Frequentist Consistency of Gaussian Process Regression

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Abstract

Gaussian Process Regression is a well-known and widely used approach to a problem of non-parametric regression. In the current study we obtain a minimax-optimal rate of convergence of its predictive mean to the true underlying function. We provide results for both random and deterministic designs.

1 Introduction

We observe $n$ response-covariance pairs $\mathcal{X} \times \mathbb{R}$ such that

$$y_i = f^*(X_i) + \varepsilon_i$$

for compact $\mathcal{X} \subseteq \mathbb{R}^p$, centered independent sub-Gaussian with proxy-variance $\sigma^2$ and second moment $\sigma^2$ noise $\varepsilon_i$. In the paper we investigate the behaviour of one of the most popular non-parametric approaches to estimation of $f^*$ – the Gaussian Process Regression (GPR). The method attains bias-variance trade-off via imposing a Gaussian Process prior over the function in question. A GP prior is driven by its mean (typically, assumed to be constant and zero) and covariance function $\sigma^2 (n\rho)^{-1} k(\cdot, \cdot)$. In the current study we focus on Matérn kernels, yet the results are also applicable to any covariance function satisfying the following two assumptions.

Alternatively, one can arrive to the same estimate via Kernel Ridge Regression (KRR) [2]

$$\hat{f} := \arg \max_f L(f) - \frac{\rho}{2} \|f\|_k^2,$$  \hspace{1cm} (1.1)

where $\|\cdot\|_k$ refers to the RKHS norm, induced by the kernel $k(\cdot, \cdot)$, and the likelihood $L$ is defined as

$$L(f) = -\frac{1}{2n} \sum_i (y_i - f(X_i))^2.$$
The goal of the current study is to provide a minimax-optimal high-probability bound on \( \|f^* - \hat{f}\|_2^2 \). An earlier study [6] provided a sup-norm bound in a univariate case, assuming \( X_i \sim U[\mathcal{X}] \), while we allow for any continuous distribution of \( X_i \) over a multivariate compact. Another line of study aims to bound the mean-squared prediction error \( \mathbb{E} \left[ \|f^* - \hat{f}\|_2^2 \right] \), leaving a large deviation probability out of the scope [7].

In the paper we heavily rely on a spectral decomposition of the kernel operator \( k(\cdot, \cdot) \). Choose a measure \( \pi \) over \( \mathcal{X} \). Mercer’s theorem [2] provides existence of normalized eigenfunctions \( \phi_j \in L_2(\mathcal{X}, \pi) \) along with the corresponding eigenvalues \( \mu_j \) (in decreasing order). For a function \( \|\cdot\|_2 \) denotes an \( L_2(\mathcal{X}, \pi) \)-norm, namely \( \|f\|_2^2 = \int f^2 d\pi \), the dot-product is also defined w.r.t. the measure \( \pi \): \( \langle f, g \rangle = \int fg d\pi \). In our random-design results \( X_i \) are presumed to be drawn independently w.r.t \( \pi \). The kernel \( k(\cdot, \cdot) \) induces a RKHS \( \mathcal{H}_k \) endowed with a norm

\[
\|f\|_k = \sum_{j=1}^{\infty} \frac{\langle f, \phi_j \rangle^2}{\mu_j}.
\]

\( \|\cdot\| \) of a vector denotes an Euclidean distance, while used with respect to a p.s.d. matrix it denotes its maximum eigenvalue. \( \|\cdot\|_F \) stands for Frobenius norm. \( I \) denotes an identity operator.

## 2 Assumptions

First of all, we impose a polynomial rate of decay for for the eigenvalues of \( k(\cdot, \cdot) \).

**Assumption 1** (Polynomial eigendecay). *Exist positive constants \( C \) and \( s \) s.t. for the \( j \)-th largest eigenvalue \( \mu_j \) of \( k(\cdot, \cdot) \)

\[
\mu_j \leq C j^{-2s}.
\]

As demonstrated in [4], **Assumption 1** holds for Matrn kernel with smoothness \( \alpha \) in a \( p \)-dimensional space with \( s = (2\alpha + p)/p \). Another popular example is a Gaussian or Squared Exponential kernel. It is known to exhibit an exponential rate of eigendecay. With some abuse of formality, our results can be applied in this case with \( s = \infty \). Alternatively, the argument can be carefully repeated with minimal augmentation in this case as well.

We also presume the eigenfunctions of the kernel are bounded. The eigenfunctions of Matrn kernel are also Lipschitz.

**Assumption 2** (Boundness of eigenfunctions). *Denote a normalized eigenfunction corresponding the the \( j \)-th largest eigenvalue as \( \phi_j(\cdot) \). Let there exist a positive constant \( C_\phi \) s.t. \( \sup_j \max_{X \in \mathcal{X}} |\phi_j(X)| \leq C_\phi \).

Consider the eigenvalues \( \{\mu_j\}_{j=1}^\infty \) and normalized eigenfunctions \( \{\phi_j(\cdot)\}_{j=1}^\infty \) of \( k(\cdot, \cdot) \). Now for \( f \in \mathcal{H}_k \) we have the vector \( f \) of expansion coefficients \( f_j := \)
\langle f, \phi_j \rangle$. Further, we introduce the design matrix $\Phi \in \mathbb{R}^{n \times \infty}$ s.t. $\Phi_{ij} = \phi_j(X_i)$. At this point the estimator (1.1) can be rewritten as

$$\hat{f} := \arg \max_f \left( -\frac{1}{2n} \| \Phi f - y \|^2 - \frac{\rho}{2} \sum_j \frac{f_j^2}{\mu_j} \right).$$

Next, consider a diagonal matrix $M \in \mathbb{R}^{\infty \times \infty}$ s.t. $M_{jj} = \sqrt{\mu_j}$ and define $\theta_j := f_j/M_{jj}$, $\Psi := \Phi M$, rewriting (1.1) again

$$\hat{\theta} := \arg \max_\theta \left( -\frac{1}{2n} \| \Psi \theta - y \|^2 - \frac{\rho}{2} \| \theta \|^2 \right).$$

At this point we are ready to formulate an assumption we impose on the design $\{X_i\}_{i=1}^n$.

**Assumption 3** (Design regularity). Let there exist some positive $\delta$ s.t.

$$\left\| \frac{1}{n} (M^2 + \rho I)^{-1/2} (\Psi^T \Psi + \rho I) (M^2 + \rho I)^{-1/2} - I \right\| \leq \delta < 1.$$  

Assumption 3 can seem to be obscure, but Lemma 2 guaranties it to hold for a random design with $X_i$ being i.i.d. and distributed w.r.t. a continuous and bounded measure. Note, we do not assume $\delta \to 0$, it only needs to be bounded away from 1. We also define

$$\theta^* := \arg \max_\theta \mathbb{E} [L(\theta)]$$

and its penalized counterpart

$$\theta^*_\rho := \arg \max_\theta \mathbb{E} [L(\theta)] - \frac{\rho}{2} \| \theta \|^2.$$  

### 3 Results

We open the section with a random-design consistency result. Note, it gives a bound in terms of $L_2(\mathcal{X}, \pi)$-norm, which is natural, as an increase of density of $X_i$ in some subset of $\mathcal{X}$ leads to better predictions on the subset.

**Theorem 1.** Let $X_i$ be drawn independently from $\mathcal{X}$ w.r.t. some continuous measure $\pi$. Choose $k(\cdot, \cdot)$ to be Matrn kernel with smoothness $\alpha > 1/2$. Presume, $f^* \in \mathcal{H}_k$. Choose $\rho = n^{-\frac{\alpha+3\alpha}{2\alpha+3}}$. Then on a set of an arbitrarily high probability

$$\left\| \hat{f} - f^* \right\|_2 \leq C \rho n^{-\frac{\alpha+3\alpha}{2\alpha+3}}$$

for some $C > 0$ independent of $n$ and $\rho$.  

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Proof. First of all, as shown in [4], Assumption 1 holds for Matern kernel with smoothness \( \alpha \) in a \( p \)-dimensional space with \( s = (2\alpha + p)/p \). Assumption 2 holds for it as well. The rest of the proof consists in application of Lemma 2 followed by application of Theorem 2.

The proof of the random-design bound relies on the bound, established for a deterministic design. Again, we bound an \( L_2(\mathcal{X}, \pi) \)-norm. Note, the choice of \( \pi \) also affects Assumption 3.

**Theorem 2.** Let \( X_i \) be deterministic. Impose Assumption 2 and Assumption 3, let Assumption 1 hold for positive \( C, s \), choose \( \rho = n^{-2s/(s+1)} \). Let \( f^* \in H_k \). Then for some positive \( C \) on a set of probability at least \( 1 - e^{-x} \)

\[
\|\hat{f} - f^*\|_2 \leq \frac{Cg\sqrt{1 + \sqrt{x} + 2x + \|f^*\|_k^2}}{(1 - \delta)^{3/2}n^{-2s/(s+1)}}.
\]

Proof. By the means of trivial calculus we have

\[
\nabla \zeta := \nabla (L(\theta) - \mathbb{E}[L(\theta)]) = \frac{1}{n} \Psi^T \varepsilon
\]

and

\[
D^2 \rho := -\nabla^2 \mathbb{E}[L(\theta) - 2\rho \|\theta\|] = \frac{1}{n} \Psi^T \Psi + \rho I.
\]

Now we apply Lemma 1, justifying applicability of Theorem 2.1 from [5], which yields for some positive \( C \) on a set of probability at least \( 1 - e^{-x} \) for a positive \( x \)

\[
\|D \rho (\hat{\theta} - \theta^*_\rho)\| \leq Cg\sqrt{\frac{\rho (1 + \sqrt{x} + 2x)}{1 - \delta}}.
\]

Finally, apply Theorem 2.3 from [5], arriving to

\[
\|D \rho (\hat{\theta} - \theta^*_\rho)\| = \|D^{-1} \rho \theta^*\| \leq \frac{\rho}{\sqrt{\rho}} \|\theta^*\| = \sqrt{\rho} \|f^*\|_k.
\]

Combination of the two bounds yields

\[
\|D \rho (\hat{\theta} - \theta^*_\rho)\|^2 \leq r^2 := C^2 g^2 \rho \left(1 + \sqrt{x} + 2x + \|f^*\|_k\right) \frac{1}{1 - \delta}.
\]

But clearly,

\[
(1 - \delta)^2 \|\hat{f} - f\|^2 = (1 - \delta) M^2 (\hat{\theta} - \theta^*)\| \leq \|D \rho (\hat{\theta} - \theta^*_\rho)\|^2 \leq r^2,
\]

which is exactly the bound we have claimed. 

\[\Box\]
A Technical Results

The following lemma verifies one of the conditions of Theorem 2.1 by [5].

**Lemma 1.** Impose Assumption 3, let Assumption 1 hold for positive $C, s$, choose $\rho = n^{-\frac{s}{2s+1}}$. Then for some positive $C$

$$\mathbb{P} \left\{ \left\| D_{\rho}^{-1} \nabla \zeta \right\| \leq C_0 \sqrt{\rho \frac{(1 + \sqrt{x} + 2x)}{1 - \delta}} \right\} \geq 1 - e^{-x}.$$ 

**Proof.** By the definition of $\nabla \zeta$

$$\left\| D_{\rho}^{-1} \nabla \zeta \right\|^2 = \frac{1}{n^2} \varepsilon^T \Psi^T \left( \frac{1}{n} \Psi^T \Psi + \rho I \right)^{-1} \Psi \varepsilon.$$ 

Clearly,

$$\left( \frac{1}{n} \Psi^T \Psi + \rho I \right) \geq (1 - \delta) M^2 + \rho I$$

and hence

$$\left\| D_{\rho}^{-1} \nabla \zeta \right\|^2 \leq \varepsilon^T \frac{1}{n^2} \Psi^T \left( (1 - \delta) M^2 + \rho I \right)^{-1} \Psi \varepsilon.$$ 

Now we bound every diagonal element of the matrix $A$.

$$\max_i A_{ii} \leq \frac{1}{n^2} \sum_{j=1}^{\infty} C_\phi^2 \frac{\mu_j}{(1 - \delta) \mu_j + \rho}$$

$$\leq \frac{C_\phi^2}{n^2(1 - \delta)} \sum_{j=1}^{\infty} \frac{\mu_j}{\mu_j + \rho}$$

$$= \frac{C_\phi^2}{n^2(1 - \delta)} \sum_{j=1}^{\infty} \frac{1}{1 + \rho/\mu_j}.$$ 

Now employ Assumption 1 and obtain

$$\max_i A_{ii} \leq \frac{C_\phi^2}{n^2(1 - \delta)} \sum_{j=1}^{\infty} \frac{C_j^{-2s}}{C_j^{-2s} + \rho} \tag{A.1}$$

and recalling the definition of $\rho$ we have for some positive $C$

$$\max_i A_{ii} \leq \frac{C_\rho}{n(1 - \delta)}.$$ 

Therefore,

$$\text{tr} \ (A) \leq C_\rho/(1 - \delta)$$

and trivially

$$\text{tr} \ (A^2) \leq (C_\rho/(1 - \delta))^2.$$
Finally, we are ready to employ Hanson-Wright inequality \[3\], constituting the claim.

Below we demonstrate that Assumption 3 holds with high probability under general assumptions.

**Lemma 2.** Let \(X_i\) be drawn independently from \(X\) under some continuous measure \(\pi\). Let \(\{\phi_j\}\) and \(\{\mu_j\}\) be eigenvalues and eigenfunctions of \(k(\cdot, \cdot)\) w.r.t. \(\pi\). Also impose Assumption 1 for \(C\) and \(s\). Choose \(\rho = n^{-\frac{C}{2s^2}}\). Then Assumption 3 holds for some \(C > 0\) with \(\delta = C n \frac{n^{-\frac{C}{2s^2}}}{\sqrt{t}}\) on a set of probability at least \(t (e^{-t} - t - 1)\).

**Proof.** Consider matrices \(\Psi^i \in \mathbb{R}^{\infty \times \infty}\) s.t. \(\Psi^i_{jk} = \sqrt{\mu_j \mu_k} \phi_j(X_i) \phi_k(X_i)\). Denote

\[
\Omega_i = \left( M^2 - \rho I \right)^{-1/2} \Psi^i \left( M^2 - \rho I \right)^{-1/2} - I.
\]

Observe

\[
\frac{1}{n} \sum_i \Omega_i = \frac{1}{n} \left( M^2 + \rho I \right)^{-1/2} \left( \Psi^T \Psi + \rho I \right) \left( M^2 + \rho I \right)^{-1/2}.
\]

Due to the fact that the eigenfunctions are normalized, \(\mathbb{E} [\Omega_i] = 0\). Below we use \(C\) as a generalized constant independent of \(n\), whose value may differ line-to-line. \(j\) and \(k\), being summation indexes, always run from 1 to \(\infty\) unless specified otherwise.

Clearly the maximum eigenvalue of a p.s.d. matrix does not exceed its trace. Hence, using the trick used in (A.1)

\[
\left\| \left( M^2 - \rho I \right)^{-1/2} \Psi^i \left( M^2 - \rho I \right)^{-1/2} \right\| \leq C \sum_j \frac{\mu_j}{\mu + \rho} \leq C \rho n.
\]

Further, using the choice of \(\rho\) we have

\[
\left\| \Omega_i \right\| \leq C \rho n - 1 \leq C \rho n.
\]

Now the goal is to bound \(\text{tr} \left( \mathbb{E} [\Omega_i^2] \right)\). First, we observe

\[
\mathbb{E} \left[ \left( M^2 + \rho I \right)^{-1/2} \left( \Psi^i + \rho I \right) \left( M^2 + \rho I \right)^{-1/2} \right] = I
\]
due to the fact that $E[\Psi^2] = M^2$. Therefore,
\[
E[\Omega^2_i] = \left( (M^2 + \rho I)^{-\frac{1}{2}} (\Psi^i + \rho I) (M^2 + \rho I)^{-\frac{1}{2}} \right)^2 - I.
\]

For an arbitrary diagonal element of $A$ we have
\[
\text{tr} \left( E[\Omega^2_i] \right) \leq \sum_j \left( \sum_k \frac{C^2 L j \mu_k + \rho I [j = k]}{(\mu_j + \rho)(\mu_k + \rho)} - 1 \right)
\]
\[
\leq \sum_j \sum_k \frac{C^2 L j \mu_k}{(\mu_j + \rho)(\mu_k + \rho)} + \left| \sum_j \left( \frac{C^2 L j \mu_j}{\mu_j + \rho} \right)^2 - 1 \right|
\]
\[
=: T_1 + T_2.
\]

Using the same trick as in (A.1) twice, relying on the choice of $\rho$ we have
\[
T_1 \leq C \sum_j \left( \frac{\mu_j}{\mu_j + \rho} \sum_k \frac{\mu_k}{\mu_k + \rho} \right)
\]
\[
\leq C \sum_j \frac{\mu_j}{\mu_j + \rho} \times \rho n
\]
\[
\leq C(\rho n)^2.
\]

The treatment of the second term uses decay of $\mu_j$
\[
T_2 \leq C \left| \sum_j \frac{\mu_j^2 + \rho \mu_j}{(\mu_j + \rho \mu_j)^2} \right|
\]
\[
\leq C \sum_j \frac{\rho \mu_j}{\mu_j^2 + 2 \mu_j \rho + \rho^2}
\]
\[
\leq C \sum_j \frac{\mu_j}{\mu_j + \rho}
\]
\[
\leq C(\rho n),
\]

where the trick from (A.1) was used again. Therefore, we have
\[
\text{tr} \left( E[\Omega^2_i] \right) \leq C(\rho n)^2
\]
due to the choice of $\rho$. Finally, we notice that the matrix $\Omega^2_i$ is p.s.d. and its maximal eigenvalue does not exceed its trace and apply the Theorem 4 by [1], demonstrating that Assumption 3 holds for
\[
\delta = \sqrt{\frac{2(\rho n)^2 t}{n}} + C\rho t
\]
with probability at least $t(e^{-t} - t - 1)$. Substitution of $\rho$ establishes the claim. □
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