
Rates of Convergence for Sparse Variational Gaussian Process Regression

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Abstract

Excellent variational approximations to Gaussian process posteriors have been developed which avoid the $\mathcal{O}(N^3)$ scaling with dataset size N . They reduce the computational cost to $\mathcal{O}(NM^2)$, with $M \ll N$ the number of *inducing variables*, which summarise the process. While the computational cost seems to be linear in N , the true complexity of the algorithm depends on how M must increase to ensure a certain quality of approximation. We show that with high probability the KL divergence can be made arbitrarily small by growing M more slowly than N . A particular case is that for regression with normally distributed inputs in D -dimensions with the Squared Exponential kernel, $M = \mathcal{O}(\log^D N)$ suffices. Our results show that as datasets grow, Gaussian process posteriors can be approximated cheaply, and provide a concrete rule for how to increase M in continual learning scenarios.

1. Introduction

Gaussian processes (GPs) [Rasmussen & Williams, 2006] are distributions over functions that are convenient priors in Bayesian models. They can be seen as infinitely wide neural networks [Neal, 1996], and are particularly popular in regression models, as they produce good uncertainty estimates, and have closed-form expressions for the posterior and marginal likelihood. The most well known drawback of GP regression is the computational cost of the exact calculation of these quantities, which scales as $\mathcal{O}(N^3)$ in time and $\mathcal{O}(N^2)$ in memory where N is the number of training examples. Low-rank approximations [Quiñonero Candela & Rasmussen, 2005] choose M *inducing variables* which summarise the entire posterior, reducing the cost to $\mathcal{O}(NM^2 + M^3)$ time and $\mathcal{O}(NM + M^2)$ memory.

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While the computational cost of adding inducing variables is well understood, results on how many are needed to achieve a good approximation are lacking. As the dataset size increases, we cannot expect to keep the capacity of the approximation constant without the quality deteriorating. Taking into account the rate at which M must increase with N to achieve a particular approximation accuracy, as well as the cost of initializing or optimizing the inducing points, determines a more realistic sense of the costs of scaling Gaussian processes.

Approximate GPs are often trained using variational inference [Titsias, 2009], which minimizes the KL divergence from an approximate posterior to the full posterior process [Matthews et al., 2016]. We use this KL divergence as our metric for the approximate posterior's quality. We show that under intuitive assumptions the number of inducing variables only needs to grow at a sublinear rate for the KL between the approximation and the posterior to go to zero. This shows that very sparse approximations can be used for large datasets, without introducing much bias into hyperparameter selection through evidence lower bound (ELBO) maximisation, and with approximate posteriors that are accurate in terms of their prediction and uncertainty.

The core idea of our proof is to use upper bounds on the KL divergence that depend on the quality of a Nyström approximation to the data covariance matrix. Using existing results, we show this error can be understood in terms of the spectrum of an infinite-dimensional integral operator. In the case of stationary kernels, our main result proves that priors with smoother sample functions, and datasets with more concentrated inputs admit sparser approximations.

Main results We assume that training inputs are drawn i.i.d. from a fixed distribution, and prove bounds of the form

$$\text{KL}\left(Q\|\hat{P}\right) \leq \mathcal{O}\left(\frac{g(M, N)}{\sigma_n^2 \delta} \left(1 + \frac{c\|\mathbf{y}\|_2^2}{\sigma_n^2}\right) + N\epsilon\right)$$

with probability at least $1 - \delta$, where \hat{P} is the posterior Gaussian process, Q is a variational approximation, and \mathbf{y} are the training targets. The function $g(M, N)$ depends on both the kernel and input distribution, and grows linearly in N and generally decays rapidly in M . The quality of the initialization determines ϵ , which can be made arbitrarily small (e.g. an inverse power of N) at some additional com-

putational cost. Theorems 1 and 2 give results of this form for a collection of inducing variables defined using spectral information, theorems 3 and 4 hold for inducing points.

2. Background and notation

2.1. Gaussian process regression

We consider Gaussian process regression, where we observe *training data*, $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^N$ with $\mathbf{x}_i \in \mathcal{X}$ and $y_i \in \mathbb{R}$. Our goal is to predict outputs y^* for new inputs \mathbf{x}^* while taking into account the uncertainty we have about $f(\cdot)$ due to the limited size of the training set. We follow a Bayesian approach by placing a prior over f , and a likelihood to relate f to the observed data through some noise. Our model is

$$f \sim \mathcal{GP}(\nu(\cdot), k(\cdot, \cdot)), \quad y_i = f(\mathbf{x}_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma_n^2),$$

where $\nu : \mathcal{X} \rightarrow \mathbb{R}$ is the *mean function* and $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is the *covariance function*. We take $\nu \equiv 0$; the general case can be derived similarly after first centering the process. We use the posterior for making predictions, and the marginal likelihood for selecting hyperparameters, both of which have closed-form expressions [Rasmussen & Williams, 2006]. The log marginal likelihood is of particular interest to us, as the quality of its approximation and our posterior approximation is linked. Its form is

$$\mathcal{L} = -\frac{1}{2}\mathbf{y}^\top \mathbf{K}_n^{-1} \mathbf{y} - \frac{1}{2} \log|\mathbf{K}_n| - \frac{N}{2} \log(2\pi), \quad (1)$$

where $\mathbf{K}_n = \mathbf{K}_{\text{ff}} + \sigma_n^2 \mathbf{I}$, and $[\mathbf{K}_{\text{ff}}]_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j)$.

2.2. Sparse variational Gaussian process regression

While all quantities of interest have analytic expressions, their computation is infeasible for large datasets due to the $\mathcal{O}(N^3)$ time complexity of the determinant and inverse. Many approaches have been proposed that rely on a low-rank approximation to \mathbf{K}_{ff} [Quiñonero Candela & Rasmussen, 2005; Rahimi & Recht, 2008], which allow the determinant and inverse to be computed in $\mathcal{O}(NM^2)$, where M is the rank of the approximating matrix.

We consider the variational framework developed by Titsias [2009], which minimizes the KL divergence from the posterior process to an approximate GP

$$\mathcal{GP}(\mathbf{k}_{\mathbf{u}} \mathbf{K}_{\mathbf{uu}}^{-1} \boldsymbol{\mu}, \mathbf{k}_{..} + \mathbf{k}_{\mathbf{u}} \mathbf{K}_{\mathbf{uu}}^{-1} (\boldsymbol{\Sigma} - \mathbf{K}_{\mathbf{uu}}) \mathbf{K}_{\mathbf{uu}}^{-1} \mathbf{k}_{\mathbf{u}}), \quad (2)$$

where $[\mathbf{k}_{\mathbf{u}}]_i = k(\cdot, \mathbf{z}_i)$, $[\mathbf{K}_{\mathbf{uf}}]_{m,i} := k(\mathbf{z}_m, \mathbf{x}_i)$ and $[\mathbf{K}_{\mathbf{uu}}]_{m,n} := k(\mathbf{z}_m, \mathbf{z}_n)$. This variational distribution is determined through defining the density of the function values $\mathbf{u} \in \mathbb{R}^M$ at *inducing inputs* $Z = \{\mathbf{z}_m\}_{m=1}^M$ to be $q(\mathbf{u}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Z , $\boldsymbol{\mu}$, and $\boldsymbol{\Sigma}$ are variational parameters. Titsias [2009] solved the convex optimization problem for $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ explicitly, resulting in the evidence lower bound

(ELBO):

$$\mathcal{L}_{\text{lower}} = -\frac{1}{2}\mathbf{y}^\top \mathbf{Q}_n^{-1} \mathbf{y} - \frac{1}{2} \log|\mathbf{Q}_n| - \frac{N}{2} \log(2\pi) - \frac{t}{2\sigma_n^2} \quad (3)$$

where $\mathbf{Q}_n = \mathbf{Q}_{\text{ff}} + \sigma_n^2 \mathbf{I}$, $\mathbf{Q}_{\text{ff}} = \mathbf{K}_{\mathbf{uf}}^\top \mathbf{K}_{\mathbf{uu}}^{-1} \mathbf{K}_{\mathbf{uf}}$ and $t = \text{Tr}(\mathbf{K}_{\text{ff}} - \mathbf{Q}_{\text{ff}})$. Hensman et al. [2013] proposed optimising over $\{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}$ numerically, which allows minibatch optimization. In both cases, $\mathcal{L} = \mathcal{L}_{\text{lower}} + \text{KL}(Q||\hat{P})$ [Matthews et al., 2016], so any bounds on the KL-divergence we prove hold for Hensman et al. [2013] as well, as long as $\{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}$ is at the optimum value.

Titsias [2009] suggests jointly maximizing the ELBO (eq. 3) w.r.t. the variational and hyperparameters. This comes at the cost of introducing bias in hyperparameter estimation [Turner & Sahani, 2011], notably the overestimation of the σ_n^2 [Bauer et al., 2016]. Adding inducing points reduces the KL gap [Titsias, 2009], and the bias is practically eliminated when enough inducing variables are used.

2.3. Interdomain inducing features

Lázaro-Gredilla & Figueiras-Vidal [2009] showed that one can specify the distribution $q(\mathbf{u})$, on integral transformations of $f(\cdot)$. Using these *interdomain* inducing variables can lead to sparser representations, or computational benefits [Hensman et al., 2018]. Interdomain inducing variables are defined by

$$u_m = \int_{\mathcal{X}} f(\mathbf{x}) g(\mathbf{x}; \mathbf{z}_m) d\mathbf{x}.$$

When $g(\mathbf{x}; \mathbf{z}_m) = \delta(\mathbf{x} - \mathbf{z}_m)$ the u_m are inducing points. Interdomain features require replacing $\mathbf{k}_{\mathbf{u}}$ and $\mathbf{K}_{\mathbf{uu}}$ in eq. 2 with integral transforms of the kernel. In later sections, we investigate particular interdomain transformations with interesting convergence properties.

2.4. Upper bounds on the marginal likelihood

Combined with eq. 3, an upper bound on eq. 1 can show when the KL divergence is small, which indicates inference has been successful and hyperparameter estimates are likely to have little bias. Titsias [2014] introduced an upper bound that can be computed in $\mathcal{O}(NM^2)$:

$$\mathcal{L}_{\text{upper}} := -\frac{1}{2}\mathbf{y}^\top (\mathbf{Q}_n + t\mathbf{I})^{-1} \mathbf{y} - \frac{1}{2} \log(|\mathbf{Q}_n|) - \frac{N}{2} \log 2\pi. \quad (4)$$

This gives a *data-dependent* upper bound, that can be computed after seeing the data, and for given inducing inputs.

2.5. Spectral properties of the covariance matrix

While for small datasets spectral properties of the covariance matrix can be analyzed numerically, we need a different

approach for understanding these properties for a typical large dataset. The *covariance operator*, \mathcal{K} , captures the limiting properties of \mathbf{K}_{ff} for large N . It is defined by

$$\mathcal{K}g(\mathbf{x}') = \int_{\mathcal{X}} g(\mathbf{x})k(\mathbf{x}, \mathbf{x}')p(\mathbf{x})d\mathbf{x}, \quad (5)$$

where $p(\mathbf{x})$ is a probability density from which the inputs are assumed to be drawn. We assume that \mathcal{K} is compact, which is the case if $k(\mathbf{x}, \mathbf{x}')$ is bounded. Under this assumption, the spectral theorem tells us that \mathcal{K} has a discrete spectrum. The (finite) sequence of eigenvalues of $\frac{1}{N}\mathbf{K}_{\text{ff}}$ converges to the (infinite) sequence of eigenvalues of \mathcal{K} [Koltchinskii & Giné, 2000]. Mercer's Theorem [Mercer, 1909] tells us that for continuous kernel functions,

$$k(\mathbf{x}, \mathbf{x}') = \sum_{m=1}^{\infty} \lambda_m \phi_m(\mathbf{x}) \phi_m(\mathbf{x}'), \quad (6)$$

where the $(\lambda_m, \phi_m)_{i=1}^{\infty}$ are eigenvalue-eigenfunction pairs of the operator \mathcal{K} , with the eigenfunctions orthonormal in $L^2(\mathcal{X})_p$. Additionally, $\sum_{m=1}^{\infty} \lambda_m < \infty$.

2.6. Selecting the number of inducing variables

Ideally, the number of inducing variables should be selected to make the $KL(Q||\hat{P})$ small. Currently, the most common advice is to increase the number of inducing variables M until the lower bound (eq. 3) no longer improves. This is a necessary, but not a sufficient condition for the ELBO to be tight and the KL to be small. Taking the upper bound (eq. 4) into consideration, we can guarantee a good approximation when difference between the upper and lower bounds converges to zero, as this upper bounds the KL.

Both these procedures rely on bounds computed for a given dataset, and a specific setting of variational parameters. While practically useful, they do not tell us how many inducing variables we should expect to use *before* observing any data. In this work, we focus on *a priori* bounds, and asymptotic behavior as $N \rightarrow \infty$ and M grows as a function of N . These bounds guarantee how the variational method scales computationally for *any* dataset satisfying intuitive conditions. This is particularly important for continual learning scenarios, where we incrementally observe more data. With our *a priori* results we can guarantee that the growth in required computation will not exceed a certain rate.

3. Bounds on the KL divergence for eigenfunction inducing features

In this section, we prove *a priori* bounds on the KL divergence using inducing features that rely on spectral information about the covariance matrix or the associated operator. The results in this section form the basis for bounds on the KL divergence for inducing points (section 4).

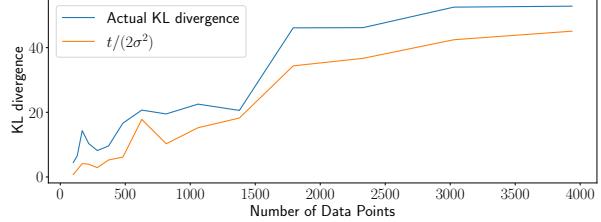


Figure 1. Increasing N with fixed M increases the expected KL divergence. $t/(2\sigma_n^2)$ is a lower bound for the expected value over the KL divergence when \mathbf{y} is generated according to our prior model.

3.1. A Posteriori Bounds on the KL Divergence

We first consider *a posteriori* bounds on the KL divergence that hold for any \mathbf{y} , derived by looking at the difference between $\mathcal{L}_{\text{upper}}$ and $\mathcal{L}_{\text{lower}}$. We will use these bounds in later sections to analyze asymptotic convergence properties.

Lemma 1. Let $\tilde{\mathbf{K}}_{\text{ff}} = \mathbf{K}_{\text{ff}} - \mathbf{Q}_{\text{ff}}$, $t = \text{Tr}(\tilde{\mathbf{K}}_{\text{ff}})$ and $\tilde{\lambda}_{\max}$ denote the largest eigenvalue of $\tilde{\mathbf{K}}_{\text{ff}}$. Then,

$$KL(Q||\hat{P}) \leq \frac{1}{2\sigma_n^2} \left(t + \frac{\tilde{\lambda}_{\max} \|\mathbf{y}\|_2^2}{\sigma_n^2 + \tilde{\lambda}_{\max}} \right) \leq \frac{t}{2\sigma_n^2} \left(1 + \frac{\|\mathbf{y}\|_2^2}{\sigma_n^2 + t} \right).$$

The proof bounds the difference between a refinement of $\mathcal{L}_{\text{upper}}$ also proven by Titsias [2014] and $\mathcal{L}_{\text{lower}}$ through an algebraic manipulation and is given in appendix A. The second inequality is a consequence of $t \geq \tilde{\lambda}_{\max}$. We typically expect $\|\mathbf{y}\|_2^2 = \mathcal{O}(N)$, which is the case when the variance of the observed y s is bounded, so if $t \ll 1/N$ the KL divergence will be small.

3.2. A priori bounds: averaging over \mathbf{y}

Lemma 1 is typically overly pessimistic, as it assumes \mathbf{y} can be parallel to the largest eigenvector of $\tilde{\mathbf{K}}_{\text{ff}}$. In this section, we consider a bound that holds *a priori* over the training outputs, when they are drawn from the model. This allows us to bound the KL divergence for a ‘typical’ dataset.

Lemma 2. For any set of $\{\mathbf{x}_i\}_{i=1}^N$, if the outputs $\{y_i\}_{i=1}^N$ are generated according to our generative model, then

$$\frac{t}{2\sigma_n^2} \leq \mathbb{E}_{\mathbf{y}} [KL(Q||\hat{P})] \leq \frac{t}{\sigma_n^2} \quad (7)$$

The lower bound tells us that *even if the training data is contained in an interval of fixed length, we need to use more inducing points for problems with large N if we want to ensure the sparse approximation has converged*. This is shown in Figure 1 for data uniformly sampled on the interval $[0, 5]$ with 15 inducing points.

Sketch of Proof.

$$\begin{aligned} \mathbb{E}_y \left[\text{KL}(Q \parallel \hat{P}) \right] &= \frac{t}{2\sigma_n^2} + \int \mathcal{N}(\mathbf{y}; 0, \mathbf{K}_n) \\ &\quad \times \log \left(\frac{\mathcal{N}(\mathbf{y}; 0, \mathbf{K}_n)}{\mathcal{N}(\mathbf{y}; 0, \mathbf{Q}_n)} \right) d\mathbf{y} \end{aligned}$$

The second term on the right is a KL divergence between centered Gaussian distributions. The lower bound follows from Jensen's inequality. The proof of the upper bound (appendix B) bounds this KL divergence above by $t/(2\sigma_n^2)$.

3.3. Minimizing the upper bound: an idealized case

We now consider the set of M interdomain inducing features that minimize the upper bounds in Lemmas 1 and 2. Taking into account the lower bound in Lemma 2, they must be within a factor of two of the optimal features defined without reference to training outputs under the assumption of Lemma 2. Consider

$$u_m := \sum_{i=1}^N w_i^{(m)} f(\mathbf{x}_i)$$

where $w_i^{(m)}$ is the i^{th} entry in the m^{th} eigenvector of \mathbf{K}_{ff} . That is, u_m is a linear combination of inducing points placed at each data point, with weights coming from the entries of the m^{th} eigenvector of \mathbf{K}_{ff} . We show in appendix C that

$$\text{cov}(u_m, u_k) = \mathbf{w}^{(m)\top} \mathbf{K}_{ff} \mathbf{w}^{(k)} = \lambda_k(\mathbf{K}_{ff}) \delta_{m,k}, \quad (8)$$

$$\text{cov}(u_m, f(\mathbf{x}_i)) = [\mathbf{K}_{ff} \mathbf{w}^{(m)}]_i = \lambda_m(\mathbf{K}_{ff}) w_i^{(m)}. \quad (9)$$

Inference with these features can be seen as the variational equivalent of the optimal parametric projection of the model derived by Ferrari-Trecate et al. [1999].

Computation with these features requires computing the matrices \mathbf{K}_{uf} and \mathbf{K}_{uu} . \mathbf{K}_{uu} contains the first M eigenvalues of \mathbf{K}_{ff} , \mathbf{K}_{uf} contains the corresponding eigenvectors. Computing the first M eigenvalues and vectors (i.e. performing a truncated SVD of \mathbf{K}_{ff}) can be done in $\mathcal{O}(N^2 M)$ using, for example, Lanczos iteration [Lanczos, 1950]. With these features \mathbf{Q}_{ff} is the *optimal* rank- M approximation to \mathbf{K}_{ff} and leads to $\lambda_{max} = \lambda_{M+1}(\mathbf{K}_{ff})$ and $t = \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{ff})$.

3.4. Eigenfunction inducing features

We now modify the construction given in section 3.3 to no longer depend on \mathbf{K}_{ff} explicitly (which depends on the specific training inputs) and instead depend on assumptions about the training data. This construction is the *a priori* counterpart of the eigenvector inducing features, as it is defined prior to observing a specific set of training inputs.

Consider the limit as we have observed a large amount of data, so that $\frac{1}{N} \mathbf{K}_{ff} \rightarrow \mathcal{K}$. This leads us to replace the eigenvalues, $\{\lambda_m(\mathbf{K}_{ff})\}_{m=1}^M$, with the operator eigenvalues, $\{\lambda_m\}_{m=1}^M$, and the eigenvectors, $\{\mathbf{w}^{(m)}\}_{m=1}^M$, with the eigenfunctions, $\{\phi_m\}_{m=1}^M$, yielding

$$u_m = \int_{\mathcal{X}} f(\mathbf{x}) \phi_m(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}. \quad (10)$$

Note that $p(\mathbf{x})$ influences u_m . In appendix C, we show

$$\text{cov}(u_m, u_k) = \lambda_m \delta_{m,k} \text{ and } \text{cov}(u_m, f(\mathbf{x}_i)) = \lambda_m \phi_m(\mathbf{x}_i).$$

These features can be seen as the variational equivalent of methods utilizing truncated priors proposed in Zhu et al. [1997], which are the optimal linear M dimensional parametric GP approximation defined *a priori*, in terms of minimizing expected mean square error.

In the case of the SE kernel and Gaussian inputs, closed form expressions for eigenfunctions and values are known [Zhu et al., 1997]. For Matérn kernels with inputs uniform on $[a, b]$, expressions for the eigenfunctions and eigenvalues needed in order to compute \mathbf{K}_{uf} and \mathbf{K}_{uu} can be found in Youla [1957]. However, the formulas involve solving systems of transcendental equations limiting the practical applicability of these features for Matérn kernels.

3.5. A priori bounds on the KL divergence for eigenfunction features

Having developed the necessary preliminary results, we now prove the first a priori bounds on the KL divergence. We start with eigenfunction features, which can be implemented practically in certain instances discussed above.

Theorem 1. Suppose N training inputs are drawn i.i.d. according to input density $p(\mathbf{x})$. For inference with M eigenfunction inducing variables defined with respect to the prior kernel and $p(\mathbf{x})$, with probability at least $1 - \delta$,

$$\text{KL}(Q \parallel \hat{P}) \leq \frac{C}{2\sigma_n^2 \delta} \left(1 + \frac{\|\mathbf{y}\|_2^2}{\sigma_n^2} \right) \quad (11)$$

where we have defined $C = N \sum_{m=M+1}^{\infty} \lambda_m$, and the λ_m are the eigenvalues of the integral operator \mathcal{K} associated to the prior kernel and $p(\mathbf{x})$.

Theorem 2. With the assumptions and notation of Theorem 1 if \mathbf{y} is distributed according to a sample from the prior generative model, with probability at least $1 - \delta$,

$$\text{KL}(Q \parallel \hat{P}) \leq \frac{C}{\delta \sigma_n^2}, \quad (12)$$

Sketch of Proof of Theorems 1 and 2. We first prove a bound on t that holds in expectation over input data matrices of size N with entries drawn i.i.d. from $p(\mathbf{x})$.

A direct computation of \mathbf{Q}_{ff} shows that $[\mathbf{Q}_{\text{ff}}]_{i,j} = \sum_{m=1}^M \lambda_m \phi_m(\mathbf{x}_i) \phi_m(\mathbf{x}_j)$. Using the Mercer expansion of the kernel matrix and subtracting,

$$[\tilde{\mathbf{K}}_{\text{ff}}]_{i,i} = \sum_{m=M+1}^{\infty} \lambda_m \phi_m^2(\mathbf{x}_i).$$

Summing this and taking the expectation,

$$\mathbb{E}_{\mathbf{X}}[t] = N \sum_{m=M+1}^{\infty} \lambda_m \mathbb{E}_{\mathbf{x}_i} [\phi_m^2(\mathbf{x}_i)] = N \sum_{m=M+1}^{\infty} \lambda_m.$$

The second equality follows from the eigenfunctions having norm 1. Applying Markov's inequality and Lemmas 1 and 2 yields Theorems 1 and 2 respectively. \square

3.6. Squared exponential kernel and Gaussian inputs

For the SE kernel in one-dimension with hyperparameters (v, ℓ^2) and $p(x) \sim \mathcal{N}(0, \sigma^2)$,

$$\lambda_m = v \sqrt{2a/AB^{m-1}}$$

where $a = 1/(4\sigma^2)$, $b = 1/(2\ell^2)$, $c = \sqrt{a^2 + 2ab}$, $A = a + b + c$ and $B = b/A$ [Zhu et al., 1997]. In this case, using the geometric series formula,

$$\sum_{m=M+1}^{\infty} \lambda_m = \frac{v \sqrt{2a}}{(1-B)\sqrt{A}} B^M.$$

Using this bound with Theorems 1 and 2, we see that by choosing $M = \mathcal{O}(\log N)$, under the assumptions of either theorem, we can obtain a bound on the KL divergence that tends to 0 as N tends to infinity.

3.7. Matérn kernels and uniform measure

For the Matérn $k + 1/2$ kernel, $\lambda_m \asymp m^{-2k-2}$ [Ritter et al., 1995], so $\sum_{m=M+1}^{\infty} \lambda_m = \mathcal{O}(M^{-2k-1})$. In order for the bound in Theorem 2 to converge to 0, we need $\lim_{N \rightarrow \infty} \frac{N}{M^{2k+1}} \rightarrow 0$. This holds if $M = N^\alpha$ for $\alpha > \frac{1}{2k+1}$. For $k > 0$, this bound indicates the number of inducing features can grow sublinearly with the amount of data.

4. Bounds for inducing points

We have shown that using spectral knowledge of either \mathbf{K}_{ff} or \mathcal{K} we obtain bounds on the KL divergence indicating that the number of inducing features can be much smaller than the number of data points. While mathematically convenient, the practical applicability of the interdomain features used is limited by computational considerations in the case of the eigenvector features and by the lack of analytic expressions for \mathbf{K}_{uf} in most cases for the eigenfunction features, as well not knowing the true input density, $p(\mathbf{x})$.

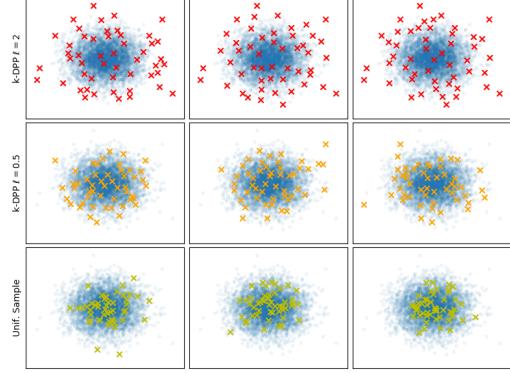


Figure 2. Determinant based sampling, with a SE kernel with $\ell = 2$ (top) and with $\ell = .5$ (middle) leads to more dispersed inducing points than uniform sampling (bottom).

In contrast, inducing points can be efficiently applied to any kernel. In this section, we show that with a good initialization based on the empirical input data distribution, inducing points lead to bounds that are only slightly weaker than the interdomain approaches suggested so far.

Proving this amounts to obtaining bounds on the trace of the error of a Nyström approximation to \mathbf{K}_{ff} . The Nyström approximation, popularized for kernel methods by Williams & Seeger [2001], approximates a positive semi-definite symmetric matrix by subsampling columns. If M columns, $\{\mathbf{c}_i\}_{i=1}^M$, are selected from \mathbf{K}_{ff} , the approximation used is $\mathbf{K}_{\text{ff}} \approx \mathbf{C} \bar{\mathbf{C}}^{-1} \mathbf{C}^\top$, where $\mathbf{C} = [\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_M]$ and $\bar{\mathbf{C}}$ is the $M \times M$ principal submatrix associated to the $\{\mathbf{c}_i\}_{i=1}^M$. Note that if inducing points are placed at the points associated to each column in the data matrix, then $\mathbf{K}_{\text{uu}} = \bar{\mathbf{C}}$ and $\mathbf{K}_{\text{uf}}^\top = \mathbf{C}$, so $\mathbf{Q}_{\text{ff}} = \mathbf{C} \bar{\mathbf{C}}^{-1} \mathbf{C}^\top$.

Lemma 3. [Belabbas & Wolfe, 2009] Given a symmetric positive semidefinite matrix, \mathbf{K}_{ff} , if M columns are selected to form a Nyström approximation such that the probability of selecting a subset of columns, Z , is proportional to the determinant of the principal submatrix formed by these columns and the matching rows, then,

$$\mathbb{E}_Z [\text{Tr}(\mathbf{K}_{\text{ff}} - \mathbf{Q}_{\text{ff}})] \leq (M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{\text{ff}}). \quad (13)$$

This means that on average well-initialized inducing points lead to bounds within a factor of $M+1$ of eigenvector inducing features.

The selection scheme described introduces negative correlations between inducing points locations, leading the \mathbf{z}_i to be well-dispersed amongst the training data, as shown in fig. 2. The strength of these negative correlations is determined by the particular kernel.

The proposed initialization scheme is equivalent to sampling Z according to a discrete k-Determinantal Point Process (k-DPP), defined over \mathbf{K}_{ff} . Belabbas & Wolfe [2009] suggested that sampling from this distribution, which has support over $\binom{N}{M}$ subsets of columns, may be computationally infeasible. Kulesza & Taskar [2011] provided an exact algorithm for sampling from k-DPPs given an eigendecomposition of the kernel matrix. In our setting, we require our initialisation scheme to have similar computational cost to computing the sparse GP bounds, which prohibits us from performing eigendecomposition. Instead, we rely on cheaper “ ϵ close” sampling methods. We therefore provide the following corollary of lemma 3, proven in appendix D.

Corollary 1. Suppose the inducing points, Z , are sampled from an ϵ k-DPP, ν , i.e a distribution over subsets of \mathbf{X} of size M satisfying, $d(\mu, \nu)_{TV} \leq \epsilon$ where $d(\cdot, \cdot)_{TV}$ denotes total variation distance and μ is a k-DPP on \mathbf{K}_{ff} . Suppose the $k(\mathbf{x}, \mathbf{x}) < v$ for all $\mathbf{x} \in \mathcal{X}$. Then

$$\mathbb{E}_{Z \sim \nu}[t] \leq (M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{\text{ff}}) + 2Nv\epsilon. \quad (14)$$

4.1. A priori bounds for inducing points

We show analogues of theorems 1 and 2 for inducing points.

Theorem 3. Suppose N training inputs are drawn i.i.d according to input density $p(\mathbf{x})$, and $k(\mathbf{x}, \mathbf{x}) < v$ for all $\mathbf{x} \in \mathcal{X}$. Sample M inducing points from the training data with the probability assigned to any set of size M equal to the probability assigned to the corresponding subset by an ϵ k-DPP with $k = M$. With probability at least $1 - \delta$,

$$\text{KL}(Q \parallel \hat{P}) \leq \frac{C(M+1) + 2Nv\epsilon}{2\sigma_n^2 \delta} \left(1 + \frac{\|\mathbf{y}\|_2^2}{\sigma_n^2}\right) \quad (15)$$

where $C = N \sum_{m=M+1}^{\infty} \lambda_m$, and λ_m are the eigenvalues of the integral operator \mathcal{K} associated to kernel, k , and $p(\mathbf{x})$.

Theorem 4. With the assumptions and notation of theorem 3 and if \mathbf{y} is distributed according to a sample from the prior generative model, with probability at least $1 - \delta$,

$$\text{KL}(Q \parallel \hat{P}) \leq \frac{C(M+1) + 2Nv\epsilon}{\delta\sigma_n^2}. \quad (16)$$

Proof. We prove theorem 4. Theorem 3 follows the same argument, replacing the expectation over \mathbf{y} with the bound given by lemma 1.

$$\begin{aligned} \mathbb{E}_{\mathbf{X}} \left[\mathbb{E}_{Z|\mathbf{X}} \left[\mathbb{E}_{\mathbf{y}} \left[\text{KL}(Q \parallel \hat{P}) \right] \right] \right] &\leq \sigma_n^{-2} \mathbb{E}_{\mathbf{X}} [\mathbb{E}_{Z|\mathbf{X}}[t]] \\ &\leq \sigma_n^{-2} (M+1) \mathbb{E}_{\mathbf{X}} \left[\sum_{m=M+1}^N \lambda_m(\mathbf{K}_{\text{ff}}) \right] + 2Nv\epsilon \\ &\leq \sigma_n^{-2} (M+1) N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon. \end{aligned}$$

The first two inequalities use lemma 2 and corollary 1. The third follows from noting that the sum inside the expectation is the error in trace norm of the optimal rank M approximation to the covariance matrix for any given \mathbf{X} , and is bounded above by the error from the rank M approximation due to eigenfunction features. We showed that this error is in expectation equal to $N \sum_{m=M+1}^{\infty} \lambda_m$ so this must be an upper bound on the expectation in the second to last line.¹

We apply Markov’s inequality, yielding for any $\delta \in (0, 1)$ with probability at least $1 - \delta$,

$$\text{KL}(Q \parallel \hat{P}) \leq \frac{(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon}{\delta\sigma_n^2}. \quad \square$$

Figure 3 compares the actual KL divergence, the *a posteriori* bound derived by $\mathcal{L}_{\text{upper}} - \mathcal{L}_{\text{lower}}$, and the bounds proven in theorems 3 and 4 on a dataset with normally distributed training inputs and \mathbf{y} drawn from the generative model.

5. Consequences of theorem 3 and theorem 4

We now investigate implications of our main results for sparse GP regression. Our first two corollaries consider Gaussian inputs and the squared exponential (SE) kernel, and show that in D dimensions, choosing $M = \mathcal{O}(\log^D(N))$ is sufficient in order for the KL divergence to converge with high probability. We then briefly summarize convergence rates for other stationary kernels. Finally we point out consequences of our definition of convergence for the quality of the pointwise posterior mean and uncertainty.

5.1. Comparison of consequences of theorems

Using the explicit formula for the eigenvalues given in section 3.6, we arrive at the following corollary:

Corollary 2. Suppose that $\|\mathbf{y}\|_2^2 \leq RN$. Fix $\gamma > 0$, and take $\epsilon = \frac{\delta\sigma_n^2}{vN^{\gamma+2}}$. Assume the input data is normally distributed and regression is performed with a SE kernel. Under the assumptions of theorem 3, with probability $1 - \delta$,

$$\text{KL}(Q \parallel \hat{P}) \leq N^{-\gamma} (2R/\sigma_n^2 + 2/N). \quad (17)$$

when inference is performed with $M = \frac{(3+\gamma)\log(N)+\log D}{\log(B^{-1})}$, where $D = \frac{v\sqrt{2a}}{2\sqrt{A}\sigma_n^2 \delta(1-B)}$.

The proof is given in appendix E. If the lengthscale is much shorter than the standard deviation of the data then B will be near 1, implying that M will need to be large in order for the bound to converge.

¹ Shawe-Taylor et al. [2005, Proposition 4] gives a different proof of the final inequality.

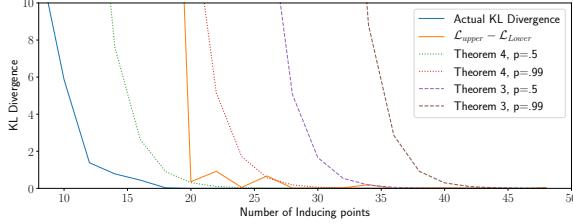


Figure 3. Rates of convergence as M increases on fixed dataset of size $N = 1000$, with a SE-kernel with $\ell = .6$, $v = 1$, $\sigma_n = 1$ and $x \sim \mathcal{N}(0, 1)$ and y sampled from the prior.

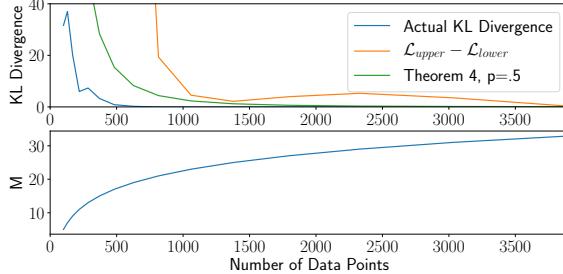


Figure 4. We increase N and take $M = C \log(N)$ for a one-dimensional SE-kernel and normally distributed inputs. The KL divergence decays rapidly, as predicted by Corollary 2.

Remark 1. The assumption $\|y\|_2^2 \leq RN$ for some R is very weak. For example, if y is a realization of an integrable function with constant noise,

$$\sum_{i=1}^N y_i^2 \leq \sum_{i=1}^N f(\mathbf{x}_i)^2 + \sum_{i=1}^N \epsilon_i^2 + o(N)$$

The first sum is asymptotically $N \int f(\mathbf{x})p(\mathbf{x})dx$, and the second is asymptotically $N\sigma_n^2$.

The consequence of corollary 2 is shown in fig. 4, in which we gradually increase N , choosing $M = C \log(N) + C_0$, and see the KL divergence converges as an inverse power of N . The training outputs are generated from a sample from the prior generative model. Note that as theorem 4 assumes y is sampled from the prior and is not derived using the upper bound (eq. 4); it may be tighter than the a posteriori bound in cases when this upper bound is not tight.

For the SE kernel and Gaussian inputs, the rate that we prove M must increase for inducing points and eigenfunction features differs by a constant factor. For the Matérn $k + 1/2$ kernel, we need to choose $M = N^\alpha$ with $\alpha > 1/(2k)$ instead of $\alpha > 1/(2k + 1)$. This difference is particularly stark in the case of the Matérn $3/2$ kernel, for which our bounds tell us that inference with inducing points requires $\alpha > 1/2$ as opposed to $\alpha > 1/3$ for the eigenfunction features. Whether this is an artifact of the proof, the initialization scheme, or an inherent limitation for inducing points is an interesting area for future work.

5.2. Multidimensional data, effect of input density and other kernels

If $\mathcal{X} = \mathbb{R}^D$, it is common to choose a *separable kernel*, i.e a kernel that can be written as a product of kernels along each dimension. If this choice is made, and input densities factor over the dimensions, the eigenvalues of \mathcal{K} are the product of the eigenvalues along each dimension. In the case of the SE-ARD kernel and Gaussian input distribution, we obtain an analogous statement to corollary 2 in D -dimensions.

Corollary 3. For any fixed $\epsilon', \delta > 0$ under the assumptions of corollary 2, with a SE-ARD kernel in D dimensions, $p(\mathbf{x})$ a multivariate Gaussian, $M = \mathcal{O}(\log^D N)$ inducing points and $\epsilon = \mathcal{O}(N^{-\gamma})$ for some fixed $\gamma > 2$, with probability at least $1 - \delta$, $\text{KL}\left(Q \parallel \hat{P}\right) \leq \delta^{-1}\epsilon'$.

The proof uses ideas from Seeger et al. [2008] and is given in appendix E. While for the SE kernel and Gaussian input density M can grow polylogarithmically in N , and the KL divergence still converges, this is not the case for regression with other kernels or input distribution.

Closed form expressions for the eigenvalues of operators associated to many kernels and input distributions are not known. For stationary kernels and compactly supported input distributions, the asymptotic rate of decay of the eigenvalues of \mathcal{K} is well-understood [Widom, 1963; 1964; Ritter et al., 1995]. The intuitive summary of these results is that smooth kernels, with concentrated input distributions have rapidly decaying eigenvalues. In contrast, kernels such as the Matérn-1/2 that define processes that are not smooth have slowly decaying eigenvalues. For Lebesgue measure on $[a, b]$ the Sacks-Ylivašker conditions of order r (appendix F), which can be roughly thought of as meaning that realizations of the process are r times differentiable with probability 1 [Ritter et al., 1995], implies an eigenvalue decay of $\lambda_m \asymp m^{-2r-2}$. Table 1 summarizes the spectral decay of several stationary kernels, as well as the implications for the number of inducing points needed for inference to provably converge with our bounds.

5.3. Computational complexity

We now have all the components necessary for analyzing the overall computational complexity of finding an arbitrarily good GP approximation. To understand the full computational complexity, we must consider the cost of initializing the inducing points using an exact or approximate k-DPP, as well as the $\mathcal{O}(NM^2)$ time complexity of variational inference. Recent work of Dereziński et al. [2019] indicate that an exact algorithm for sampling a k-DPP can be implemented in $\mathcal{O}(N \log(N)\text{poly}(M))$. We base our method on Anari et al. [2016], who show that an ϵ k-DPP can be sampled via MCMC methods in $\mathcal{O}(NM^4 \log(N) + NM^3 \log(\frac{1}{\epsilon}))$ time with memory $\mathcal{O}(N+M^2)$ (see appendix

Table 1. The number of features needed for our bounds to converge in D -dimensions these hold for some fixed $\alpha > 0$ and any $\epsilon_D > 0$.

KERNEL	INPUT DISTRIBUTION	DECAY OF λ_m	M, THEOREM 3	M, THEOREM 4
SE-KERNEL	COMPACT SUPPORT	$\mathcal{O}(\exp(-\alpha \frac{m}{d} \log \frac{m}{d}))$	$\mathcal{O}(\log^D(N))$	$\mathcal{O}(\log^D(N))$
SE-KERNEL	GAUSSIAN	$\mathcal{O}(\exp(-\alpha \frac{m}{d}))$	$\mathcal{O}(\log^D(N))$	$\mathcal{O}(\log^D(N))$
MATÉRN $k+1/2$	UNIFORM ON INTERVAL	$\mathcal{O}(M^{-2k-2} \log(M)^{2(d-1)(k+1)})$	$\mathcal{O}(N^{1/k+\epsilon_D})$	$\mathcal{O}(N^{1/(2k)+\epsilon_D})$

D).² We can choose ϵ to be any inverse power of N which only adds a constant factor to the complexity. For the SE kernel, taking $M = \mathcal{O}(\log^D N)$ inducing points leads to a complexity of $\mathcal{O}(N \log^{4D+1} N)$, a large computational saving compared to the $\mathcal{O}(N^3)$ cost of exact inference. For the Matérn $k + \frac{1}{2}$ kernel and the average case analysis of theorem 4 we need to take $M = \mathcal{O}(N^{1/(2k)+\epsilon_D})$ implying a computational complexity of $\mathcal{O}(N^{1+2/k+4\epsilon_D} \log(N))$ which is an improvement over the cost of full inference for $k > 1$. Improvements in methods for sampling exact or approximate k-DPPs (e.g. recent bounds on mixing time [Hermen & Salez, 2019]) or bounds on other selection schemes for Nyström approximations directly translate to improved bounds on the computational cost of convergent sparse Gaussian process approximations through this framework.

5.4. Pointwise approximate posterior

In many applications, pointwise estimates of the posterior mean and variance are of interest. It is therefore desirable that the approximate variational posterior gives similar estimates of these quantities as the true posterior. Huggins et al. [2019] derived an approximation method for sparse GP inference with provable guarantees about pointwise mean and variance estimates of the posterior process and showed that approximations with moderate KL divergences can still have large deviations in mean and variance estimates. However, if the KL divergence converges to zero, estimates of mean and variance converge to the posterior values. By the chain rule of KL divergence [Matthews et al., 2016],

$$\begin{aligned} \text{KL}(\mu_{\mathcal{X}} \| \nu_{\mathcal{X}}) &= \text{KL}(\mu_{\mathbf{x}_*} \| \nu_{\mathbf{x}_*}) \\ &+ \mathbb{E}_{\mu_{\mathbf{x}_*}} [\text{KL}(\mu_{\mathcal{X} \setminus \mathbf{x}_* | \mathbf{x}_*} \| \nu_{\mathcal{X} \setminus \mathbf{x}_* | \mathbf{x}_*})] \geq \text{KL}(\mu_{\mathbf{x}_*} \| \nu_{\mathbf{x}_*}). \end{aligned}$$

Therefore, bounds on the mean and variance of a one-dimensional Gaussian with a small KL divergence imply pointwise guarantees about posterior inference when the KL divergence between processes is small.

Proposition 1. Suppose q and p are one dimensional Gaussian distributions with means μ_1 and μ_2 and variances σ_1^2 and σ_2^2 , such that $2\text{KL}(q \| p) = \varepsilon \leq \frac{1}{5}$, then

$$|\mu_1 - \mu_2| \leq \sigma_2 \sqrt{\varepsilon} \leq \frac{\sigma_1 \sqrt{\varepsilon}}{\sqrt{1 - \sqrt{3\varepsilon}}} \text{ and } |1 - \sigma_1^2/\sigma_2^2| < \sqrt{3\varepsilon}.$$

²Open source implementations of approximate k-DPPs are available (e.g. [Gautier et al., 2018]).

The proof is in appendix B. If $\epsilon \rightarrow 0$, proposition 1 implies $\mu_1 \rightarrow \mu_2$ and $\sigma_1 \rightarrow \sigma_2$. Using this and theorems 3 and 4, the posterior mean and variance converge pointwise to those of the full model using $M \ll N$ inducing features.

6. Related work

Statistical guarantees for convergence of parametric GP approximations [Zhu et al., 1997; Ferrari-Trecate et al., 1999], lead to similar conclusions about the choice of approximating rank. Ferrari-Trecate et al. [1999] showed that given N data points, using a rank M truncated SVD of the prior covariance matrix, such that $\lambda_M \ll \sigma_n^2/N$ results in almost no change in the model, in terms of expected mean squared error. Our results can be considered the equivalent for variational inference, showing that theoretical guarantees can be established for non-parametric approximate inference.

Guarantees on the quality Nyström approximations have been used to bound the error of approximate kernel methods, notably for kernel ridge regression [Alaoui & Mahoney, 2015; Li et al., 2016]. The specific method for selecting columns in the Nyström approximation plays a large role in these analyses. Li et al. [2016] use an approximate k-DPP, nearly identical to the initialization we analyze; Alaoui & Mahoney [2015] sample columns according to ridge leverage scores. The substantial literature on bounds for Nyström approximations [e.g. Gittens & Mahoney, 2013] motivates considering other initialization schemes for inducing points in the context of Gaussian process regression.

7. Conclusion

We proved bounds on the KL divergence between the variational approximation of sparse GP regression to the posterior, that depend only on the decay of the eigenvalues of the covariance operator. These bounds prove the intuitive result that smooth kernels with training data concentrated in a small region admit high quality, very sparse approximations. These bounds prove that truly sparse non-parametric inference, with $M \ll N$, can provide reliable estimates of the marginal likelihood and pointwise posterior.

Extensions to models with non-conjugate likelihoods, especially within the framework of Hensman et al. [2015], pose a promising direction for future research.

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