Learning Integral Representations of Gaussian Processes

Zilong Tan
Machine Learning Department
Carnegie Mellon University
Email: zilongt@cs.cmu.edu

Sayan Mukherjee
Departments of Statistical Science
Computer Science, Mathematics,
Biostatistics & Bioinformatics
Duke University
Email: sayan@stat.duke.edu

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Abstract

We propose a representation of Gaussian processes (GPs) based on powers of the integral operator defined by a kernel function, we call these stochastic processes integral Gaussian processes (IGPs). Sample paths from IGPs are functions contained within the reproducing kernel Hilbert space (RKHS) defined by the kernel function, in contrast sample paths from the standard GP are not functions within the RKHS. We develop computationally efficient non-parametric regression models based on IGPs. The main innovation in our regression algorithm is the construction of a low dimensional subspace that captures the information most relevant to explaining variation in the response. We use ideas from supervised dimension reduction to compute this subspace. The result of using the construction we propose involves significant improvements in the computational complexity of estimating kernel hyper-parameters as well as reducing the prediction variance.

1 Introduction

Gaussian processes (GPs) (Doob, 1944) have been used extensively for non-parametric regression and density estimation in the statistics and machine learning literature (Stein, 1999; Rasmussen and Williams, 2006). Models based on GPs enjoy the flexibility that nonlinear interpolation and spatial structure can be naturally modeled. The covariance kernel of the GP is the crucial component that specifies the class of functions the GP can realize. A key observation that motivates this work is that the sample paths (realizations) of the GP with covariance kernel $\kappa(\cdot, \cdot)$ is outside the reproducing kernel Hilbert space (RKHS) $\mathcal{H}_\kappa$ with the reproducing kernel $\kappa$ almost surely by the zero-one law of GPs (Kallianpur, 1970; Driscoll, 1973; Lukić and Beder, 2001; Wahba, 1990). Thus, the GP perspective is natural for point estimates such as the posterior mean but is problematic for posterior sample paths from the RKHS (Liang et al., 2007; Pillai et al., 2007; Dunson, 2010). In this paper, we present a construction of GPs with sample paths in a given RKHS, and

*Work done while the author was at Duke University.
develop fast algorithms for non-parametric regression. The utility of our approach involves posterior based hyper-parameter inference as well as variable selection in Bayesian kernel models (Neal, 1997; Bishop, 2003; Dunson, 2010; Crawford et al., 2018).

Let \( \{ f(x) : x \in \mathcal{X} \} \) be a zero-mean GP indexed by a separable metric space \( \mathcal{X} \). The standard GP regression model is specified by

\[
y_i = f(x_i) + \epsilon_i
\]

with independent noise \( \epsilon_i \sim \mathcal{N}(0, \sigma^2) \). Denote the covariance kernel as \( \kappa \) and the the RKHS induced by \( \kappa \) as \( \mathcal{H}_\kappa \). Approaches such as Tipping (2001); Sollich (2002); Chakraborty et al. (2012) assume that the \( f(\cdot) \) is in a finite-dimensional subspace

\[
\left\{ f(\cdot) = \sum_{i=1}^{n} a_i \kappa(\cdot, x_i) \mid x_i \in \mathcal{X}, a_i \in \mathbb{R} \right\}
\]

of \( \mathcal{H}_\kappa \) dependent on the training data \( \{x_i\}_{i=1}^{n} \). Generalizing the GP regression model (1) to the infinite-dimensional \( \mathcal{H}_\kappa \), by directly placing the GP prior on \( \mathcal{H}_\kappa \) is problematic since a sample path (realization) of the GP lies almost surely outside the RKHS \( \mathcal{H}_\kappa \), i.e.,

\[
P(f(\cdot) \in \mathcal{H}_\kappa) = 0 \text{ if } \mathcal{H}_\kappa \text{ is infinite dimensional (see e.g., Theorem 5.1 of Kallianpur, 1970; Driscoll, 1973; Wahba, 1990)}.
\]

One solution to this problem was given in (Pillai et al., 2007; Liang et al., 2007) by assuming that \( f(x) \) is specified by the following integral operator

\[
f(x) = \int_{\mathcal{X}} \kappa(x, z) \nu(z) d\pi(z)
\]

where \( \nu(\cdot) \) is the sample path form a GP and \( \pi \) is a finite measure. Their approach can be viewed as the embedding of signed measures (see e.g., Chapter 4 of Berlinet and Thomas-Agnan, 2003), and the resulting \( f(\cdot) \) can be thought of as a GP (Itô, 1954; Gelfand et al., 1967). A limitation of the GP specified by equation (2) is that only a subspace of the functions in \( \mathcal{H}_\kappa \) can be realized. Indeed, the relation between the function space spanned by (2) and \( \mathcal{H}_\kappa \) has been examined by considering integral operators based on powers of the covariance kernel (Steinwart and Scovel, 2012). We combine the integral representation in equation (2) with the idea of using powers of integral operators to propose a new GP model for which we can precisely characterize both the RKHS as well as sample paths of the functions drawn from the GP.

There are three main contributions of this paper with respect to both specifying GP models as well as efficient and accurate non-parametric regression based on GPs:

1. We first introduce a GP representation which expands the function space spanned by (2) while still having the sample paths confined to an RKHS specified by the kernel function. This is accomplished by using an integral operator defined by powers of kernels (Steinwart and Scovel, 2012; Kanagawa et al., 2018). We demonstrate that the space of functions realized by this representation is strictly larger than those given by the specification in (2).

2. We then present a finite-sample variant of the GP that has nice properties in that the class of functions realized include solutions to Tikhonov regularization problems
(Cucker and Smale, 2002; Hofmann et al., 2008) as well as several Bayesian kernel models (Tipping, 2001; Sollich, 2002; Chakraborty et al., 2012). The key insight in formulating this variant is a dual construction of GPs as the class of functions

\[ f(x) = \sum_{i=1}^{n} \beta_{i} \kappa(x, x_i), \quad (\beta_1, \beta_2, \cdots, \beta_n) \sim \mathcal{N}(\mathbf{0}, \Sigma_{\beta}) \]

in contrast to the more classical construction of a GP based on eigenfunctions (elaborated in Section 3.1.1)

\[ f(x) = \sum_{j=1}^{l} \alpha_{j} e_{j}(x), \quad \alpha_{j} \text{i.i.d.} \sim \mathcal{N}(0, \lambda_{j}) \]

where \( \{e_{j}\}_{j=1}^{l} \) and \( \{\lambda_{j}\}_{j=1}^{l} \) are the eigenfunctions and the corresponding eigenvalues for the integral operator defined by the kernel \( \kappa \).

3. To speed up computation as well as to potentially reduce prediction variance, we compute a low rank approximation of the RKHS using ideas from sufficient dimension reduction (SDR) (Li, 1991; Cook, 1998; Fukumizu et al., 2004). We show that the SDR method is natural and generally yields a low-rank parameterization of the covariance kernel. Fast algorithms are developed for computing this approximation. The overall computational complexity for learning the proposed low rank GP is \( O(n^2m) \) per iteration which improves the complexity \( O(n^3) \) of the standard GP. Further speedups can be achieved by combining the algorithm with the sparse GP methods (Smola and Bartlett, 2001; Seeger et al., 2003; Snelson and Ghahramani, 2006a).

4. Our approach is grounded in the theory of RKHS and sufficient dimension reduction. An exact characterization of the function space realized by the integral representation is given, suggesting that our approach is particularly useful for kernels with rapidly decaying eigenvalues. This holds true for several widely used kernels (Zhu et al., 1998; Belkin, 2018). Second, we generalize the classic SDR likelihood (Cook and Forzani, 2009) on \( \mathbb{R}^d \) to the RKHS setting. We justify that the RKHS can be well approximated by a low-rank SDR subspace if the eigenvalue of the reproducing kernel decays at a faster rate than \( O(1/n) \).

### 1.1 Outline of the Paper

The remainder of this paper is organized as follows: in Section 2, we introduce the the GP representation using powers of the integral operators. In addition, we discuss computational issues and posterior inference based on the SDR approximation to the RKHS. In Section 3, we provide the theoretical justification for the results stated in Section 2 as well as the approximation to the RKHS using SDR subspaces. In Section 4, we develop fast algorithms for estimating the parameters of our approach. In Section 5, we illustrate the difference between our approach and the standard GP regression model, and report competitive experimental results on a diverse collection of real-life datasets. In Section 6, we conclude this paper.
1.2 Notation

We use bold lowercase letters for vectors, bold capital letters for matrices, calligraphic letters for sets. The $i$-th row and $j$-th column of a matrix $A$ are denoted by $A_i$ and $A_j$, respectively. In addition, we write $A_k$ for the orthogonal complement to the column space of $A$, $\text{tr}(\cdot)$ for the trace, and $\det(\cdot)$ for the determinant. $I_n$ and $1_n$ denote respectively the $n$-by-$n$ identity matrix and a (column) $n$-vector of all ones. Random variables $X$ and $Y$ represent the covariates vector and the response, whose realizations are the matrix $X$ and $y$ with the $i$-th row corresponding to the $i$-th observation. Similarly, $\kappa(X, Z)$ denotes the matrix whose $(i,j)$-th element is specified by $\kappa(X^i, Z^j)$. We also denote by $K_\kappa$ the kernel matrix of a kernel function $\kappa$, whose $(i,j)$-th entry is specified by $\kappa(x_i, x_j)$.

2 Integral Representations of Gaussian Processes

Let $(X, B, \mu)$ be a measure space for some finite measure $\mu$. Throughout this paper, we assume that $\kappa$ is a continuous positive definite kernel measurable on $X \times X$. In addition, $\kappa$ has an infinitely number of nonzero eigenvalues, and is of trace class, i.e., the sum of eigenvalues is finite, a property that characterizes covariance kernels (see e.g., Section 2.3 of Horváth and Kokoszka, 2012).

We consider the GP obtained by applying an integral operator $\mathcal{K}^p$ to a GP $\nu : X \times \Omega \mapsto \mathbb{R}$ on a probability space $(\Omega, \mathcal{F}, P)$ with covariance kernel $\kappa_\nu$. The integral operator $\mathcal{K}^p : L^2(X, B, \mu) \mapsto L^2(X, B, \mu)$ is based on the powers of kernels (Steinwart and Scovel, 2012; Kanagawa et al., 2018), and is given by

$$\mathcal{K}^p \nu := \int_X \kappa_p(\cdot, z) \nu(z) d\mu(z) \quad \text{with} \quad \kappa_p(x, z) := \sum_{i=1}^{\infty} \lambda_i^p e_i(x) e_i(z), \quad 1 \leq p \leq 1,$$

where $\{e_i\}$ denotes the complete set of orthonormal eigenfunctions of $\kappa$ corresponding to the non-increasing sequence of eigenvalues $\{\lambda_i\}$. This integral representation is an instance of generalized stochastic processes introduced in (Itô, 1954; Gelfand et al., 1967), where $\kappa_p(x, z)$ can be viewed as a weighting function. The resulting GP $\mathcal{K}^p \nu$ is written

$$\mathcal{M} := \left\{ f(x) := \sum_{i=1}^{\infty} \lambda_i^p \varphi_i e_i(x) \mid \varphi_i := \int_X \nu(z) e_i(z) d\mu(z), x \in X \right\}.$$

In particular, $\mathcal{M}$ is equivalent to (2) for the case that $p = 1$. Setting $p < 1$, the representation (3) becomes a superset of (2) but can still have all sample paths confined within $\mathcal{H}_\kappa$ as we will show in Section 2.1. In the remainder of this paper, the GP (3) will be termed the Integral GP (IGP), and $\gamma(f; \kappa_p, \kappa_\nu)$ denotes the corresponding prior.

Let us consider some basic properties of the IGP. For an IGP $f \in \mathcal{M}$, the curve $f(x), x \in X$, is a random element of $L^2(X, B, \mu)$, and is square integrable since

$$\mathbb{E} \|f\|^2 = \mathbb{E} \sum_{i=1}^{\infty} \left( \lambda_i^p \int_X \nu(z) e_i(z) d\mu(z) \right)^2 \leq \lambda_1^{2p} \mathbb{E} \|\nu\|_{L^2}^2 < \infty.$$
holds by Parseval's identity. Its mean and covariance functions are written

\[ E f = \sum_{i=1}^{\infty} \lambda_i^p E (\varphi_i) e_i \]  

\[ \kappa_M (x, z) = \int_{X} \int_{X} \kappa_\nu (s, t) \kappa_p (x, s) \kappa_p (z, t) d\mu (s) d\mu (t). \]  

Let \( K \) and \( K_{\kappa_M} \) be respectively the kernel matrix \( K_{ij} = \kappa (x_i, x_j) \) and the covariance matrix \( [K_{\kappa_M}]_{ij} := \kappa_M (x_i, x_j) \) on a finite sample \( \{x_i\}_{i=1}^{n} \). By analogy, Proposition 1 gives the covariance matrix \( K_{\kappa_M} \). The proof is straightforward by observing that \( \lambda_i = \eta_i / n \) and \( e_i (x_j) = \sqrt{n} b_{ij} \) for eigenvalue-eigenvector pairs \( (\eta_i, b_i) \) of \( K \).

**Proposition 1.** Suppose that \( \mu = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \) where \( \delta_{x_i} \) is the Dirac measure, the covariance matrix of (5) is given by \( K_{\kappa_M} = n^{-2p} K^p K_\nu K^p \).

Another perspective is that the covariance function \( \kappa_M \) is non-stationary which enables the IGP to model spatial data. For example, consider the setting \( \kappa_\nu = \kappa \) and \( p = 1/2 \) in (3), the covariance kernel of the IGP is simplified to

\[ \kappa_M (x, z) = \int_{X} \kappa (x, s) \kappa (z, s) d\mu (s). \]  

This gives us a non-stationary covariance kernel since it is no longer a function of the distance alone. Note that we do not require \( \kappa \) to be non-stationary as well. The covariance kernel (6) can be viewed as the correlation between two points \( x \) and \( z \) taking into account neighborhood locations \( s \). In this example, (6) is the spatial correlation kernel proposed in (Higdon et al., 1998).

### 2.1 Characterizing the Function Space

Recall that our goal is to construct a GP whose sample paths are confined in a given RKHS, and can realize the largest possible subspace of the RKHS. In this section, we outline how the IGP meets this goal, and defer the proof until Section 3.2.

First, the IGP representation (3) can realize an expanding subspace of \( \mathcal{H}_\kappa \) as \( p \) decreases, and the entire \( \mathcal{H}_\kappa \) for \( p = 1/2 \) and some \( \nu \in L^2 (X \times \Omega, F, P) \). Proposition 2 characterizes the function space of the IGP. The proof of the proposition is straightforward using Mercer's representation of the RKHS discussed in Section 3.1.

**Proposition 2.** Suppose that \( \{\nu (x) : x \in X\} \) is a GP on \( L^2 (\Omega, F, P) \). Then, the space of functions realizable by the IGP (3) is given by \( \left\{ \sum_{i=1}^{\infty} w_i e_i : \sum_{i=1}^{\infty} w_i^2 / \lambda_i^{2p} < \infty \right\} \).

Pillai et al. (2007) and Liang et al. (2007) proposed the following class of functions

\[ f (x) = \int_{X} \kappa (x, z) \nu (z) d\mu (z) = \sum_{i=1}^{\infty} \lambda_i e_i (x) \int_{X} \nu (z) e_i (z) d\mu (z) \]

which corresponds to the IGP with \( p = 1 \). From Proposition 2, the IGP can realize an expanded space of functions setting \( p < 1 \). This also holds when the Hilbert space of \( \nu (\cdot) \) is an RKHS subspace of the \( L^2 \) (see Section 3.1.1).
While a smaller $p$ allows the IGP to realize more functions, the sample path can potentially go beyond $\mathcal{H}_\kappa$. Theorem 3 provides a sufficient condition for the IGP sample paths to be confined within $\mathcal{H}_\kappa$, requiring the eigenvalue of $\kappa$ to decay rapidly. We demonstrate this condition is satisfied for several popular classes of kernels including radial kernels.

**Theorem 1.** Let $f \in \mathcal{L}^2(\mathcal{X} \times \Omega, \mathcal{F}, P)$ be an IGP. Then, it holds that $P(f(\cdot) \in \mathcal{H}_\kappa) = 1$ if the kernel $\kappa_{2p-1}$ is of trace class.

From Theorem 1, sample paths of the IGP with $p = 1$ are confined within $\mathcal{H}_\kappa$ almost surely by our assumption that $\kappa$ is of trace class. This corresponds to the case where the function space of IGP is minimized from Proposition 2. For several popular classes of kernel operators, it is possible for the IGP to realize a larger space of functions while still having its sample paths confined in $\mathcal{H}_\kappa$. Below, we give two examples.

**Radial Kernels** For any $p > 1/2$, the condition of Theorem 1 is satisfied for radial kernels of which the eigenvalue decays nearly exponentially (Belkin, 2018). For example, consider $\kappa(x,z) = \exp(-\frac{\|x-z\|^2}{2\ell^2})$ and $\mu(x)$ is Gaussian, it has been shown

$$
\lambda_j \propto b^j, \quad b < 1
$$

$$
e_j(x) \propto \exp(-(c-a)x^2) h_j\left(x\sqrt{2c}\right),
$$

where $a, b, c$ are functions of $\ell$, and $h_j$ is the $j$-th order Hermite polynomial (Zhu et al., 1998).

**Brownian Bridge** Suppose that $\mathcal{X} = [0,1]$ and $\mu$ is the Lebesgue measure, the Brownian bridge kernel reads $\kappa(x,z) = \min(x, z) - xz$ (Rogers and Williams, 2000). The corresponding eigenvalues and eigenfunctions are given by

$$
\lambda_j = \frac{1}{\pi^2j^2}, \quad e_j(x) = \sqrt{2}\sin(j\pi x).
$$

Thus, the condition of Theorem 1 holds for $p > 3/4$.

**2.2 A Finite-Sample Variant**

To obtain practical algorithms, we also present a finite-sample variant of the IGP (SIGP) on a sample $\{x_i\}_{i=1}^n$. The function space of the SIGP will be specified by the Hilbert closure $\mathcal{H}_{\kappa,n}$ of the linear subspace

$$
\left\{ \sum_{i=1}^n a_i \kappa(\cdot, x_i) \mid \{a_i\}_{i=1}^n \subset \mathbb{R}, \{x_i\}_{i=1}^n \subset \mathcal{X} \right\}.
$$

Suppose that $x_i$’s in the sample $\{x_i\}_{i=1}^n$ are i.i.d. and $\mu$ is a probability measure without loss of generality. The SIGP is defined as

$$
f_n(\cdot) := \frac{1}{n} \sum_{i=1}^n \nu(x_i) \kappa_p(\cdot, x_i), \quad (7)
$$
which converges to the IGP at a rate \( O_P \left( n^{-1/2} \right) \) by the Central Limit Theorem for Hilbert spaces (Ledoux and Talagrand, 1991; Berline and Thomas-Agnan, 2003). Compared to the standard function-space view of GPs (see Williams, 1997 and Section 3.1.1), the SIGP representation provides a dual construction of GPs where the Gaussian coefficients are assigned to the representer \( \kappa_p (\cdot, x_i) \) of each data point \( x_i \) as opposed to each eigenfunction \( e_i (\cdot) \) in the function-space view of GPs.

The SIGP can be useful for two reasons. First, the dual construction of GPs offered by the SIGP affords natural approximations and thereby fast computation, as will be discussed in Section 2.3. Second, the SIGP function space \( \mathcal{H}_{\kappa,n} \) contains “interesting” functions including the solution to Tikhonov regularization problems by the representer theorem:

\[
\min_{f \in \mathcal{H}_{\kappa,n}} L(f, D) + \rho \left( \| f \|_{\mathcal{H}_{\kappa,n}} \right)
\]

with a convex loss function \( L \) and a monotonically increasing function \( \rho \), which enjoys wide application in machine learning (Cucker and Smale, 2002; Hofmann et al., 2008). This also includes Bayesian kernel methods based on placing a prior on \( \mathcal{H}_{\kappa,n} \) (Tipping, 2001; Sollich, 2002; Chakraborty et al., 2012). These approaches implicitly assume that the prior distribution is supported on the finite-dimensional subspace \( \mathcal{H}_{\kappa,n} \) (see also Dunson, 2010 for details).

We point out that the finite-sample variant can be reduced to the setting \( p = 1 \) since \( \kappa_p \) and \( \kappa \) have the same eigenfunctions. This fact leads to simplified expressions and fast computation. Specifically, let \( K = U D U^\top \) be the eigenvalue decomposition, we can rewrite

\[
\kappa_M (x_i, x_j) = n^{-2p} \kappa(x_i, X) U D^{p-1} U^\top K_p U D^{p-1} U^\top \kappa(X, x_j).
\]

This is always possible because \( K \) is positive definite and hence \( D \) is invertible. For a centered \( f_n (\cdot) \) on the sample, it can be expressed as a linear combination of the centered representers \( \bar{\kappa} (\cdot, x_i) := \kappa (\cdot, x_i) - \sum_{j=1}^n \kappa (\cdot, x_j) / n \). Denote by \( \Gamma_n := I_n - n_1 1^\top_n / n \), we have \( \bar{\kappa} (\cdot, X) = \kappa (\cdot, X) \Gamma_n \). Using the parameterization \( \Sigma := n^{-2p} U D^{p-1} U^\top K_p U D^{p-1} U^\top \), the centered SIGP is simplified to

\[
f_n (\cdot) \sim \mathcal{GP} (0, \kappa (\cdot, X) \Gamma_n \Sigma \Gamma_n \kappa (X, \cdot)),
\]

where the matrix \( \Sigma \) is the parameter to be estimated.

### 2.3 Approximation with Sufficient Dimension Reduction Subspaces

Recall that the SIGP is supported on \( \mathcal{H}_{\kappa,n} \), we may intuitively adopt supervised dimension reduction of \( \mathcal{H}_{\kappa,n} \) to speedup the computation as well as reduce the variance in the prediction. A natural choice for this task is the sufficient dimension reduction (SDR) which is a state-of-the-art approach to supervised dimension reduction (Li, 1991; Cook and Weisberg, 1991; Cook, 1998; Fukumizu et al., 2004, 2009; Wu et al., 2009; Cook and Forzani, 2009). Below, we first briefly review the basics of the SDR.

**Background on SDR**  In a regression problem with response \( Y \) and covariate \( X \), the SDR aims to find a subspace \( S \) such that the projection of \( X \) onto \( S \) captures the statistical
dependency of $Y$ on $X$. The SDR is typically stated as the conditional independence

$$Y \perp X \mid \mathcal{P}_S X \quad \text{or} \quad P(Y \mid X) = P(Y \mid \mathcal{P}_S X) \quad (10)$$

where $\mathcal{P}_S$ denotes the orthogonal projection onto $S$. The SDR can be viewed as the supervised version of principle component analysis that takes into account the information of the response.

Suppose that $X \in \mathbb{R}^d$ and $S \in \mathbb{R}^{d \times m}$, and let $S_1^\top X, S_2^\top X, \ldots, S_m^\top X$ be the projection onto $S$. The SDR typically assumes that $X$ satisfies Condition 1, a property characterizing elliptically symmetric distributions such as the normal distribution (Eaton, 1983).

**Condition 1.** For any $a \in \mathbb{R}^d$, there exists $c_0 \in \mathbb{R}$ and $c \in \mathbb{R}^m$ such that $E(a^\top X \mid S^\top X) = c_0 + c^\top S^\top X$.

This condition leads to an important result stated in Theorem 2 which gives an algorithm for computing $S$ for an arbitrary unknown link function $f$ in (1).

**Theorem 2** (Li, 1991). Under assumption (10) and Condition 1, it holds that $E(X \mid Y) = \mathbb{E}X \in \text{span}(\text{Var}(X) S)$.

Theorem 2 implies that $S$ is given by the leading eigenvector of the generalized eigenvalue decomposition $\text{Var}(E(Y \mid X)) S = \text{Var}(X) S \Lambda$, where $\Lambda$ is the diagonal eigenvalue matrix. We will derive an RKHS variant of the theorem in Section 3.3.1, and show that the SIGP distribution satisfies the SDR assumptions. The intuition is that the analytical expression of the SIGP (7) is a linear combination of Gaussian random functions $\kappa_p(\cdot, x_i)$ which can be considered as the covariates in $\mathcal{H}_{\kappa,n}$.

**SDR Approximation to SIGP** We highlight two key results on the SDR approximation. First, the SIGP can be well-approximated with a low-rank SDR subspace when the eigenvalue of $\kappa$ decays at a faster rate than $O(1/n)$. This is consistent with the observation that many widely-used kernel operators have nearly exponential eigenvalue decay (Belkin, 2018). Second, we derive a log-likelihood

$$g(W) = -\frac{n}{2} \log \frac{\det(W^\top M W)}{\det(W^\top N W)} \quad (11)$$

for the SDR subspace of $\mathcal{H}_{\kappa,n}$ spanned by the basis

$$\sum_{i=1}^n W_{i1} \kappa(\cdot, x_i), \sum_{i=1}^n W_{i2} \kappa(\cdot, x_i), \ldots, \sum_{i=1}^n W_{im} \kappa(\cdot, x_i), \quad (12)$$

where $W$ specifies the coefficients of the basis functions of the SDR subspace, and $M$ and $N$ are computed from the kernel matrix $K$. The log-likelihood (11) extends the classic likelihood for SDR subspaces of $\mathbb{R}^d$ (Cook and Forzani, 2009) to the RKHS setting. These results will be proved in Section 3.

The approximation to the centered SIGP (9) using basis (12) is given by a random function $f_n \approx n^{-1} \sum_{j=1}^m \beta_j \sum_{i=1}^n W_{ij} \kappa(\cdot, x_i)$ with $\beta \sim \mathcal{N}(0, \Sigma_\beta)$, and the reproducing
With this approximation, we will instead estimate the parameters of the finite \( \beta \) in the approximated SIGP. It is worth pointing out that \( \Pi (z) := (\kappa (z, X) - 11^T_n K / n) W \) is the evaluation of the projection of the centered SIGP at \( z \). The approximate SIGP distribution is therefore

\[
    f_n (\cdot) \sim \mathcal{GP} \left( 0, \Pi (\cdot) \Sigma \Pi (\cdot)^T \right),
\]

(13)

In the subsequent sections, we will assume that the approximated SIGP (13) is used.

### 2.4 The Predictive Distribution

Let us first consider the predictive distribution of the vanilla SIGP (7). The posterior induced by the model (1) with the SIGP (7) is given by

\[
    \gamma (f_n | D) \propto \frac{\gamma (f_n; \kappa_p, \kappa_\nu)}{(2\pi)^{n/2} \sigma^n} \prod_{i=1}^n \exp \left( -\frac{1}{2\sigma^2} (y_i - f_n (x_i))^2 \right),
\]

(14)

where \( \gamma (f_n; \kappa_p, \kappa_\nu) \) denotes the SIGP prior on a sample \( \{x_i\}_{i=1}^n \). Thus, it remains to obtain the analytical expression of \( \gamma (f_n; \kappa_p, \kappa_\nu) \). Similar to Proposition 1, we have the covariance \( \text{Cov} (f_n (x_i), f_n (x_j)) = n^{-2p} [K^{\nu}K_\nu K^{\nu}]_{ij} \) where \( [K_\nu]_{ij} := \kappa_\nu (x_i, x_j) \) is the covariance matrix of \( \nu (\cdot) \). The SIGP prior is then expressed as the density of the multivariate Gaussian distribution \( \gamma (f_n; \kappa_p, \kappa_\nu) = \mathcal{N} (f | 0, n^{-2p} K^{\nu}K_\nu K^{\nu}) \). Denote by \( f := (f (x_1), f (x_2), \cdots, f (x_n))^T \) a column vector. The reproducing property yields \( f = K \alpha \) for some \( \alpha \in \mathbb{R}^n \). Substitute \( f = K \alpha \) into the SIGP prior density, we arrive at

\[
    \gamma (\alpha; \kappa_p, \kappa_\nu) = \mathcal{N} \left( \alpha \ igg| 0, n^{-2p} K^{p-1}K_\nu K^{p-1} \right).
\]

(15)

Combined with (14), one can select the kernel \( K_\nu \) using the maximum marginal likelihood method as in the standard GP (Rasmussen and Williams, 2006).

Now consider the the approximate SIGP (13). Denote by \( X_T \) and \( y_T \) the covariate matrix and response vector on the test set, respectively. The predictive distribution of \( y_T \) is a multivariate Gaussian, and we have the function covariance

\[
    \text{Cov} (f_n (X_T), f_n (X)) = \Pi (X_T) \Sigma \beta \Pi (X)^T.
\]

Denote by \( \Sigma_{ZY} := \text{Cov} (f_n (Z), f_n (Y)) \) the function covariance matrix, the mean of the predictive SIGP distribution is given by

\[
    \mathbb{E} (y_T | D) = u (X_T) + \Sigma_{X_T X} V^{-1} (y - u (X))
    = u (X_T) + \Pi (X_T) \hat{\beta},
\]
where \( u(X_T) \) is the mean function, and \( V := \Sigma_{XX} + \sigma^2 I \) represents the marginal variance of the SIGP.

Let \( P_Z = \Pi(Z) \Sigma_{\beta}^{1/2} \) such that \( \Sigma_{ZY} = P_Z P_Y^T \). The variance of the predictive distribution can be written

\[
\text{Var}(y_T | D) = \Sigma_{X_T X_T} - \Sigma_{X_T X} V^{-1} \Sigma_{XX_T} + \sigma^2 I
\]

\[
= P_{X_T} P_{X_T}^T - P_{X_T} P_X^T (P_X P_X^T + \sigma^2 I)^{-1} P_{X_T} + \sigma^2 I
\]

\[
= P_{X_T} P_{X_T}^T - P_{X_T} \left[ I - (\sigma^{-2} P_X^T P_X + I)^{-1} \right] P_{X_T}^T + \sigma^2 I
\]

\[
= \Pi(X_T) \Delta \Pi(X_T)^T + \sigma^2 I
\]

with \( \Delta := (\Sigma_{\beta} - 1)^{-1} \sigma^{-2} \Pi(X_T) \Pi(X_T)^T \) \( \in \mathbb{R}^{m \times m} \). We only need the diagonal elements of \( \text{Var}(y_T | D) \), among which the \( i \)-th diagonal entry is given by \( \| (\Pi(X_T) \Delta^{1/2}) e_i \|^2 + \sigma^2 \). These diagonal entries can be computed efficiently for low-rank SDR approximation with a small \( m \).

### 3 Theoretical Underpinnings and Results

In this section, we begin by providing the background on the RKHS as well as the function space of GPs. Then, we present the proofs for the main results outlined in Section 2.1 and Section 2.3. Finally, we derive a likelihood for the SDR approximation in the SIGP which can be of independent interest.

#### 3.1 Reproducing Kernel Hilbert Spaces and Gaussian Processes

We review some relevant concepts of the RKHS. More comprehensive exposition of the theory of RKHS can be found in e.g., (Aronszajn, 1950; Parzen, 1970; Cucker and Smale, 2002; Berlinet and Thomas-Agnan, 2003) and the references therein. An RKHS \( H \) is a Hilbert space of functions (on \( \mathcal{X} \)) with bounded evaluation functionals \( \delta_x(f) := f(x) \) for all \( f \in H \). Below, we recall three important properties of the RKHS.

First, the RKHS has the reproducing property. From Riesz representation theorem, the RKHS is “reproducing” in the sense that for every \( x \in \mathcal{X} \), there exists a unique representer function \( \phi(x) \in H \) satisfying

\[
(\forall f \in H) \quad f(x) = \langle f, \phi(x) \rangle_H,
\]

where \( \langle \cdot, \cdot \rangle_H \) denotes the inner product in \( H \). Each input data \( x \in \mathcal{X} \) is mapped to the corresponding representer function \( \phi(x) \) via the map \( \phi: \mathcal{X} \mapsto H \) which is commonly referred to as the feature map.

Another important property of the RKHS is the one-to-one correspondence between the RKHS and the kernel. Apply the reproducing property to \( \phi(x) \), one has

\[
[\phi(x)](x') = \langle \phi(x'), \phi(x) \rangle_H = \langle \phi(x), \phi(x') \rangle_H = [\phi(x')] (x).
\]
Suppose that $\mathcal{X}$ is a separable metric space, the reproducing kernel $\kappa : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ of $\mathcal{H}$ is a continuous symmetric function given by

$$\kappa (x, x') := \langle \phi (x), \phi (x') \rangle_\mathcal{H} = \langle \kappa (\cdot, x), \kappa (\cdot, x') \rangle_\mathcal{H}.$$ 

Note that $\kappa (\cdot, \cdot)$ is also positive semidefinite since for any countable subset $\{x_i\}$ dense in $\mathcal{X}$ and $\{a_i\} \subset \mathbb{R}$, we have $\sum_{i,j} a_i a_j \langle \phi (x_i), \phi (x_j) \rangle_\mathcal{H} = (\sum_{i=1}^{\infty} a_i \phi (x_i), \sum_{j=1}^{\infty} a_j \phi (x_j))_\mathcal{H} \geq 0$. This shows that for each RKHS $\mathcal{H}$, there is a unique symmetric positive semidefinite reproducing kernel $\kappa (\cdot, \cdot)$. The converse is also true — the Hilbert closure of

$$\left\{ \sum_{i=1}^{n} a_i \kappa (\cdot, x_i) \mid n \in \mathbb{N}, \{a_i\}_{i=1}^{n} \subset \mathbb{R}, \{x_i\}_{i=1}^{n} \subset \mathcal{X} \right\}$$

under the norm $\| \sum_{i=1}^{\infty} a_i \kappa (\cdot, x_i) \| = \sqrt{\sum_{i,j} a_i a_j \kappa (x_i, x_j)}$ is the unique RKHS $\mathcal{H}_{\kappa,n}$ of $\kappa (\cdot, \cdot)$ (Aronszajn, 1950).

Last but not least, the RKHS can be related to an $L^2(\mathcal{X}, \mathcal{B}, \mu)$ space $\mathcal{G}$ of measurable real-valued functions on $\mathcal{X}$ equipped with the inner product $\langle f, g \rangle_{L^2} := \int_{\mathcal{X}} f (x) g (x) d\mu (x)$ and the generated norm $\| f \|_{L^2} := \left( \int_{\mathcal{X}} (f (x))^2 d\mu (x) \right)^{1/2}$. Suppose that the kernel $\kappa$ is Hilbert-Schmidt, i.e., $\int_{\mathcal{X}} \int_{\mathcal{X}} \kappa (x, z) d\mu (x) d\mu (z) < \infty$, the Mercer’s theorem (Mercer, 1909) states

$$\kappa (x, z) = \sum_{i=1}^{\infty} \lambda_i e_i (x) e_i (z),$$

where convergence is absolute and uniform for a non-increasing sequence of eigenvalues $\{\lambda_i\}$ and the corresponding eigenfunctions $\{e_i\}$. These eigenfunctions are orthonormal and satisfy $\int_{\mathcal{X}} \kappa (x, z) e_i (z) d\mu (z) = \lambda_i e_i (x)$. From (18), there is an isomorphism between $\mathcal{H}$ and $\mathcal{G}$ under the linear map $\mathcal{F} \phi (x) := \sum_{i=1}^{\infty} \sqrt{\lambda_i} e_i (x) \left( \sqrt{\lambda_i} e_i \right)$. Thus, $\mathcal{G}$ consists of functions $\sum_{i=1}^{\infty} w_i \sqrt{\lambda_i} e_i$ for $w_i \in \mathbb{R}$. In particular, one can compute the RKHS inner product using (18) as $\langle \sum_{i=1}^{\infty} a_i \sqrt{\lambda_i} e_i, \sum_{i=1}^{\infty} b_i \sqrt{\lambda_i} e_i \rangle_\mathcal{H} = \sum_{i=1}^{\infty} a_i b_i$. For any function $\sum_{i=1}^{\infty} w_i \sqrt{\lambda_i} e_i$ in $\mathcal{H}$, it holds that $\sum_{i=1}^{\infty} w_i^2 < \infty$. This yields the following Mercer’s representation of $\mathcal{H}$:

$$\mathcal{G} = \left\{ \sum_{i=1}^{\infty} w_i \sqrt{\lambda_i} e_i \mid \sum_{i=1}^{\infty} w_i^2 < \infty \right\}.$$ (19)

Denote by $a_i := \int_{\mathcal{X}} f (x) e_i (x) d\mu (x)$, the constraint $\sum_{i=1}^{\infty} w_i^2 < \infty$ is alternatively written as $\sum_{i=1}^{\infty} a_i^2 / \lambda_i < \infty$. The Mercer’s representation (19) establishes a duality between the RKHS $\mathcal{H}$ and the corresponding $L^2$ space $\mathcal{G}$ in which GPs are typically defined.

### 3.1.1 Reproducing Kernel Hilbert Space of a Gaussian process

We now recall the function perspectives of GPs, focusing on its connection to the RKHS. Let $(\Omega, \mathcal{F}, P)$ be a probability space, where $\Omega$ is a sample space, $\mathcal{F}$ is an appropriate $\sigma$-algebra on $\Omega$, and $P$ is a probability measure. Denote by $L^2(\Omega, \mathcal{F}, P)$ the Hilbert space of real-valued square integrable random variables on $\Omega$:

$$L^2(\Omega, \mathcal{F}, P) := \left\{ Z : \Omega \mapsto \mathbb{R} : \int_{\Omega} |Z (\omega)|^2 dP (\omega) < \infty \right\}.$$
A GP \( f \in L^2(\mathcal{X} \times \Omega, \mathcal{F}, \mathbb{P}) \) is a family of Gaussian random variables \( \{ f(x) : x \in \mathcal{X} \} \) indexed by \( \mathcal{X} \). Fixing some \( \omega \in \Omega \), \( f(\cdot) := f(\cdot, \omega) \) is called a realization or a sample path of the GP. We will refer to the smallest Hilbert subspace of \( L^2(\Omega, \mathcal{F}, \mathbb{P}) \) that contains all sample paths as the Hilbert space spanned by the GP \( f \), or the Hilbert space of \( f \). The Hilbert space of \( f \) is related to an RKHS through the following Loève’s lemma.

**Lemma 1** (Loève, 1948). Let \( \{ f(x) : x \in \mathcal{X} \} \) be a centered second-order process with covariance \( k_f(x,z) := \mathbb{E}(f(x)f(z)) \). Then, the Hilbert space \( H_f \) of \( f \) is congruent to the RKHS \( H_{k_f} \) under the isometry \( \mathcal{L} : H_f \mapsto H_{k_f} \) given by

\[
(\mathcal{L} g)(x) := \mathbb{E}(g f(x)), \quad g \in H_f, \ x \in \mathcal{X}.
\]

The function space of GPs can be characterized via the duality specified by the Mercer’s representation (19) which states that a function is contained in RKHS \( H_k \) if and only if it can be expressed as \( f = \sum_{i=1}^{\infty} a_i e_i \in G \) for some \( \{a_i\} \) satisfying \( \sum_{i=1}^{\infty} a_i^2/\lambda_i < \infty \). Suppose that \( \{ f(z) : z \in \mathcal{X} \} \) is a zero-mean GP with Hilbert-Schmidt covariance kernel \( k(x,z) := \mathbb{E}(f(x)f(z)) \). Then it follows from (18) that \( \sum_{i=1}^{\infty} a_i^2 = \lambda_i \). This is formalized by the Karhunen-Loève expansion (Ghanem and Spanos, 1991) which states that \( f(x) \) has the following expansion:

\[
f(x) = \sum_{i=1}^{\infty} a_i e_i(x) \in L^2(\mathcal{X}, \mathcal{F}, \mathbb{P}), \quad a_i := \int_{\mathcal{X}} f(x) e_i(x) d\mathbb{P}(x)
\]

and the coefficients \( a_i \) are mutually uncorrelated random variables with

\[
\mathbb{E}a_i = 0, \quad \mathbb{E}a_i^2 = \lambda_i,
\]

where convergence is in quadratic mean.

For Gaussian processes, \( a_i \) are independent and distributed as \( a_i \sim \mathcal{N}(0, \lambda_i) \). Often times, the eigenfunctions \( e_i \) are difficult to compute and may not have closed analytic expressions. One can alternatively use a few basis functions \( \psi_i : \mathcal{X} \mapsto \mathbb{R} \) in \( G \), and this leads to the function-space view of GPs (Williams, 1997):

\[
f(x) = \sum_{i=1}^{\infty} a_i \psi_i(x), \quad \alpha \sim \mathcal{N}(0, \Sigma),
\]

where we slightly abused the notation to write \( a_i \) for the coefficients associated with \( \psi_i \). The covariance kernel under the above GP specification is given by

\[
\text{Cov}(f(x), f(z)) = \psi_x^\top \Sigma_x \psi_z, \quad \psi_x = (\psi_1(x), \psi_2(x), \cdots)^\top.
\]

**3.2 Proof of Theorems**

We now provide the missing proofs in Section 2.1 and Section 2.3. Recall that Proposition 2 states that as \( p \) increases the space of functions realizable by the IGP shrinks. This holds in general for a GP \( \nu \) in either an RKHS generated by a kernel \( \kappa_q \), \( q \geq 0 \), or the \( L^2(\mathcal{X} \times \Omega, \mathcal{F}, \mathbb{P}) \), as shown by the following simple Proposition 3.
Proposition 3. Let \( \{e_i\} \) and \( \{\lambda_i\} \) be the eigenfunctions and eigenvalues of the kernel \( \kappa \). For any function \( h \in \left\{ \sum_{i=1}^{\infty} w_i e_i : \sum_{i=1}^{\infty} w_i^2 / \lambda_i^{2p+q} < \infty \right\} \) and \( q \geq 0 \), the curve \( h(\cdot) \) is a sample path of the IGP (3) with kernel \( \kappa \) and some \( \nu \in \mathcal{H}_{\kappa_q} \).

Proof. By Mercer’s representation (19) of the RKHS, any sample path \( h \) of the IGP admits the representation \( h = \sum_{i=1}^{\infty} a_i e_i \) with \( a_i = \int_X h(x) e_i(x) d\mu(x) \). Similarly, we can also express \( \nu \) as \( \nu = \sum_{i=1}^{\infty} b_i e_i \) with \( \sum_{i=1}^{\infty} b_i^2 / \lambda_i^q < \infty \). Now rewrite \( h \) in the form of (3), we have \( \varphi_i = a_i / \lambda_i^p \). Together with the condition \( \nu \in \mathcal{H}_{\kappa_q} \), we obtain \( \sum_{i=1}^{\infty} \varphi_i^2 / \lambda_i^q = \sum_{i=1}^{\infty} a_i^2 / \lambda_i^{2p+q} < \infty \), completing the proof.

Note that Proposition 2 is the special case of Proposition 3 with \( q = 0 \) where \( \mathcal{H}_{\kappa_q} \) is equivalent to the \( L^2 \) for a non-degenerate kernel \( \kappa \).

As for the proof of Theorem 1, we first construct an RKHS \( \mathcal{H}_{\kappa_0}' \) that contains \( \mathcal{H}_{\kappa_M} \) using Lemma 2. Then, we use the dominance operator argument in Lemma 3 to show that sample paths of \( \mathcal{H}_{\kappa_0}' \) are contained in \( \mathcal{H}_{\kappa} \).

Lemma 2 (Aronszajn, 1950). \( \mathcal{H}_{\kappa'} \subset \mathcal{H}_{\kappa} \) if there is a constant \( C < \infty \) such that \( C^2 \kappa - \kappa' \) is a nonnegative kernel.

Lemma 3 (Lukić and Beder, 2001). Let \( \{f(x) : x \in \mathcal{X}\} \) be a Gaussian process with covariance kernel \( k_f \) and let \( \mathcal{H}_{\kappa} \) be an RKHS with reproducing kernel \( \kappa \). Then, a sufficient and necessary condition for \( P(f(\cdot) \in \mathcal{H}_{\kappa}) = 1 \) is that there exists a trace class dominance operator \( \mathcal{T} : \mathcal{H}_{\kappa} \to \mathcal{H}_{\kappa} \) with range contained in \( \mathcal{H}_f \) and satisfies

\[
(\forall f \in \mathcal{H}_{\kappa}, \forall g \in \mathcal{H}_f) \quad \langle f, g \rangle_{\mathcal{H}_{\kappa}} = \langle \mathcal{T} f, g \rangle_{\mathcal{H}_f}.
\]

Note that if the kernel operator of \( \kappa_{\nu} \) has a finite number of nonzero eigenvalues, i.e., \( \kappa_{\nu} \) is degenerate, \( \kappa_M \) will also be degenerate and \( \mathcal{H}_{\kappa_M} \subset \mathcal{H}_{\kappa} \). Thus, we only need to consider the case where \( \kappa_{\nu} \) is non-degenerate. The following theorem provides a sufficient condition for the IGP sample paths to be contained in \( \mathcal{H}_{\kappa} \).

Theorem 3. Let \( f \in L^2(\mathcal{X} \times \Omega, \mathcal{F}, P) \) be an IGP specified by prior \( \gamma(f; \kappa_p, \kappa_{\nu}) \). It holds that \( P(f(\cdot) \in \mathcal{H}_{\kappa}) = 1 \) if the kernel \( \kappa_{2p-1} \) is of trace class.

Proof. First, we show that the mean (4) is contained in \( \mathcal{H}_{\kappa} \). Denote by \( \{e_i\} \) the complete set of orthonormal eigenfunctions of \( \kappa \) corresponding the non-increasing sequence of eigenvalues \( \{\lambda_i\} \), and let \( a_i = \int_X (\mathbb{E} f(x)) e_i(x) d\mu(x) \). We have

\[
a_i^2 = \left( \lambda_i^p \int_X [\mathbb{E} \nu(x)] e_i(x) d\mu(x) \right)^2 = \lambda_i^{2p} \mathbb{E} \langle \nu, e_i \rangle_{L^2}^2 \leq \lambda_i^{2p} \mathbb{E} \langle \nu, e_i \rangle_{L^2}^2,
\]

where the last inequality follows from Jensen’s inequality. From Mercer’s representation (19), the squared RKHS norm of the mean function is given by \( \|f\|_{\mathcal{H}_{\kappa}}^2 = \sum_{i=1}^{\infty} a_i^2 / \lambda_i \leq \sum_{i=1}^{\infty} \lambda_i^{2p-1} \mathbb{E} \langle \nu, e_i \rangle_{L^2}^2 \). By Parseval’s identity, \( \sum_{i=1}^{\infty} \lambda_i^{2p-1} \mathbb{E} \langle \nu, e_i \rangle_{L^2}^2 = \lambda_1^{2p-1} \mathbb{E} \|\nu\|_{L^2}^2 < \infty \), yielding \( \mathbb{E} f \in \mathcal{H}_{\kappa} \) as desired.

Let \( \lambda_1' \) denote the largest eigenvalue of the kernel operator of \( \kappa_{\nu} \), it is easy to verify that \( \lambda'_M(x,z) := \lambda_1' \sum_{i=1}^{\infty} \lambda_i^{2p} e_i(x) e_i(z) \) is a kernel that satisfies \( \lambda'_M - \lambda_M \) is nonnegative definite. By Lemma 2, we then have \( \mathcal{H}_{\kappa_M} \subset \mathcal{H}_{\lambda'_M} \).
Now we use the dominance operator in Lemma 3 to show that sample paths of \( \mathcal{H}_{\kappa, n} \) are contained in \( \mathcal{H}_{\kappa} \). Denote by \( \mathcal{T}: \mathcal{H}_{\kappa} \rightarrow \mathcal{H}_{\kappa} \) the dominance operator. From Mercer’s representation (19), the complete orthonormal basis of \( \mathcal{H}_{\kappa} \) and \( \mathcal{H}_{\kappa, M} \) are respectively \( \{\sqrt{\lambda_i} e_i\} \) and \( \{\sqrt{\lambda_i^p} e_i\} \). Recall that the dominance operator satisfies

\[
(\forall i \in \mathbb{N}) \quad \left\langle \mathcal{T} \sqrt{\lambda_i} e_i, \sqrt{\lambda_i} e_i \right\rangle_{\mathcal{H}_{\kappa, M}} = \left\langle \sqrt{\lambda_i} e_i, \sqrt{\lambda_i} e_i \right\rangle_{\mathcal{H}_{\kappa}} = \sqrt{\lambda_i^p}. 
\]

We obtain \( \mathcal{T} \sqrt{\lambda_i} e_i = \sqrt{\lambda_i^p} \sqrt{\lambda_i} e_i \), for all \( i \in \mathbb{N} \). Thus, the trace of \( \mathcal{T} \) is given by \( \sum_{i=1}^{\infty} \left\langle \mathcal{T} \sqrt{\lambda_i} e_i, \sqrt{\lambda_i} e_i \right\rangle_{\mathcal{H}_{\kappa}} = \lambda_i^p \sum_{i=1}^{\infty} \lambda_i < \infty \), which holds for trace class \( \kappa_{2p-1} \). Invoking Lemma 3 completes the proof.

Theorem 4 states that if the reproducing kernel \( \kappa \) of the SIGP function space \( \mathcal{H}_{\kappa, n} \) has fast eigenvalue decay, then \( \mathcal{H}_{\kappa, n} \) can be well-approximated by a low-rank SDR subspace, and hence the approximate SIGP (13) has a low-rank covariance.

**Theorem 4.** Under the assumption (10) and let \( \tau_1 \geq \tau_2 \geq \cdots \geq \tau_n \) be the eigenvalues for \( \text{Var}(\mathbb{E}(Y \mid X)) S = \tau_i \text{Var}(X) S_i \). Then, with probability at least \( 1 - \delta \) the true SDR rank \( m_* \) for the model (1) with the SIGP prior (9) satisfies

\[
\tau_{m_*} \geq \frac{1}{n} - \sqrt{\frac{8}{n^3 \log \frac{2}{\delta}}}. 
\]  
(24)

**Proof.** We first start with a result (Theorem 5.1 of Li, 1991) which states that \( n \sum_{i=m_*+1}^{n} \tau_i \) follows a chi-squared distribution with \( (n - m_*) (s - m_* - 1) \) degree of freedom, where \( s \) is the number of slices used for computing the sample \( \text{Var}(\mathbb{E}(Y \mid X)) \). Set \( s = m_* + 2 \) to get \( n \sum_{i=m_*+1}^{n} \tau_i \sim \chi^2_{n-m_*} \). It can be easily shown that \( \chi^2_k \) is sub-exponential with the tail bound

\[
P\left(|\chi^2_k/k - 1| \geq t\right) \leq 2 \exp\left(-nt^2/8\right), \quad \forall 0 < t < 1.
\]

Denote by \( \overline{\tau} = \sum_{i=m_*+1}^{n} \tau_i / (n - m_*) \), we obtain from the tail bound that

\[
\left| \overline{\tau} - \frac{1}{n} \right| \leq \frac{1}{n} \sqrt{\frac{8}{n \log \frac{2}{\delta}}} \quad (25)
\]

holds with probability at least \( 1 - \delta \). From (25) and note that \( \tau_{m_*} \geq \overline{\tau} \), we arrive at (24). 

**3.3 The Likelihood over SDR Subspaces of \( \mathcal{H}_{\kappa, n} \)**

In this section, we derive the likelihood over SDR subspaces of the RKHS. Our point of departure is provided by Lemma 4 proposed in (Cook and Forzani, 2009) which specifies the likelihood over SDR subspace in \( \mathbb{R}^d \). Cook and Forzani (2009) showed that the likelihood achieves more robust SDR subspace estimation compared to the generalized eigenvalue decomposition implied by Theorem 2 which essentially yields the intersection of SDR subspaces known as the central subspace (Cook, 1998).
Lemma 4 (Cook and Forzani, 2009). Consider the regression problem with the response $Y \in \mathbb{R}$ and covariates $X \in \mathbb{R}^d$. If the conditional distribution $X \mid Y$ is normal, then the log-likelihood for the SDR subspace spanned by the columns of $S$ is given by

$$l(S) \propto -\frac{1}{2} \sum_y n_y \log \det \left[ S^\top \text{Var}(X \mid y) S \right] + \frac{n}{2} \log \det \left[ S^\top \text{Var}(X) S \right]$$

(26)

where $y$ is the index over the slices of the range of $Y$, and $n_y$ denotes the number of data points in the slice.

Here we denote by $S$ the SDR basis of $\mathbb{R}^d$ in contrast to the SDR basis $W$ in the RKHS setting. Similar to (Li, 1991), Cook’s method also computes the sample $\text{Var}(X \mid Y)$ by slicing the range of $Y$, and $\text{Var}(X \mid y)$ in Lemma 4 represents the sample variance of $X$ within the $y$-th slice.

We show in Theorem 5 an equivalent form of the Cook’s likelihood (26), but with an explicit maximizer. We first give the likelihood over SDR subspaces of $\mathbb{R}^d$, and then extend the result to the RKHS setting in Section 3.3.1.

Theorem 5. Under the same conditions of Lemma 4, the likelihood for the SDR subspace with basis $S \in \mathbb{R}^{d \times m}$ is written

$$g(S) \propto -\frac{n}{2} \log \frac{\det \left[ S^\top \mathbb{E}(\text{Var}(X \mid Y)) S \right]}{\det (S^\top \text{Var}(X) S)}$$

(27)

Proof. We will use the SDR subspace characterization given by Proposition 1(i) of (Cook and Forzani, 2009), which states

$$S^\top \text{Var}^{-1}(X \mid Y) = S^\top \mathbb{E}^{-1}(\text{Var}(X \mid Y)),$$

(28)

where $S_\perp$ denotes the orthogonal complement of $S$. It is clear that $g(S)$ is invariant to linear transformations of $S$, thus we can assume without loss of generality that $S$ is semi-orthogonal.

The following identity (29) is from (Rao, 1973): Let $A \in \mathbb{R}^{p \times n}$ be of rank $n$ and let $S \in \mathbb{R}^{p \times (p-n)}$ be of rank $p-n$ such that $A^\top B = 0$. Then

$$\Sigma = B \left( B^\top \Sigma^{-1} B \right)^{-1} B^\top + \Sigma A \left( A^\top \Sigma A \right)^{-1} A^\top \Sigma.$$

(29)

Note that if both $A$ and $B$ are semi-orthogonal, then due to (29):

$$S^\top \Sigma S - S^\top \Sigma S_\perp \left( S^\top \Sigma S_\perp \right)^{-1} S^\top_\perp \Sigma S = \left( S^\top \Sigma^{-1} S \right)^{-1}.$$

Observe that the left hand side is the Schur’s complement. We then rewrite $\det(\Sigma)$ as

$$\det \left( \begin{bmatrix} S & S_\perp \end{bmatrix}^\top \Sigma \begin{bmatrix} S & S_\perp \end{bmatrix} \right) = \det \left( \begin{bmatrix} S^\top \Sigma S & S^\top \Sigma S_\perp \\ S_\perp^\top \Sigma S & S_\perp^\top \Sigma S_\perp \end{bmatrix} \right) = \det \left( S^\top \Sigma S_\perp \right) \det \left( S_C \right),$$

15
where $S_C := S^T \Sigma S - S^T \Sigma S_{\perp} (S_{\perp}^T \Sigma S_{\perp})^{-1} S_{\perp}^T \Sigma S$ is the Schur’s complement. We obtain
\[
\det (S_{\perp}^T \Sigma S_{\perp}) = \det (\Sigma) \det (S_{\perp}^T \Sigma S_{\perp})^{-1}
\]
Together with (28), we have
\[
\det \left[ S^T \text{Var} (X | y) S \right] = \det (\Sigma) \det \left[ S^T \text{Var} (X | y) S \right].
\]
Note that $\sum_y n_y \log \det \left[ S^T \text{Var} (X | y) S \right] = n \mathbb{E} \left\{ \log \det \left[ S^T \text{Var} (X | y) S \right] \right\}$ in (26). Also, (30) yields
\[
\mathbb{E} \left\{ \log \det \left[ \text{Var} (X | y) S \right] \right\} = \log \det \left[ \text{Var} (X | y) S \right] + \log \det (\Sigma) + \mathbb{E} \left\{ \log \det \left[ \text{Var} (X | y) \right] \right\}.
\]
The first term on the right is the numerator in (27), and the last two terms do not involve $S$. This shows that $g (S) - l (S)$ is a constant. By Lemma 4, $g (S)$ gives unbiased estimation of the SDR subspace.

The utility of Theorem 5 is that the log-likelihood (27) has an explicit maximizer $S_*$ whose columns are the leading eigenvectors of $\Sigma^{-1} \left( \text{Var} (X | Y) \right) \Sigma (X)$. This is an immediate consequence of the following Lemma 5.

**Lemma 5.** For positive definite matrices $M, N \in \mathbb{R}^{n \times n}$, the column space of an optimal full-rank $S_* \in \mathbb{R}^{n \times m}$, $m \leq n$, for
\[
\min_S \frac{\det (S^T MS)}{\det (S^T NS)}
\]
coincides with the span of the d leading eigenvectors of $M^{-1} N$.

**Proof.** Since $M$ is positive definite, we denote by $S = M^{-1/2} T$ and let $T = QR$ be the QR decomposition. Observe that both $S$ and $R$ are of full rank. The objective of (31) can be rewritten as
\[
\frac{1}{\det (Q^T M^{-1/2} N M^{-1/2} Q)}.
\]
The minimum is attained by setting the columns of $Q$ to the leading eigenvectors of $M^{-1/2} N M^{-1/2}$. Then, the columns of $M^{-1/2} Q$ are the leading eigenvectors of $M^{-1} N$, and the column space of $S = M^{-1/2} T = (M^{-1/2} Q) R$ is the same as the eigenspace spanned by the leading eigenvectors of $M^{-1} N$.

The log-likelihood (27) has several desirable properties. First, $g (S) = g (S')$ whenever $S$ and $S'$ are bases of the same subspace. Thus, the maximizer $S_*$ for (27) is not unique, but they span the same SDR subspace. Second, the log-likelihood yields the same $S_*$ as Fisher linear discriminant analysis (FDA) for two groups, i.e., $Y$ is binary, when $S$ is a vector. In this case,
\[
g (S) \propto - \log \left( 1 - \frac{S^T \text{Var} (\mathbb{E} (X | Y)) S}{S^T \text{Var} (X) S} \right),
\]
where the fraction in (32) is the objective of FDA. Moreover, Proposition 4 states that the SDR subspace basis given by the sliced inverse regression (SIR) (Li, 1991) are in the vector space spanned by a maximizer of (27).
Proposition 4. Suppose that \( \mathbb{E} ( \text{Var} (X \mid Y) ) \) and \( \text{Var} (X) \) are positive definite. Then, the column space of a maximizer \( S \) to \( g(S) \) contains the central subspace estimated by the sliced inverse regression.

Proof. The SIR solves for the basis \( b_i \) of the SDR (central) subspace via the following generalized eigenvalue decomposition:

\[
\text{Var} (\mathbb{E} (X \mid Y)) b_i = \tau_i \text{Var} (X) b_i.
\]

The variance decomposition gives \([\text{Var} (X) - \mathbb{E} (\text{Var} (X \mid Y))] b_i = \tau_i \text{Var} (X) b_i\). Rearrange the terms, we obtain

\[
[\mathbb{E} (\text{Var} (X \mid Y))]^{-1} \text{Var} (X) b_i = \frac{1}{1 - \tau_i} b_i.
\]

From Theorem 5 and Lemma 5, \( S \), is specified by the eigenvectors of (34). Clearly, any eigenvector \( b_i \) of (33) corresponding to a nonzero eigenvalue is an eigenvector of (34). However, when \( \mathbb{E} (X \mid Y) \equiv 0 \), (33) fails to recover the SDR direction \( b_i \) corresponding to the \( \tau_i = 0 \) as reported in (Cook and Weisberg, 1991). Note that we have \( \tau_i < 1 \) due to the variance decomposition. Thus, the central subspace basis given by SIR corresponding to the largest \( \tau_i \) are also the leading eigenvectors of (34).

3.3.1 Extension to RKHS

Theorem 5 can be extended to the RKHS setting under an analogous Condition 2 to Condition 1. The condition is basically a restatement of Condition 1 in terms of the basis \( \kappa (\cdot, x_1), \ldots, \kappa (\cdot, x_n) \) of the finite-dimensional subspace of \( \mathcal{H}_K \). It has been shown that Condition 2 is fairly reasonable in the setting of cross-covariance operators on Hilbert spaces (Fukumizu et al., 2004). Recall that the SDR subspace of the RKHS is spanned by (12), we aim to estimate the basis coefficients \( W \) on a finite sample.

Condition 2. Suppose that \( \kappa \) is of trace class. For any \( f (\cdot) = \sum_{i=1}^n a_i \kappa (\cdot, x_i), \{a_i\}_{i=1}^n \subset \mathbb{R} \), there exists \( \{c_i\}_{i=0}^m \subset \mathbb{R} \) such that \( \mathbb{E} (f (x) \mid \sum_{i=1}^n W_{ij} \kappa (x, x_i), \ldots, \sum_{i=1}^n W_{im} \kappa (x, x_i)) = c_0 + \sum_{j=1}^m c_j \sum_{i=1}^n W_{ij} \kappa (x, x_i) \) for all \( x \in \mathcal{X} \).

Denote by \( \phi := (\kappa (\cdot, x_1), \ldots, \kappa (\cdot, x_n)) \) the feature vector on the sample \( \{x_i\}_{i=1}^n \), and \( \bar{\phi} := (\bar{\kappa} (\cdot, x_1), \ldots, \bar{\kappa} (\cdot, x_n)) = \phi \Gamma_n \) the centered feature vector with \( \bar{\kappa} (\cdot, x_i) \) and \( \Gamma_n \) as defined in (9). Observe that \( K = \phi^\top \phi \) and \( \Gamma_n \) is idempotent. In the following, we provide two methods for estimating \( W \).

First consider a slicing based estimation of \( W \) as in SIR. Suppose that the data \( \mathcal{D} \) is sorted by the response value. Partition the data into slices \( \{(x_1, y_1), \ldots, (x_{n_1}, y_{n_1})\}, \{(x_{n_1+1}, y_{n_1+1}), \ldots, (x_{n_1+n_2}, y_{n_1+n_2})\}, \) and so forth, where \( n_i \) denotes the size of the \( i \)-th slice. We replace \( X \) with \( \bar{\phi} \) in the log-likelihood (27), and compute \( \mathbb{E} (\text{Var} (\phi \mid Y)) \) as the weighted average of the slice sample variances. Specifically, we have

\[
\text{Var} (\phi) = \frac{1}{n} \bar{\phi} \bar{\phi}^\top = \frac{1}{n} \phi \Gamma_n \phi^\top
\]

\[
\mathbb{E} (\text{Var} (\phi \mid Y)) = \phi \left[ \frac{1}{n} J_n - \frac{1}{n} \text{diag} \left( \frac{1_{n_i} 1_{n_i}^\top}{n_i} \right) \right] \phi^\top = \frac{1}{n} \phi \text{diag} (\Gamma_{n_i}) \phi^\top,
\]
where $\text{diag}(\Gamma_n)$ denotes the block diagonal matrix with diagonal blocks $\Gamma_n$. Thus, the log-likelihood (27) over SDR subspaces of the RKHS is written

$$g(W) = -\frac{n}{2} \log \frac{\det(W^\top MW)}{\det(W^\top NW)}$$

with $M := K\text{diag}(\Gamma_n) + n\zeta K$ and $N := K\Gamma_n K$. Here, $M$ is obtained by adding a small constant $\zeta$ to $E(\text{Var} (\phi | Y))$ in order for the conditions of Proposition 4 to hold. It is well-known that adding the constant imposes Tikhonov regularization on $W$ from the Lagrange multiplier perspective.

Under some mild conditions, the sample $E(\text{Var} (\phi | Y))$ can be computed without slicing as stated in the following theorem.

Theorem 6 (Fukumizu et al., 2004). Assume $\kappa$ is of trace class, and there exists a function $f_Y : \mathbb{R} \mapsto \mathbb{R}$ in an RKHS $H_{\kappa Y}$ with trace class reproducing kernel $\kappa_Y$ satisfying $E(f(x) | y) = f_Y(y)$ for any $f \in H_{\kappa}$ and almost every $y$, then

$$E(\text{Var}(\phi(X) | Y)) = \text{Var}(\phi(X)) - \text{Cov}(\phi(X), Y) \text{Var}^{-1}(Y) \text{Cov}(Y, \phi(X)).$$

Let $K_{\kappa_Y}$ be the kernel matrix generated by the response $\{y_i\}_{i=1}^n$ and $\kappa_Y$. Denote by $\phi_Y := (\kappa_Y(\cdot, y_1), \cdots, \kappa_Y(\cdot, y_n))$, then it follows from Theorem 6

$$E(\text{Var}(\phi | Y)) = \frac{1}{n} \phi \Gamma_n \phi^\top - \frac{1}{n^2} \phi \Gamma_n \phi^\top \left( \frac{1}{n} \phi \Gamma_n \phi^\top + \zeta_1 I \right)^{-1} \phi \Gamma_n \phi^\top$$

$$= \frac{1}{n} \phi \Gamma_n \phi^\top - \frac{1}{n} \phi \left( \Gamma_n K_{\kappa_Y} \Gamma_n + n\zeta_1 I \right)^{-1} \Gamma_n K_{\kappa_Y} \Gamma_n \phi^\top$$

$$= \frac{1}{n} \phi \left[ \Gamma_n - (K_{\kappa_Y} + n\zeta_1 I)^{-1} K_{\kappa_Y} \right] \phi^\top,$$

where $K_{\kappa_Y} := \Gamma_n K_{\kappa_Y} \Gamma_n$ represents the centered kernel matrix of $y$ (see e.g., Schölkopf et al., 1998), and $\zeta_1 > 0$ is a small constant added to ensure the positive definiteness of $\text{Var}(Y)$. Note that $\Gamma_n$ is symmetric as well as idempotent in deriving the second equality.

4 Algorithms for Parameter Inference

In this section, we develop fast algorithms for estimating the parameters of the SIGP (13). Learning the IGP (3) can be carried out similarly as in training the standard GP by maximizing the marginal likelihood (14) (Rasmussen and Williams, 2006).

The estimation task is to infer parameters of both the mean function and (13), namely the SDR basis $W$, $\Sigma_\beta$, as well as $\sigma^2$. Specifically, the estimation of $W$ uses the log-likelihood (11), and can be computed directly by Lemma 5. In addition, inference of the covariance parameters leverages the low-rank SDR parameterization via an Expectation-Maximization (EM) algorithm. While $\kappa$ is assumed to be given and fixed, inferring the hyper-parameters of $\kappa$ is also possible.
4.1 Selecting the Sufficient Dimension Reduction Subspace

Recall the log-likelihood (11) of the SDR subspace basis $W$, whose maximizer from Lemma 5 is given by the leading eigenvectors for the generalized eigenvalue decomposition

$$\Gamma_n K W = \tau_i (A + n \zeta I_n) W_i,$$

(36)

where $\Gamma_n$ is as defined in (9), $\zeta > 0$ is a regularization parameter, and $A$ is computed from the kernel matrix $K$ discussed next.

As we discussed in Section 3.3.1, there are two ways for computing $A$: 1) a fast slicing-based approach as in the sliced inverse regression; and 2) the method that uses an additional kernel of the response $Y$ which potentially yields improved estimates in regression by exploiting the local information in $Y$.

For the slicing-based approach, first partition the data into slices $\{(x_1, y_1), \ldots, (x_{n_1}, y_{n_1})\}, \{(x_{n_1+1}, y_{n_1+1}), \ldots, (x_{n_1+n_2}, y_{n_1+n_2})\},$ and so forth, where $n_i$ denotes the size of the $i$-th slice. Then, let $A = \text{diag} (\Gamma_n) K_i$ and solve the generalized eigenvalue decomposition (36). The overall computational complexity in this case is $O(n^2 m)$. As for the other method, the sorting is not needed, but instead a kernel matrix $\bar{K}_{\kappa Y}$ for $Y$ is needed. We will instead let $A = \Gamma_n K - (\bar{K}_{\kappa Y} + n \zeta I)^{-1} \bar{K}_{\kappa Y} K$ in (36), where $\zeta > 0$ is a constant for the inverse to be well-defined (see also Fukumizu et al., 2004). Clearly, the computational complexity for solving the slicing-free SDR estimation is $O(n^3)$.

4.2 Estimating the Covariance via Expectation Maximization

The SIGP regression model (1) with the approximate SIGP prior (13) can be viewed as a latent variable model $Y(\cdot) \sim u(\cdot) + \Pi(\cdot) \beta + \epsilon$, where $u$ is the mean function and $\beta \sim N(0, \Sigma_\beta)$ is a latent vector. Intuitively, we may consider an EM algorithm for estimating the variance components $\Sigma_\beta$ as well as $\sigma^2$. Parameter inference for the mean can also be performed during the M-step. For ease of exposition, we will use the mean function $u(\cdot) = \Pi(\cdot) \alpha + c$ with parameters $\alpha$ and $c$.

First, the log-likelihood of the SIGP regression model after dropping irrelevant terms is written

$$l(\Sigma_\beta, \sigma^2) \propto -\frac{1}{2} \log \det \Sigma_\beta - \frac{n}{2} \log \sigma^2 - \frac{1}{2} \beta^\top \Sigma_\beta^{-1} \beta - \frac{\epsilon^\top \epsilon}{2\sigma^2}.$$  

(37)

For notational convenience, denote by $\Pi := \Pi(X) = \Gamma_n K W$. From the latent variable model view of the SIGP, we obtain the posterior distribution of $\beta$

$$\mathcal{N} \left( \hat{\Sigma}_\beta \Pi^\top \hat{V}^{-1} (y - u(X)), \hat{\Sigma}_\beta - \hat{\Sigma}_\beta \Pi^\top \hat{V}^{-1} \Pi \hat{\Sigma}_\beta \right).$$  

(38)

The above posterior distribution gives the MAP estimator $\hat{\beta}$ for the latent variable, which will be used in the M-step. Let $\hat{r} := y - u(X)$ denote the random effect, the MAP estimator $\hat{\beta}$ can be equivalently expressed as

$$\hat{\beta} = \left( \sigma^2 \hat{\Sigma}_\beta^{-1} + \Pi^\top \Pi \right)^{-1} \Pi^\top \hat{r} = \sigma^{-2} \hat{\Delta} \Pi^\top \hat{r}$$  

(39)
Algorithm 1: EM algorithm for learning the SIGP

Input: \( K, y \), SDR rank \( m \) as well as regularization parameter \( \zeta, \xi \)

Output: \( \hat{\alpha}, \hat{c}, \hat{\Sigma}_\beta, \hat{\sigma}^2 \)

[1] Estimate \( W \) by solving generalized eigenvalue decomposition (36);
[2] Initialize \( \Pi := \Gamma_nKW, \Lambda := \Pi^\top\Pi \);

repeat

[3] \( \hat{V}^{-1} \leftarrow \hat{\sigma}^{-2} \left[ I - \Pi \left( \hat{\sigma}^2 \hat{\Sigma}_\beta^{-1} + \Lambda \right)^{-1} \Pi^\top \right] \);
[4] \( \hat{L} \leftarrow I - 11^\top \hat{V}^{-1} \left( 1^\top \hat{V}^{-1} 1 \right)^{-1} \);
[5] \( \hat{\alpha} \leftarrow \left( \Pi^\top \hat{V}^{-1} \hat{L} \Pi + n\xi W^\top KW \right)^{-1} \Pi^\top \hat{V}^{-1} \hat{L} y \);
[6] \( \hat{\Delta} \leftarrow \left( \hat{\Sigma}_\beta^{-1} + \Lambda/\hat{\sigma}^2 \right)^{-1} \);
[7] \( \hat{\beta} \leftarrow \hat{\sigma}^{-2} \hat{\Delta} \Pi^\top (y - \Pi \hat{\alpha} - 1\hat{c}) \);
[8] \( \hat{\Sigma}_\beta \leftarrow \hat{\beta} \hat{\beta}^\top + \hat{\Delta} \);
[9] \( \hat{\sigma}^2 \leftarrow \hat{\sigma}^2 + n^{-1} \left( \| y - \Pi (\hat{\beta} + \hat{\alpha}) - 1\hat{c} \|^2 - \hat{\sigma}^4 \text{tr} \hat{V}^{-1} \right) \);

until log-likelihood (37) converges;

where \( \hat{\Delta} \) is as defined in (16).

By taking the expectation of (37) with respect to the posterior distribution (38), we arrive at the E-step:

\[
\mathbb{E}_{\beta|D} \left[ l \left( \Sigma_\beta, \sigma^2 \right) \right] \propto -\frac{1}{2} \log \det \Sigma_\beta - \frac{n}{2} \log \sigma^2 - \frac{1}{2} \hat{\beta}^\top \Sigma_\beta^{-1} \hat{\beta} - \frac{1}{2} \text{tr} \hat{\Delta} \Sigma_\beta^{-1} \\
- \frac{1}{2\sigma^2} \left( \| \hat{r} - \Pi \hat{\beta} \|^2 + \text{tr} \left( \Pi \hat{\Delta} \Pi^\top \right) \right),
\]

where we used the fact that the covariance of (38) satisfies \( \hat{\Sigma}_\beta - \hat{\Sigma}_\beta \Pi^\top \hat{V}^{-1} \Pi \hat{\Sigma}_\beta = \left( \hat{\Sigma}_\beta^{-1} + \hat{\sigma}^{-2} \Pi^\top \Pi \right)^{-1} = \hat{\Delta} \). Also note that \( \hat{\beta} \) and \( \hat{\Delta} \) are computed based on the estimated \( \hat{\Sigma}_\beta \) and \( \hat{\sigma}^2 \) from the previous iteration.

The M-step maximizes the expectation given in the E-step. The optimization is straightforward by setting the partial derivatives with respect to both \( \Sigma_\beta^{-1} \) and \( \sigma^2 \) to zero. The resulting updates are given by

\[
\hat{\Sigma}_\beta \leftarrow \hat{\beta} \hat{\beta}^\top + \hat{\Delta} \\
\hat{\sigma}^2 \leftarrow \hat{\sigma}^2 + \frac{1}{n} \left( \| \hat{r} - \Pi \hat{\beta} \|^2 - \hat{\sigma}^4 \text{tr} \hat{V}^{-1} \right).
\]

Note that the random effect \( \hat{r} \) also depends on the mean function which has parameters \( \hat{\alpha} \) and \( \hat{c} \). These parameters can be optimized in the M-step as well. For example, the
Tikhonov regularization (8) with the a quadratic loss can be used:

$$\arg \min_{\alpha, c} \frac{1}{n} (y - \Pi \alpha - c 1) ^ {\top} \hat{V}^{-1} (y - \Pi \alpha - c 1) + \xi \alpha ^ {\top} W ^ {\top} K W \alpha,$$

where $\xi > 0$ is the regularization parameter. Denote by $L := I - 11 ^ {\top} \hat{V}^{-1} \left(1 ^ {\top} \hat{V}^{-1} 1 \right)^{-1}$ the centering matrix, it is easy to obtain the following estimates

$$\hat{\alpha} = \left(\Pi ^ {\top} \hat{V}^{-1} L \Pi + n \xi W ^ {\top} K W \right)^{-1} \Pi ^ {\top} \hat{V}^{-1} L y$$

$$\hat{c} = 1 ^ {\top} \hat{V}^{-1} (y - \Pi \hat{\alpha}) \left(1 ^ {\top} \hat{V}^{-1} 1 \right)^{-1}.$$ (42)

Algorithm 1 gives the pseudo-code for the above EM algorithm. We remark that the computation of Algorithm 1 is efficient, requiring $O(n^2 m)$ time per iteration by taking advantage of the low-rank SDR parameterization. Furthermore, $\hat{V}^{-1}$ is computed via the Woodbury identity

$$V^{-1} = \sigma^{-2} \left[ I - \Pi \left(\sigma^2 \Sigma^{-1} + \Pi ^ {\top} \Pi \right)^{-1} \Pi ^ {\top} \right],$$

which reduces the computational complexity $O(n^3)$ of the inverse to $O(n^2 m)$. In practice, $m$ can be very small as we will show on several real datasets.

5 Experiments

We present experiments to 1) highlight the difference in the predictive distribution between the SIGP and the standard GP regression model; 2) illustrate the impact of the SDR approximation on the SIGP prediction; and 3) demonstrate that the SIGP with low-rank SDR approximation achieves competitive performance compared to state-of-the-art GP inference methods on a diverse collection of real-life datasets.

For the comparison, we consider several state-of-the-art GP inference methods, namely the Laplace’s approximation (Laplace) (Rasmussen and Williams, 2006), Kullback-Leibler divergence minimization (KL) (Nickisch and Rasmussen, 2008), expectation propagation (EP) (Minka, 2001), and fully independent training conditional (FITC) (Snelson and Ghahramani, 2006a). The experiments are based on the GP implementation in GPML toolbox (Rasmussen and Nickisch, 2010) which is generally considered to be amongst the best implementation of these algorithms. The support vector machine (SVM) results are based on the fitcsvm function from the Matlab. All methods use the radial basis kernel of which the parameters for SVM and SIGP are obtained via cross-validation. For all other GP inference methods, we optimize hyper-parameters using L-BFGS (Liu and Nocedal, 1989) for 1000 iterations. In addition to learning kernel hyper-parameters, we fit a linear mean function.

5.1 Illustration on Synthetic Data

Since the SDR approximation in the SIGP captures the functional dependence of $Y$ on $X$, the SIGP is particularly well-suited to modeling data with sampling biases.
Figure 1: Inference in a sinusoidal function with training data sampled at different locations.

Figure 1 depicts two samples at different locations, and the data is generated from a sine function with an additive Gaussian noise \( \mathcal{N}(0, 0.01) \). The posterior means and 95% credible intervals produced by the GP and SIGP are shown. The SIGP recovered the ground truth sine function on both samples, and tend to give more realistic uncertainty estimates at the unseen positions. This suggests that the SIGP can be useful to address problems such as covariate shift.

5.1.1 Impact of the SDR Approximation

Now consider a classification example shown in Figure 2. The toy dataset consists of 2D points from four classes. Note that each corner consists of points from two distinct classes. The figure shows the contours generated by the GP and SIGP. The SIGP-\( m \) denote the SIGP with rank-\( m \) SDR approximation.

For SIGP-1, the contours only separate the classes at the corners. This is because the basis functions of the SDR subspace correspond to principal components of the normal vectors (functions in the RKHS) to the contours (Li et al., 2011). Consequently, a rank-1 SDR subspace is insufficient to separate the four classes. However, as we increase the SDR rank all classes are successfully separated by the contours of the SIGP. In general, a rank-\( m \) SIGP suffices to classify at least \( m + 1 \) classes.

Figure 3 plots the projection of the data onto the first two dimensions of the SDR subspace estimated by the SIGP. As can be seen, the data is well-separated in the SDR subspace representation of the SIGP. In addition, the eigenvalue drops quickly to zero at
5.2 Results on Real-Life Data

We compare the performance of the SIGP and several state-of-the-art methods for classification and regression on UCI datasets as well as real-world environmental datasets from WCCI-2006 Predictive Uncertainty in Environmental Modeling Competition. Table 1 reports the total number of observations, the number of attributes, as well as the number of test cases for each dataset.

Table 1: The size as well as the training/testing splits of each dataset.

| Dataset   | #Obser. | #Attr. | #Test | Dataset   | #Obser. | #Attr. | #Test  |
|-----------|---------|--------|-------|-----------|---------|--------|-------|
| Arcene    | 200     | 10000  | 100   | Cancer    | 699     | 10     | 200   |
| Gisette   | 7000    | 5000   | 1000  | Housing   | 506     | 13     | 106   |
| Madelon   | 2600    | 500    | 600   | Temp      | 7117    | 106    | 3558  |
| German    | 1000    | 24     | 300   | Wine      | 3098    | 11     | 1800  |
| Heart     | 270     | 13     | 100   | Precip    | 7031    | 106    | 3515  |
Binary Classification  For the binary classification task, we use the F1 score, i.e., $2 \times \text{precision} \times \text{recall}/(\text{precision} + \text{recall})$, as the balanced accuracy metric. Since the classification is binary, we use the SIGP with rank-1 SDR approximation.

Table 2: Comparing F1 scores in binary classification.

| DATASET  | LAPLACE | KL   | EP   | FITC$^1$ | SVM   | SIGP-1  |
|----------|---------|------|------|---------|-------|---------|
| Arcene   | 0.8235  | 0.8269| 0.8235| 0.8352  | 0.8571|
| Gisette  | 0.9570  | 0.9541| 0.9571| 0.9571  | 0.9670| 0.9780  |
| Madelon  | 0.5695  | 0.5695| 0.5695| 0.5695  | 0.5990| 0.6367  |
| German   | 0.6211  | 0.6211| 0.6211| 0.6125  | 0.6182| 0.6424  |
| Heart    | 0.8409  | 0.8409| 0.8409| 0.8506  | 0.8605| 0.8605  |
| Cancer   | 0.9425  | 0.9213| 0.9438| 0.9778  | 0.9778| 0.9888  |

$^1$ Using $\lfloor n/2 \rfloor$ pseudo-inputs.

Table 2 reports the F1 scores on the benchmark datasets. From the table, the SIGP performs competitively compared to state-of-the-art methods, particularly on the high-dimensional dataset Arcene.

Regression  For regression, we report the negative log predictive density (NLPD) and mean squared error (MSE) for the SIGP and the GP with the FITC inference which is known to yield better NLPD than the other inference methods (Snelson and Ghahramani, 2006b).

Table 3: Prediction performance on the held-out validation data. FITC-$t$ denotes the FITC method using $t$ pseudo-inputs. Since the Housing dataset is relatively small, the entire training data is used.

| METHOD      | HOUSING NLPD | HOUSING MSE | TEMP NLPD | TEMP MSE | WINE NLPD | WINE MSE | PRECIP NLPD | PRECIP MSE |
|-------------|--------------|-------------|-----------|----------|-----------|----------|-------------|------------|
| LINEAR REG. | 3.2363       | 37.8938     | 0.1265    | 0.0754   | 1.1052    | 0.5340   | 1.8268      | 2.2607     |
| FITC-1500   | 3.1200       | 28.8048     | 0.0522    | 0.0649   | 1.1002    | 0.5417   | 1.7258      | 1.8298     |
| FITC-2000   | 3.1200       | 28.8048     | 0.0527    | 0.0650   | 1.0972    | 0.5724   | 1.7229      | 1.8353     |
| FITC-2500   | 3.1200       | 28.8048     | 0.0520    | 0.0647   | 1.0966    | 0.5628   | 1.7204      | 1.8302     |
| SIGP-1      | 2.7756       | 15.0003     | 0.0531    | 0.0640   | 1.0953    | 0.5228   | 1.7221      | 1.8349     |
| SIGP-2      | **2.7459**   | **14.2078** | 0.0513    | 0.0628   | **1.0905**| **0.5177**| **1.7135**  | **1.7664**  |
| SIGP-3      | 2.8393       | 16.5767     | **0.0498**| **0.0617**| 1.0911    | 0.5181   | 1.7163      | 1.7783     |

Table 3 compares the NLPD (smaller is better) as well as MSE on the held-out validation data. The experiment shows that higher rank SDR approximation in the SIGP may not necessarily improve the predictive performance. This is reasonable as increasing the rank may also overfit the data, and the optimal rank actually depends on the structure of data, e.g., the number of classes as discussed in Section 5.1.1. The result in Table 3 suggests that
the SIGP performs consistently in both MSE as well as NLPD, and is a state-of-the-art method for regression.

6 Conclusions

In this paper, we introduce novel non-parametric stochastic regression models based on integral representations of Gaussian processes. We provide a characterization of the sample paths of these GP models with respect to the RKHS that contains the sample paths. The theoretical ideas developed in formulating the novel GP is of interest in itself. We then show how we can use the GP defined by the integral representations for computationally efficient and statistically accurate non-parametric regression using a data-dependent kernel model. We illustrate the practical utility of this via results on simulated and real data. From a machine learning perspective we provide a way to efficiently infer hyper-parameters in a data-dependent way that takes prediction into account for Gaussian processes.

We suspect that there are extensions to the IGP and our sample-based implementation of the IGP both from a theoretical and practical perspective. In addition, considering powers of integral operators fits into the perspective of understanding the power of deep learning as interpolation (Belkin, 2018) and the idea of analyzing deep learning via kernel models that interpolate (Belkin et al., 2018).

Code and Data

The datasets as well as the sample-based implementation of the IGP are available on the Git repository: https://github.com/ZilongTan/sigp.

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