^{-1}) + \text{tr}(QQ^{-1}yy^\top(\tilde{Q}^{-1} - \tilde{K}^{-1}))$$

$$\leq \text{tr}(K\tilde{K}^{-1} - QQ^{-1})\|yy^\top\|_{op}\|\tilde{K}^{-1}\|_{op} + \text{tr}(\tilde{Q}^{-1} - \tilde{K}^{-1})\|QQ^{-1}\|_{op}\|yy^\top\|_{op}$$

$$\leq \frac{1}{n\lambda}\text{tr}(K\tilde{K}^{-1} - QQ^{-1})\|y\|^2 + \text{tr}(\tilde{Q}^{-1} - \tilde{K}^{-1})\|y\|^2$$

$$= \frac{1}{n\lambda}\left(\text{tr}((K - Q)\tilde{K}^{-1}) + \text{tr}(Q(\tilde{K}^{-1} - \tilde{Q}^{-1}))\right)\|y\|^2 + \text{tr}(\tilde{Q}^{-1}(K - Q)\tilde{K}^{-1})\|y\|^2$$

Since $Q$ is SPSD and $\tilde{K}^{-1} - \tilde{Q}^{-1}$ is SNSD, we have

$$\text{tr}(Q(\tilde{K}^{-1} - \tilde{Q}^{-1})) \leq 0$$
due to (60). Using this and (59), we obtain

\[
\leq \frac{1}{n\lambda} \text{tr}(K - Q)\|K^{-1}\|_{\text{op}}\|y\|^2 + \text{tr}(K - Q)\|K^{-1}\|_{\text{op}}\|Q^{-1}\|_{\text{op}}\|y\|^2
\]

\[
\leq \frac{2}{(n\lambda)^2} \text{tr}(K - Q)\|y\|^2,
\]

which concludes the proof.

References

Vincent Adam, Stefanos Eleftheriadis, Artem Artemev, Nicolas Durrande, and James Hensman. Doubly sparse variational gaussian processes. In International Conference on Artificial Intelligence and Statistics, pages 2874–2884. PMLR, 2020.

Raja Hafiz Affandi, Alex Kulesza, Emily Fox, and Ben Taskar. Nyström approximation for large-scale determinantal processes. In Artificial Intelligence and Statistics, pages 85–98. PMLR, 2013.

Nachman Aronszajn. Theory of reproducing kernels. Transactions of the American Mathematical Society, 68(3):337–404, 1950.

Francis Bach. Sharp analysis of low-rank kernel matrix approximations. In Conference on Learning Theory, pages 185–209. PMLR, 2013.

Matthias Bauer. Advances in Probabilistic Modelling: Sparse Gaussian Processes, Autoencoders, and Few-shot Learning. PhD thesis, University of Cambridge, 2020.

Matthias Bauer, Mark van der Wilk, and Carl Edward Rasmussen. Understanding probabilistic sparse Gaussian process approximations. Advances in neural information processing systems, 29, 2016.

Mohamed-Ali Belabbas and Patrick J Wolfe. Spectral methods in machine learning and new strategies for very large datasets. Proceedings of the National Academy of Sciences, 106(2):369–374, 2009.

A. Berlinet and C. Thomas-Agnan. Reproducing Kernel Hilbert Spaces in Probability and Statistics. Kluwer, 2004.

David Burt, Carl Edward Rasmussen, and Mark Van Der Wilk. Rates of convergence for sparse variational Gaussian process regression. In Proceedings of the 36th International Conference on Machine Learning, pages 862–871, 2019.

David R. Burt, Carl Edward Rasmussen, and Mark van der Wilk. Convergence of sparse variational inference in Gaussian processes regression. Journal of Machine Learning Research, 21(131):1–63, 2020.
Yifan Chen and Yun Yang. Fast statistical leverage score approximation in kernel ridge regression. In *International Conference on Artificial Intelligence and Statistics*, pages 2935–2943. PMLR, 2021.

Corinna Cortes, Mehryar Mohri, and Ameet Talwalkar. On the impact of kernel approximation on learning accuracy. In *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, pages 113–120. JMLR Workshop and Conference Proceedings, 2010.

Lehel Csató and Manfred Opper. Sparse on-line Gaussian processes. *Neural Computation*, 14(3):641–668, 2002.

Imre Csiszár. I-divergence geometry of probability distributions and minimization problems. *The annals of probability*, pages 146–158, 1975.

Michal Derezinski, Rajiv Khanna, and Michael W Mahoney. Improved guarantees and a multiple-descent curve for Column Subset Selection and the Nyström method. In H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, editors, *Advances in Neural Information Processing Systems*, volume 33, pages 4953–4964. Curran Associates, Inc., 2020.

Monroe D Donsker and SR Srinivasa Varadhan. Asymptotic evaluation of certain markov process expectations for large time, i. *Communications on Pure and Applied Mathematics*, 28(1):1–47, 1975.

Petros Drineas and Michael W. Mahoney. On the Nyström method for approximating a Gram matrix for improved kernel-based learning. *Journal of Machine Learning Research*, 6(72):2153–2175, 2005.

Vincent Dutordoir, Nicolas Durrande, and James Hensman. Sparse Gaussian processes with spherical harmonic features. In Hal Daumé III and Aarti Singh, editors, *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pages 2793–2802. PMLR, 2020.

Ahmed El Alaoui and Michael W Mahoney. Fast randomized kernel ridge regression with statistical guarantees. In *Advances in Neural Information Processing Systems*, pages 775–783, 2015.

Charless Fowlkes, Serge Belongie, Fan Chung, and Jitendra Malik. Spectral grouping using the Nyström method. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 26(2):214–225, 2004.

Alex Gittens and Michael W Mahoney. Revisiting the nyström method for improved large-scale machine learning. *The Journal of Machine Learning Research*, 17(1):3977–4041, 2016.

James Hensman, Nicolò Fusi, and Neil D Lawrence. Gaussian processes for big data. In *Proceedings of the Twenty-Ninth Conference on Uncertainty in Artificial Intelligence*, pages 282–290, 2013.
James Hensman, Alexander Matthews, and Zoubin Ghahramani. Scalable variational Gaussian process classification. In Artificial Intelligence and Statistics, pages 351–360. PMLR, 2015a.

James Hensman, Alexander G Matthews, Maurizio Filippone, and Zoubin Ghahramani. MCMC for variationally sparse Gaussian processes. In C. Cortes, N. Lawrence, D. Lee, M. Sugiyama, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 28. Curran Associates, Inc., 2015b.

James Hensman, Nicolas Durrande, and Arno Solin. Variational Fourier features for Gaussian processes. Journal of Machine Learning Research, 18(151):1–52, 2018.

Thomas Hofmann, Bernhard Schölkopf, and Alexander J Smola. Kernel methods in machine learning. Annals of Statistics, 36(3):1171–1220, 2008.

Michael I Jordan, Zoubin Ghahramani, Tommi S Jaakkola, and Lawrence K Saul. An introduction to variational methods for graphical models. Machine Learning, 37(2):183–233, 1999.

Motonobu Kanagawa, Philipp Hennig, Dino Sejdinovic, and Bharath K Sriperumbudur. Gaussian processes and kernel methods: A review on connections and equivalences. arXiv preprint arXiv:1807.02582, 2018.

Mohammad Emtiyaz Khan and Håvard Rue. The Bayesian Learning Rule. arXiv preprint arXiv:2107.04562, 2021.

G. S. Kimeldorf and G. Wahba. A correspondence between Bayesian estimation on stochastic processes and smoothing by splines. The Annals of Mathematical Statistics, 41(2):495–502, 1970.

Jeremias Knoblauch, Jack Jewson, and Theodoros Damoulas. Generalized variational inference: Three arguments for deriving new posteriors. arXiv preprint arXiv:1904.02063, 2019.

Sanjiv Kumar, Mehryar Mohri, and Ameet Talwalkar. Ensemble Nyström method. In Y. Bengio, D. Schuurmans, J. Lafferty, C. Williams, and A. Culotta, editors, Advances in Neural Information Processing Systems, volume 22. Curran Associates, Inc., 2009.

Sanjiv Kumar, Mehryar Mohri, and Ameet Talwalkar. Sampling methods for the nyström method. Journal of Machine Learning Research, 13(34):981–1006, 2012.

Felix Leibfried, Vincent Dutordoir, ST John, and Nicolas Durrande. A tutorial on sparse Gaussian processes and variational inference. arXiv preprint arXiv:2012.15962, 2020.

Chengtao Li, Stefanie Jegelka, and Suvrit Sra. Fast DPP sampling for Nyström with application to kernel methods. In Maria Florina Balcan and Kilian Q. Weinberger, editors, Proceedings of The 33rd International Conference on Machine Learning, volume 48 of Proceedings of Machine Learning Research, pages 2061–2070, New York, New York, USA, 20–22 Jun 2016. PMLR.
Alexander G de G Matthews, James Hensman, Richard Turner, and Zoubin Ghahramani. On sparse variational methods and the Kullback-Leibler divergence between stochastic processes. In Artificial Intelligence and Statistics, pages 231–239, 2016.

Giacomo Meanti, Luigi Carratino, Lorenzo Rosasco, and Alessandro Rudi. Kernel methods through the roof: Handling billions of points efficiently. In H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, editors, Advances in Neural Information Processing Systems, volume 33, pages 14410–14422. Curran Associates, Inc., 2020. URL https://proceedings.neurips.cc/paper/2020/file/a59af8b1b7d82ee353921a55c579ee26d-Paper.pdf.

Cameron Musco and Christopher Musco. Recursive sampling for the Nyström method. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.

Dennis Nieman, Botond Szabo, and Harry van Zanten. Contraction rates for sparse variational approximations in Gaussian process regression. Journal of Machine Learning Research, 23(205):1–26, 2022. URL http://jmlr.org/papers/v23/21-1128.html.

Manfred Opper and Cédric Archambeau. The variational Gaussian approximation revisited. Neural Computation, 21(3):786–792, 2009.

E. Parzen. An approach to time series analysis. The Annals of Mathematical Statistics, 32(4):951–989, 1961.

Joaquin Quiñonero-Candela and Carl Edward Rasmussen. A unifying view of sparse approximate Gaussian process regression. Journal of Machine Learning Research, 6:1939–1959, 2005.

C.E. Rasmussen and C.K.I. Williams. Gaussian Processes for Machine Learning. MIT Press, 2006.

Simone Rossi, Markus Heinonen, Edwin Bonilla, Zheyang Shen, and Maurizio Filippone. Sparse Gaussian processes revisited: Bayesian approaches to inducing-variable approximations. In Arindam Banerjee and Kenji Fukumizu, editors, Proceedings of The 24th International Conference on Artificial Intelligence and Statistics, volume 130 of Proceedings of Machine Learning Research, pages 1837–1845. PMLR, 13–15 Apr 2021.

Alessandro Rudi, Raffaello Camoriano, and Lorenzo Rosasco. Less is more: Nyström computational regularization. In Advances in Neural Information Processing Systems, pages 1657–1665, 2015.

Alessandro Rudi, Luigi Carratino, and Lorenzo Rosasco. FALKON: An optimal large scale kernel method. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.
J Saniuk and I Rhodes. A matrix inequality associated with bounds on solutions of algebraic Riccati and Lyapunov equations. *IEEE Transactions on Automatic Control*, 32(8):739–740, 1987.

Bernhard Schölkopf and Alexander J Smola. *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*. MIT press, 2002.

Bernhard Schölkopf, Ralf Herbrich, and Alex J Smola. A generalized representer theorem. In *International Conference on Computational Learning Theory*, pages 416–426. Springer, 2001.

Matthias Seeger, Christopher Williams, and Neil Lawrence. Fast forward selection to speed up sparse Gaussian process regression. In *Artificial Intelligence and Statistics*, 2003.

Jiaxin Shi, Michalis Titsias, and Andriy Mnih. Sparse orthogonal variational inference for Gaussian processes. In Silvia Chiappa and Roberto Calandra, editors, *Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics*, volume 108 of *Proceedings of Machine Learning Research*, pages 1932–1942. PMLR, 26–28 Aug 2020.

Alex J Smola and Bernhard Schölkopf. Sparse greedy matrix approximation for machine learning. In *Proceedings of the Seventeenth International Conference on Machine Learning*, pages 911–918, 2000.

Edward Snelson and Zoubin Ghahramani. Sparse Gaussian processes using pseudo-inputs. In *Advances in Neural Information Processing Systems*, pages 1257–1264, 2006.

Edward Snelson and Zoubin Ghahramani. Local and global sparse Gaussian process approximations. In *Artificial Intelligence and Statistics*, pages 524–531, 2007.

I. Steinwart and A. Christmann. *Support Vector Machines*. Springer, 2008.

Ameet Talwalkar, Sanjiv Kumar, and Henry Rowley. Large-scale manifold learning. In *2008 IEEE Conference on Computer Vision and Pattern Recognition*. IEEE, 2008.

Ameet Talwalkar, Sanjiv Kumar, Mehryar Mohri, and Henry Rowley. Large-scale SVD and manifold learning. *Journal of Machine Learning Research*, 14(60):3129–3152, 2013.

Michalis Titsias. Variational learning of inducing variables in sparse Gaussian processes. In *Artificial Intelligence and Statistics*, pages 567–574, 2009a.

Michalis K Titsias. Variational model selection for sparse Gaussian process regression. *Technical Report, University of Manchester, UK*, 2009b.

Gia-Lac Tran, Dimitrios Milios, Pietro Michiardi, and Maurizio Filippone. Sparse within sparse Gaussian processes using neighbor information. In *Proceedings of the Thirty-eighth International Conference on Machine Learning*, 2021.
Sattar Vakili, Jonathan Scarlett, Da-Shan Shiu, and Alberto Bernacchia. Improved Convergence Rates for Sparse Approximation Methods in Kernel-Based Learning. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvari, Gang Niu, and Sivan Sabato, editors, Proceedings of the 39th International Conference on Machine Learning, volume 162 of Proceedings of Machine Learning Research, pages 21960–21983. PMLR, 17–23 Jul 2022. URL https://proceedings.mlr.press/v162/vakili22a.html.

Grace Wahba. Spline Models for Observational Data. SIAM, 1990.

Christopher KI Williams and Matthias Seeger. Using the Nyström method to speed up kernel machines. In Advances in Neural Information Processing Systems, pages 682–688, 2001.

Jian Wu, Matthias Poloczek, Andrew G Wilson, and Peter Frazier. Bayesian optimization with gradients. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.