Rethinking Sparse Gaussian Processes: Bayesian Approaches to Inducing-Variable Approximations

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Abstract

Variational inference techniques based on inducing variables provide an elegant framework for scalable posterior estimation in Gaussian process (GP) models. Most previous works treat the locations of the inducing variables, i.e. the inducing inputs, as variational hyperparameters, and these are then optimized together with GP covariance hyper-parameters. While some approaches point to the benefits of a Bayesian treatment of GP hyper-parameters, this has been largely overlooked for the inducing inputs. In this work, we show that treating both inducing locations and GP hyper-parameters in a Bayesian way, by inferring their full posterior, further significantly improves performance. Based on stochastic gradient Hamiltonian Monte Carlo, we develop a fully Bayesian approach to scalable GP and deep GP models, and demonstrate its competitive performance through an extensive experimental campaign across several regression and classification problems.

1. Introduction and Motivation

Bayesian kernel machines based on Gaussian processes (GPs) offer the modeling flexibility of kernel methods combined with the ability to characterize the uncertainty in predictions and model parameters (Rasmussen & Williams, 2006). The field of GPs has considerably evolved in the last few years with key contributions in modeling and inference in the direction of making GPs scalable to virtually any number of data points, using mini-batches, and suitable for implementations in languages featuring automatic differentiation (Matthews et al., 2017; Krauth et al., 2017), thus making them easy to implement and use. This has been possible thanks to the combination of variational inference techniques with popular GP approximations, such as inducing points (Titsias, 2009; Lázaro-Gredilla & Figueiras-Vidal, 2009; Hensman et al., 2013), random features (Rahimi & Recht, 2008; Cutajar et al., 2017; Gal & Ghahramani, 2016), and structured approximations (Wilson & Nickisch, 2015; Wilson et al., 2016b). These advancements have now put GPs in the position to be attractive models for a variety of applications using a variety of likelihoods (Matthews et al., 2017; Bonilla et al., 2019).

Despite these significant insights, the common practice in GP models to date is to only carry out point estimation of the inducing inputs, usually via continuous optimization. In fact, the original work of Titsias (2009) advocates for the introduction of a new variable, which we refer to as the inducing inputs, and these are then optimized along with covariance hyper-parameters. In line with previous evidence that a fully Bayesian treatment of GPs is beneficial for performance of GP models (Neal, 1997; Barber & Williams, 1997; Murray & Adams, 2010; Filippone & Girolami, 2014), following up on the works on variational sparse GPs, there have been studies showing that full posterior inference of the inducing variables jointly with covariance hyper-parameters improves performance (Hensman et al., 2015b).

In this work, we focus in particular on variationally sparse GPs as originally formulated by Titsias (2009) and later developed by Hensman et al. (2013) to scale up to very large datasets via stochastic (mini-batch) optimization. In these formulations, the GP prior is augmented with inducing variables (drawn from the same prior) and their posterior is estimated via variational inference. In contrast, the locations of the inducing variables, which we refer to as the inducing inputs, are only optimized along with covariance hyper-parameters. In line with previous evidence that a fully Bayesian treatment of GPs is beneficial for performance of GP models (Neal, 1997; Barber & Williams, 1997; Murray & Adams, 2010; Filippone & Girolami, 2014), following up on the works on variational sparse GPs, there have been studies showing that full posterior inference of the inducing variables jointly with covariance hyper-parameters improves performance (Hensman et al., 2015b).

Table 1: A comparison of inference methods for GP models. \( \theta, U, Z \) refer to the GP latent function values, covariance hyper-parameters, inducing variables and inducing inputs, respectively. Notably, the variational methods do not infer exact posteriors.

| Model       | \( \theta \) | \( U \) | \( Z \) | Reference                     |
|-------------|-------------|--------|--------|--------------------------------|
| MCMC-GP     | \checkmark  | -      | -      | Neal (1997); Barber & Williams (1997) |
| SGHMC-DGP   | \xmark      | \checkmark | \checkmark | Hensman et al. (2015a)        |
| IPVI-DGP    | \checkmark  | \checkmark | \checkmark | Yang et al. (2019)            |
| MCMC-SVGP   | \checkmark  | \checkmark | \xmark  | Hensman et al. (2015b)        |
| BSGP        | \checkmark  | \checkmark | \checkmark | this work                     |

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Figure 1: Comparison of test mean negative loglikelihood (MNLL) on NAVAL (left) and PROTEIN (right) for different number of inducing variables and for determinantal point process prior (○), normal prior (○)), Strauss process prior (○) and uniform prior (○). Finally, (□) corresponds to the case of inducing points optimized and covariance hyper-parameters inferred similarly to Hensman et al. (2015a), while (--) is the performance reached by SGHMC-DGP with 100 points from Havasi et al. (2018b).

Figure 1 shows a preview of such results. By jointly inferring a free-form posterior on covariance hyper-parameters, inducing variables and inducing inputs one can considerably improve GP inference over state-of-the-art methods.

2. Preliminaries and Related Works

A GP defines a distribution over functions \( f: \mathbb{R}^D \rightarrow \mathbb{R} \), for which any finite marginal follows a Gaussian distribution (Rasmussen & Williams, 2005). A GP is fully described by a mean function \( m(x) \) and a covariance function \( k(x, x'; \theta) \) with hyper-parameters \( \theta \). Given a supervised learning problem with \( N \) pairs of inputs \( x_i \) and labels \( y_i \), \( D = \{(x_i, y_i)\} | x_i \in \mathbb{R}^D, y_i \in \mathbb{R} \}_{i=1,...,N} \), we consider a GP prior over functions which are fed to a suitable likelihood function to model the observed labels.

Denoting by \( f \in \mathbb{R}^N \) the realizations of the GP random variables at the \( N \) inputs \( X = \{x_1, \ldots, x_N\} \) and assuming a zero-mean GP prior, we have that \( p(f) = N(0, K_{xx; \theta}) \), where \( K_{xx; \theta} \) is the covariance matrix obtained by evaluating \( k(x, x'; \theta) \) over all input pairs \( x_i, x_j \) (we will drop the explicit parameterization on \( \theta \) to keep the notation uncluttered). In the Bayesian setting, given a suitable likelihood function \( p(y|f) \), the objective is to characterize the posterior \( p(f|y) \) given \( N \) pairs of inputs and labels (see Figure 2a). This inference problem is analytically tractable only in the case of a Gaussian likelihood \( y|f \sim N(f, \sigma^2 I) \), but it involves the costly \( O(N^3) \) inversion of the covariance matrix \( K_{xx} \).

Sparse GPs are a family of approximate models that address the scalability issue by introducing a set of \( M \) inducing variables \( u = (u_1, \ldots, u_M) \) at corresponding inducing inputs \( Z = (z_1, \ldots, z_M) \) such that \( u = f(z) \) (Snelson & Ghahramani, 2005). These inducing variables are assumed to be drawn from the same GP as the original process, yielding the joint prior \( p(f, u) = p(u)p(f|u) \) with

\[
p(u) = N(0, K_{zz})
p(f|u) = N(K_{xz}K_{zz}^{-1}u, K_{xx} - K_{xz}K_{zz}^{-1}K_{zx}) ,
\]

where \( K_{zz} = k(Z, Z) \), \( K_{xz} = k(X, Z) \) and \( K_{zx} = K_{xz}^T \) (see Figure 2b). After introducing the inducing variables, the interest is in obtaining a posterior distribution over \( f \) by relying on the set of inducing variables \( u \) so as to avoid costly algebraic operations with \( K_{xx} \in \mathbb{R}^{N \times N} \). A general framework to do this for any likelihood and at scale (using mini-batches) can be obtained using variational inference techniques (Titsias, 2009; Hensman et al., 2013; Bonilla et al., 2019). The main innovation in Titsias (2009) is the formulation of an approximate posterior \( q(f, u) \) within variational inference (Jordan et al., 1999) so as to develop such a framework. This variational distribution formulation has
An alternative treatment of the inducing variables under Bayesian Sparse Gaussian Processes (a), sparse GPs (b), and the proposed Bayesian sparse GPs (c) with priors on hyperparameters \( \theta \), inducing inputs \( Z \) and outputs \( u \).

come to be known as Titsias’ trick and has the form:

\[
q(f, u) = q(u) p(f|u).
\]

Following the variational inference approach, and using the above approximate posterior, we introduce the evidence lower bound (ELBO),

\[
\log p(y) \geq -KL [q(u) \parallel p(u)] + \mathbb{E}_{q(f,u)} \log p(y | f),
\]

where the Kullback-Leibler divergence \( KL \) term only involves \( M \)-dimensional distributions, as the exact conditional prior \( \text{Equation 1} \) is also used in the approximate posterior \( \text{Equation 2} \), which results in the KL involving \( N \)-dimensional distributions vanish. The second term in the expression above is usually referred to as the expected log likelihood (ELL) and, for factorized conditional likelihoods, it can be computed efficiently using quadrature or Monte Carlo (MC) sampling \( \text{Hensman et al., 2015a; Bonilla et al., 2019} \). Thus, posterior estimation under this framework involves constraining \( q(u) \) to have a parametric form (usually a Gaussian) and finding its parameters so as to optimize the ELBO above. This optimization can be carried out using stochastic-gradient methods operating on mini-batches yielding a time complexity of \( O(M^3) \).

### 2.1. MCMC for Variationally Sparse GPs

An alternative treatment of the inducing variables under the variational framework described above is to avoid constraining \( q(u) \) to have any parametric form or admitting simplistic factorizing assumptions. As shown by Hensman et al. (2015b), this can be, in fact, achieved by finding the optimal (unconstrained) distribution \( q(u) \) that maximizes the ELBO in \text{Equation 3} and sampling from it using techniques such as Markov chain Monte Carlo (MCMC). This optimal distribution can be shown to have the form

\[
\log q(u) = \mathbb{E}_{p(f|u)} \log p(y|f) + \log p(u) + C,
\]

where \( C \) is an unknown normalizing constant. This expression makes it apparent that sparse variational GPs can be seen as GP models with a Gaussian prior over the inducing variables and a likelihood which has a complicated form due to the expectation under the conditional \( p(f|u) \). This observation makes it possible to derive MCMC samplers for the posterior over \( u \), thus relaxing the constraint of having to deal with a fixed form approximation. The only difficulty is that the likelihood requires the computation of an expectation; however, as mentioned above, for most modeling problems where the likelihood factorizes, this expectation can be calculated as a sum of univariate integrals, for which it is easy to employ numerical quadrature.

Hensman et al. (2015b) also include the sampling of the hyper-parameters \( \theta \) jointly with \( u \); however, in order to do this efficiently, a whitening representation is employed, whereby the inducing variables are reparameterized as \( u = \text{L}_{uu}\nu \), with \( \text{K}_{zz} = \text{L}_{zz}\text{L}_{zz}^T \). The sampling scheme then amounts to sampling from the joint posterior over \( \nu, \theta \).

The actual sampling scheme proposed by Hensman et al. (2015b) employs a more efficient method based on Hamiltonian Monte Carlo (HMC, Duane et al., 1987; Neal, 2010). Given a potential energy function defined as \( U(u) = -\log p(u, y) = -\log p(u|y) + C \), Hamiltonian Monte Carlo (HMC) introduces auxiliary momentum variables \( \nu \) and it generates samples from the joint distribution \( p(u, \nu) \) by simulation of the Hamiltonian dynamics

\[
du = \text{M}^{-1}\nu dt,
\]

\[
d\nu = -\nabla U(u) dt,
\]

where \( \text{M} \) is the so called mass matrix, followed by a Metropolis accept/reject step.

### 2.2. Stochastic gradient HMC for Deep models

Different from classic HMC where it is required to compute the full gradients \( \nabla U(u) = -\nabla \log p(u|y) \), Stochastic Gradient Hamiltonian Monte Carlo (SGHMC) (Chen et al., 2014) allows to sample from the true intractable posterior by means of stochastic gradients, and without the need of Metropolis accept/reject steps, which would require access to the whole data set. By modeling the stochastic gradient noise as normally distributed \( \mathcal{N}(0, \Sigma) \), the (discretized) Hamiltonian dynamics are updated as follows

\[
u_{t+1} = \nu_t + \varepsilon \text{M}^{-1}\nu_t,
\]

\[
\nu_{t+1} = \nu_t - \varepsilon \nabla U(u) - \varepsilon \text{CM}^{-1}\nu_t + \mathcal{N}(0, 2\varepsilon(C - \tilde{B}))
\]

where \( \varepsilon \) is the step size, \( C \) is a user defined friction term and \( \text{B} \) is the estimated diffusion matrix of the gradient noise; see
e.g., Springenberg et al. (2016) for ideas on how to estimate these parameters.

A similar approach can be adopted for deep Gaussian processes (DGPs) (Damianou & Lawrence, 2013). A DGP is a model obtained by composing layers parameterized by GPs. Each layer is associated with a set of inducing inputs \{Z_i\}_{i=1}^{L} and a set of inducing variables \{U_i\}_{i=1}^{L} (Salimbeni & Deisenroth, 2017). SGHMC is the primary inference method used by Havasi et al. (2018a) for obtaining samples from the posterior distribution over the latent variables at all layers \{U_i\}_{i=1}^{L}. Recently, this has been approached using adversarial inference methods (Yu et al., 2019).

2.3. Other Approaches to Scalable and Bayesian GPs

It is worth mentioning that, as mentioned in section 1, other approaches to scalable inference in GPs have been proposed, which feature the possibility to operate using mini-batches. For example, looking at the feature-space view of kernel machines, Rahimi & Recht (2008) show how random features can be obtained for shift invariant covariance functions, like the commonly used squared exponential. These approximations are also useful for addressing the scalability of GPs and DGPs, as showed by Lázaro-Gredilla et al. (2010) and Cutajar et al. (2017). Similarly, the work on structured approximations of GPs (Saatçi, 2011) has found applications to develop a scalable framework for GPs, later developed to include the possibility to learn deep learning-based representations for the input (Wilson et al., 2016b).

The Gaussian process latent variable model (GPLVM) proposed by Lawrence (2005) is a popular approach to Bayesian nonlinear dimensionality reduction and its Bayesian extensions such as those developed by Titsias & Lawrence (2010) consider a prior over the inputs of a GP. Although these methods can be used for training GPs with missing or uncertain inputs, we are not aware of previous work adopting such methodologies for inducing inputs within scalable sparse GP models.

3. Fully Bayesian Sparse Deep Gaussian Process

In this section, we question the common practice of treating inducing inputs as variational parameters, and propose our Bayesian Sparse Gaussian Process (BSGP) framework, where we carry out full posterior estimation of these variables.

While GPs are advocated as fully probabilistic models, it is common practice to treat covariance hyper-parameters and inducing inputs through optimization, which somewhat goes against this philosophy. We argue that in the spirit of Bayesian modeling, any uncertainty in the covariance should be accounted for.

3.1. Bayesian treatment of sparse Gaussian processes

Given that the inducing inputs do have an imprint on the modeling capabilities of sparse GPs, it is natural to consider them as model parameters and attempt to infer these along with inducing variables and covariance hyper-parameters. For this purpose, we propose Bayesian Sparse Gaussian Process (BSGP)—a fully-Bayesian treatment of sparse Gaussian process. The corresponding generative model, illustrated in Figure 2c, is given as

\[
\begin{align*}
\theta & \sim p_\phi(\theta), \\
Z & \sim p_k(Z), \\
u | Z, \theta & \sim N(0, K_{zz}(\theta)), \\
f | u, Z, \theta & \sim N(K_{xz}(\theta)K_{zz}^{-1}u, K_{xx}(\theta)Z), \\
y | f, \sigma^2 & \sim N(f, \sigma^2I),
\end{align*}
\]

Figure 3: Representation of the posterior induced distribution on the covariance function computed at location \(x'\).
where $K_{xx|\theta,z}$ denotes the covariance matrix obtained by conditioning in the joint model, i.e. $K_{xx|\theta} = K_{xx|\theta} - K_{xz|\theta} K_{zz|\theta}^{-1} K_{xz|\theta}$. Although for simplicity we have specified a Gaussian conditional likelihood above, our approach does, in fact, handle other factorized conditional likelihood models. Figure 3 gives a pictorial illustration of the distribution over the covariance function induced by the posterior over inducing inputs computed at $x'$ for an RBF covariance function $k(x,x') = \sigma \exp(-||x-x'||^2\lambda^{-2})$.

Given the model above, and following a similar analysis as that described in Section 2.1, we can obtain the optimal variational form that minimizes $KL[q(\mathbf{f}^*, \mathbf{f}, \mathbf{u}, \theta) \| p(\mathbf{f}^*, \mathbf{f}, \mathbf{u}, \theta|\mathbf{y})]$, where $\mathbf{f}^*$ denotes functional values on all points of interest, a term well-defined even on infinite index sets (Matthews et al., 2016), which consider distributions over point sets (González et al., 2015). DPP is a repulsive point process, which gives higher probabilities to location diversity, controlled by the hyper-parameters $\lambda \equiv \theta$. Alternatively we also consider the Strauss process (see e.g. Daley & Vere-Jones, 2003; Strauss, 1975),

$$p_D(\mathbf{Z}) \propto \det K_{zz|\theta},$$

relates the probability of inducing locations to the volume of space spanned by the covariance (Lavancier et al., 2015). DPP is a repulsive point process, which gives higher probabilities to location diversity, controlled by the hyper-parameters $\xi \equiv \theta$. Alternatively we also consider the Strauss process (see e.g. Daley & Vere-Jones, 2003; Strauss, 1975),

$$p_S(\mathbf{Z}) \propto \lambda^M \gamma \sum_{\mathbf{x',x} \in \mathbf{Z}} \delta(||\mathbf{x} - \mathbf{x}'|| < r),$$

where $\lambda > 0$ is the intensity, and $0 < \gamma \leq 1$ is the repulsion coefficient which decays the prior as a function of the number of location pairs that are within distance $r$. The Strauss prior (S) tends to maintain the minimum distance between inducing locations, parameterised by $\xi = (\lambda, \gamma, r)$. We finally include a vanishing uninformative uniform prior (U), $\log p_U(\mathbf{Z}) = 0$, as a naive baseline for reference.

Figure 4: Comparison of the posterior over the inducing position $p(\mathbf{Z}|\mathbf{y})$ for different choices of prior. On the right, the posterior over covariance hyper-parameters $p(\lambda|\mathbf{y})$ and $p(\sigma|\mathbf{y})$. We therefore obtain stochastic gradient estimates of

$$U(\mathbf{u}, \mathbf{z}, \theta) = -\log q(\mathbf{u}, \mathbf{z}, \theta) + \log C,$$

where $C$ is the prior over covariance hyper-parameters. We begin by proposing a simple Normal (N) prior

$$p_N(\mathbf{Z}) = \prod_{j=1}^{M} N(\mathbf{z}_j|0, \mathbf{I}),$$

which matches the mean and variance of the normalized data distribution, and favors inducing locations toward the barcenter of the data inputs.
To gain insights on the choice of these priors, we set up a comparative analysis on a toy 1D regression task and on the BANANA dataset. Figure 4 visualizes the inducing location and kernel parameter posteriors with respect to the four priors on a 1D simulated toy dataset. We observe that the posterior densities on the inducing position are multimodal and highly non-Gaussian, further confirming the necessity of free form inference. Both Strauss and DPP priors lead approximately to evenly spread inducing locations. Figure 5 shows the inducing posteriors on a two-dimensional banana classification example, where accurate decision boundaries require some inducing location proximity, which results in the superior performance obtained by the Normal prior (N).

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Prior on covariance hyper-parameters. Choosing a proper prior on the hyper-parameters has been discussed in previous works on Bayesian inference for GPs (see e.g. Filippone & Girolami, 2014). Throughout the paper, we use the RBF covariance with marginal variance $\sigma$ and one lengthscale $\lambda_i$ per feature (automatic relevance determination (Mackay, 1994)). On these two hyper-parameters we place a lognormal prior with unit variance and means equal to 1 and 0.05 for $\lambda$ and $\sigma$, respectively.

4. Experiments

In this section, we will provide empirical evidence of the benefits of BSGP in shallow and deep GPs.

4.1. UCI benchmark

We start our evaluation with a benchmark on 8 small to moderate sized UCI regression datasets. The input points and targets are normalized with zero mean and unit variance. We perform 8 different splits of train/test set with 0.8/0.2 ratio, and train the different models for 10,000 iterations with a learning rate fixed at 0.01 and a minibatch size of 1,000 samples. We then proceed to collect 256 samples, used for computing the predictive test metrics. We compare against two current state-of-the-art deep GP methods SGHMC-DGP (Havasi et al., 2018b) and IPVI-DGP (Yu et al., 2019), and against the shallow SVGP baseline (Hensman et al., 2015a).

Choosing the prior. As described in Section 3.2, we propose different types of priors on the inducing positions: determinantal point process prior, standard normal prior, Strauss prior and uniform. Next, we compare the performance of the four priors on a single layer BSGP over the UCI datasets (see Figure 7). The results show that the
Normal prior consistently outperforms other priors. The uniform and Strauss priors behave similarly, while the Determinantal prior has the largest variance.

A comment on computational efficiency. Similarly to the competing baseline algorithms, each iteration of BSGP involves the computation of the covariance matrix and its inverse with complexity $O(M^3)$. Computing the predictive distribution, on the other hand, is more challenging as it requires recomputing the covariance matrices $K_{xx}$, $K_{xz}$ for each posterior sample $z$, for an overall complexity linear on the number of posterior samples. Nonetheless, this operation can be parallelized, thus taking full advantage of the high-performance parallel computing power of GPUs.

We show this trade-off in practice for a shallow GP and a 2-layer DGP in Figure 8, where we compare the three main methods with a fixed training time budget of one hour. The experiment is repeated four times on the same fold and
After a burn-in phase of 10,000 iterations, we draw 200 (although the single gradient step requires a bit more time – AIRLINE

The Average number of gradient evaluations per second on Table 2:

\[ \hat{\text{R}} \text{ compares the within-chain vari-} \]

ance to between-chain variance. This diagnostic yielded a \( \hat{\text{R}} = 1.02 \pm 0.045 \), which indicates good convergence. Finally, we visualise the prediction marginals and the trace for 3 test points for further indication of mixing in the Supplements.

As a final large scale test, we opt for the HIGGS dataset (Baldi et al., 2014). With 11 millions data points and 28 features each, this dataset was created by Monte Carlo simulations of particle dynamics in accelerators to help detecting the Higgs boson. We select 90% of the these points for training, while the rest is kept for testing. Table 4 reports the final test performance, showing that BSGP outperforms the competitive methods. Interestingly, in both these large scale experiments, SGHMC-GP always falls back considerably w.r.t. BSGP and even SVGP. We argue that, with these large sized datasets, the continuous alternation of optimization of \( \mathbf{Z} \) and \( \mathbf{\theta} \) and sampling of \( \mathbf{U} \) used by the Authors (called Moving Window MCEM – see Havasi et al. (2018a) for further details) might have lead to suboptimal solutions.

4.2. Large scale classification

The AIRLINE dataset is a classic benchmark for large scale prediction task. It collects all commercial flights in USA during 2008, counting more than 5 millions data points. The goal is to find if a flight will be delayed based on 8 features, namely month, day of month, day of week, airtime, distance, arrival time, departure time and age of the plane. We pre-process the dataset following the guidelines provided by Hensman et al. (2015b) and Wilson et al. (2016a).

After a burn-in phase of 10,000 iterations, we draw 200 samples with 1000 simulation steps in between. We test on 100,000 randomly selected held-out points. We fit three models with \( M = 100 \) inducing points. Table 3 shows the predictive performance of three shallow GP models over test fold. The BSGP improves upon both inference methods of SGHMC-GP and SVGP over all criteria of test error, test MNLL and test area under the curve (AUC). We assess the convergence of the predictive posterior by evaluating the \( \hat{\text{R}} \)-statistics (Gelman et al., 2004) over 4 SGHMC sampler chains. The \( \hat{\text{R}} \) compares the within-chain vari-

\begin{table}[h]
\centering
\caption{AIRLINE dataset predictive test performance.} \label{tab:airline}
\begin{tabular}{lccc}
\hline
Model & error (\%) & MNLL (\$) & AUC (\$) \\
\hline
SGHMC-GP & 35.85 & 0.646 & 0.671 \\
SVGP & 31.26 & 0.595 & 0.730 \\
BSGP & 30.46 & 0.580 & 0.749 \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{HIGGS dataset predictive test performance.} \label{tab:higgs}
\begin{tabular}{lccc}
\hline
Model & error (\%) & MNLL (\$) & AUC (\$) \\
\hline
SGHMC-GP & 35.39 & 0.628 & 0.698 \\
SVGP & 27.79 & 0.544 & 0.796 \\
BSGP & 26.97 & 0.530 & 0.808 \\
\hline
\end{tabular}
\end{table}

the results are then averaged. Each run is performed on an isolated instance in a cloud computing platform with 8 CPU cores and 8 GB of memory reserved. Inference on the test set is performed every 250 iterations.

BSGP converges dramatically faster in wall-clock time into superior solutions over state-of-the-art competing methods (although the single gradient step requires a bit more time – see Table 2).

5. Conclusion & Discussion

We have developed a fully Bayesian treatment of sparse Gaussian process models that considers the inducing inputs, along with the inducing variables and covariance hyper-parameters, as random variables, places suitable priors and carries out approximate inference over them. Our approach, based on SGHMC, investigated two conventional priors (Gaussian and uniform) for the inducing inputs as well as two point process based priors (the Determinantal and the Strauss processes).

By challenging the standard belief of most previous work on sparse GP inference that assumes the inducing inputs can be estimated point-wisely, we have developed a state-of-the-art inference method and have demonstrated its outstanding performance on both accuracy and running time on regression and classification problems. We hope this work can have an impact similar (or better) to other works in machine learning that have adopted more elaborate Bayesian machinery (e.g. Wallach et al., 2009) for long-standing inference problems in commonly used probabilistic models.

Finally, we believe it is worth investigating further more structured priors similar to those presented here (e.g. exploring different hyper-parameter settings), including a full joint treatment of inducing inputs and their number, i.e. \( p(\mathbf{Z}, M) \). We leave this as future work. We are currently investigating ways to extend BSGP to convolutional Gaussian process (van der Wilk et al., 2017; Dutordoir et al., 2019; Blomqvist et al., 2018).

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Yu, H., Chen, Y., Low, B. K. H., Jaillet, P., and Dai, Z. Implicit Posterior Variational Inference for Deep Gaussian Processes. In Wallach, H., Larochelle, H., Beygelzimer, A., d’Alché Buc, F., Fox, E., and Garnett, R. (eds.), Advances in Neural Information Processing Systems 32, pp. 14475–14486. Curran Associates, Inc., 2019.
A. Derivation for Deep Gaussian Processes

In this section, we derive the mathematical basis for the Bayesian treatment of inducing inputs in a DGP setting (Damianou & Lawrence, 2013). This derivation extends the one in Section 2 of Hensman et al. (2015b), where we add deep GPs, prior on inducing inputs and stochastic gradients. We assume a deep Gaussian process prior \( f^L \circ f^{L-1} \circ \cdots \circ f^1 \), where each \( f^\ell \) is a GP. For notational brevity, we use \( \theta^\ell \) as both kernel hyper-parameters and inducing inputs of the \( \ell \)-th layer, and \( f^\ell_\ell \) as the input vector \( X \). We also denote \( f^\ell_\ell \) as the latent function values for layer \( \ell \) at other input points of interest. Then we can write down the joint distribution over visible and latent variables (omitting the dependency on \( X \) for clarity) as

\[
p \left( y, \{ \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) = p \left( y \mid \mathbf{f}^L \right) \prod_{\ell=1}^L p \left( \mathbf{f}^\ell \mid \mathbf{u}^\ell, \mathbf{f}^{\ell-1}, \theta^\ell \right) p \left( \mathbf{u}^\ell \mid \theta^\ell \right) p(\theta^\ell). \tag{10}
\]

Our goal is to estimate the posterior \( p \left( \{ \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \mid y \right) \), which we can use to compute the predictive distribution

\[
p \left( \mathbf{f}^L \mid y \right) = \int p \left( \{ \mathbf{f}^\ell \}_{\ell=1}^L \mid \{ \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) p \left( \{ \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \mid y \right) d\{ \mathbf{f}^\ell \}_{\ell=1}^{L-1}, \{ \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L. \tag{11}
\]

Given that the posterior \( p \left( \{ \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \mid y \right) \) is intractable, we can use the following variational approximation over all latent variables (including \( \{ f^\ell_\ell \} \)):

\[
q \left( \{ \mathbf{f}^\ell_\ell, \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) = p \left( \{ \mathbf{f}^\ell_\ell \}_{\ell=1}^L \mid \{ \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) \prod_{\ell=1}^L p \left( \mathbf{f}^\ell \mid \mathbf{u}^\ell, \mathbf{f}^{\ell-1}, \theta^\ell \right) q \left( \{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right). \tag{12}
\]

where, analogously to the GP case, we have used the exact conditionals \( p(\{ f^\ell_\ell \}_{\ell=1}^L \mid \{ f^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L ) \) and \( p(\mathbf{f}^\ell \mid \mathbf{u}^\ell, \mathbf{f}^{\ell-1}, \theta^\ell ) \). More importantly, we will let the variational posterior over inducing variables and hyper-parameters (including inducing inputs) \( q(\{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L ) \) be a free-form distribution which we will sample from. In order to obtain this optimal posterior, we can thus minimize the KL-divergence between the approximate posterior \( q(\{ f^\ell_\ell, \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L ) \) and the true posterior \( p(\{ f^\ell_\ell, \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \mid y ) \) as follows,

\[
\text{KL} \left[ q \left( \{ f^\ell_\ell, \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) \parallel p \left( \{ f^\ell_\ell, \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \mid y \right) \right] = - \mathbb{E}_{q(\{ f^\ell_\ell, \mathbf{f}^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L )} \left[ \log \frac{p \left( \{ f^\ell_\ell \}_{\ell=1}^L \mid \{ f^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) p \left( \{ f^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \mid y \right)}{p \left( \{ f^\ell_\ell \}_{\ell=1}^L \mid \{ f^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) q \left( \{ f^\ell, \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right)} \right]
\]

\[
= - \mathbb{E}_{q(\{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L )} \left[ \log \frac{p \left( y \mid \mathbf{f}^L \right) \prod_{\ell=1}^L p \left( \mathbf{f}^\ell \mid \mathbf{u}^\ell, \mathbf{f}^{\ell-1}, \theta^\ell \right) \prod_{\ell=1}^L p \left( \mathbf{u}^\ell \mid \theta^\ell \right) p(\theta^\ell) / p(y)}{\prod_{\ell=1}^L p \left( \mathbf{f}^\ell \mid \mathbf{u}^\ell, \mathbf{f}^{\ell-1}, \theta^\ell \right) q \left( \{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right)} \right] + \log p(y)
\]

\[
= - \mathbb{E}_{q(\{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L )} \left[ \log \frac{\sum_{\ell=1}^L p \left( y \mid \mathbf{f}^\ell \right) \prod_{\ell=1}^L p \left( \mathbf{f}^\ell \mid \mathbf{u}^\ell, \theta^\ell \right) p(\theta^\ell) / p(y)}{\prod_{\ell=1}^L q \left( \{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) } \right] + \log p(y)
\]

\[
= - \mathbb{E}_{q(\{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L )} \left[ \log \frac{e^{\mathbb{E}_{p(\{ f^\ell \mid \mathbf{u}^\ell, \theta^\ell \})} \log p(y) \mid f^\ell} \prod_{\ell=1}^L p \left( \mathbf{f}^\ell \mid \theta^\ell \right) p(\theta^\ell)}{\prod_{\ell=1}^L q \left( \{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) } \right] - \log C + \log p(y)
\]

\[
= - \mathbb{E}_{q(\{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L )} \left[ \log \frac{e^{\mathbb{E}_{p(\{ f^\ell \mid \mathbf{u}^\ell, \theta^\ell \})} \log p(y) \mid f^\ell} \prod_{\ell=1}^L p \left( \mathbf{f}^\ell \mid \theta^\ell \right) p(\theta^\ell)}{\prod_{\ell=1}^L q \left( \{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L \right) } \right] - \log C + \log p(y)
\]

\[
= - \mathbb{E}_{q(\{ \mathbf{u}^\ell, \theta^\ell \}_{\ell=1}^L )} \left[ \log \frac{e^{\text{Bayesian Sparse Gaussian Processes}}}{} \right]
\]
\[\text{KL}\left[q\left(\{u^\ell, \theta^\ell\}_{\ell=1}^L\right)\right] = \sum_{\ell=1}^L \log p\left(y_j | f^\ell_j\right) - \log C + \log p(y) \]  

\[\geq - \log C + \log p(y). \]  

Here $C$ is a normalizing constant $C = \int \mathbb{E}_{p(\{u^\ell\}|\{u^\ell, \theta^\ell\})} \log p(y | f^\ell) \prod_{\ell=1}^L p\left(u^\ell | \theta^\ell\right) p(\theta^\ell) d\{u^\ell, \theta^\ell\}_{\ell=1}^L$, and the KL-divergence term is minimized when the KL term in Equation 13 equals 0, i.e.,

\[
\log \hat{q}\left(\{u^\ell, \theta^\ell\}_{\ell=1}^L\right) = \mathbb{E}_{p(\{u^\ell\}|\{u^\ell, \theta^\ell\})} \left[\log p\left(y | f^L\right)\right] + \sum_{\ell=1}^L \left(\log p\left(u^\ell | \theta^\ell\right) + \log p(\theta^\ell)\right) - \log C. \]  

While the optimal distribution $\hat{q}$ is intractable, we have obtained the form of its (un-normalized) log joint, from which we can sample using Monte Carlo and data subsampling (Salimbeni & Deisenroth, 2017), assuming that the conditional likelihood $p(y | f^L)$ factorizes over datapoints,

\[
\mathbb{E}_{p(\{u^\ell\}|\{u^\ell, \theta^\ell\})} \left[\log p\left(y | f^L\right)\right] \approx \mathbb{E}_{p(\{u^\ell\}|\{u^\ell, \theta^\ell\})} \left[\log p\left(y | f^L\right)\right], \hat{y}^3 \sim p\left(y^3 | u^1, \theta^1, \theta^0\right),
\]

\[
\approx \ldots
\]

\[
\approx \mathbb{E}_{p(\{u^\ell\}|\{u^\ell, \theta^\ell\})} \left[\log p\left(y | f^L\right)\right], \hat{y}^L \sim p\left(y^L | u^{L-1}, \theta^{L-1}, \theta^{L-2}\right),
\]

\[
= \sum_{j=1}^N \mathbb{E}_{p(\{u^\ell\}|\{u^\ell, \theta^\ell\})} \left[\log p\left(y_j | f^L_j\right)\right]
\]

\[
\approx N \mathbb{E}_{p(\{u^\ell\}|\{u^\ell, \theta^\ell\})} \left[\log p\left(y_i | f^L_i\right)\right], i \sim \text{Uniform}\{1, 2, \ldots, N\}. \]  

Because of the layer-wise factorization of the joint likelihood Equation 10, each step of the approximation is unbiased. While it is possible to approximate the last-layer expectation with a Monte Carlo sample $f^L_j$, the expectation is tractable when $y_j | f^L_j$ is a Gaussian or Poisson distribution, or is computable with one-dimensional quadrature (Hensman et al., 2015b).

**B. Additional Results**

**Figure 9:** Traces for three test points (4 chains/200 samples).

| NAME       | N.  | D-IN | D-OUT |
|------------|-----|------|-------|
| BOSTON     | 506 | 13   | 1     |
| CONCRETE   | 1,030 | 8    | 1     |
| ENERGY     | 768 | 8    | 2     |
| KINSHNM    | 8,192 | 8    | 1     |
| NAVAL      | 11,934 | 16   | 2     |
| POWERPLANT | 9,568 | 4    | 1     |
| PROTEIN    | 45,730 | 9    | 1     |
| YACHT      | 408 | 6    | 1     |
| AIRLINE    | 5,934,530 | 8    | 2     |
| HIGGS      | 11,000,000 | 28   | 2     |

**Table 5:** Datasets used, including number of datapoints and their dimensionality.
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Table 6: Tabular version of Figure 6 in the main paper.

| DATASET NAME | BOSTON | CONCRETE | ENERGY | KINSNM | NAVAL | POWERPLANT | PROTEIN | YACHT |
|--------------|--------|----------|--------|--------|-------|------------|---------|-------|
| BSGP         | 2.47 ± 0.16 | 3.12 ± 0.04 | 0.97 ± 0.13 | −1.12 ± 0.01 | −8.22 ± 0.04 | 2.71 ± 0.02 | 2.78 ± 0.01 | −0.23 ± 0.13 | |
| BSGP 2       | 2.47 ± 0.15 | 3.04 ± 0.05 | 0.95 ± 0.16 | −1.40 ± 0.01 | −8.23 ± 0.04 | 2.67 ± 0.02 | 2.63 ± 0.02 | −0.72 ± 0.15 | |
| BSGP 3       | 2.47 ± 0.14 | 2.96 ± 0.10 | 0.95 ± 0.15 | −1.41 ± 0.01 | −8.02 ± 0.04 | 2.66 ± 0.03 | 2.57 ± 0.03 | −0.83 ± 0.10 | |
| BSGP 4       | 2.48 ± 0.14 | 2.97 ± 0.06 | 0.92 ± 0.14 | −1.43 ± 0.02 | −8.03 ± 0.05 | 2.65 ± 0.05 | 2.59 ± 0.03 | −0.76 ± 0.13 | |
| BSGP 5       | 2.48 ± 0.12 | 2.91 ± 0.08 | 0.75 ± 0.30 | −1.43 ± 0.01 | −8.09 ± 0.05 | 2.65 ± 0.03 | 2.43 ± 0.03 | −0.74 ± 0.08 | |
| IPVI GP      | 2.84 ± 0.36 | 3.19 ± 0.11 | 1.27 ± 0.07 | −1.12 ± 0.02 | −5.96 ± 0.89 | 2.79 ± 0.03 | 2.81 ± 0.02 | 1.21 ± 1.50 | |
| IPVI GP 2    | 2.73 ± 0.35 | 3.13 ± 0.11 | 1.31 ± 0.28 | −1.34 ± 0.02 | −4.98 ± 0.48 | 2.76 ± 0.07 | 2.65 ± 0.02 | 0.74 ± 1.13 | |
| IPVI GP 3    | 2.61 ± 0.25 | 3.08 ± 0.13 | 1.21 ± 0.12 | −1.33 ± 0.03 | −4.86 ± 0.23 | 2.72 ± 0.06 | 2.74 ± 0.05 | 1.05 ± 1.77 | |
| IPVI GP 4    | 2.64 ± 0.44 | 3.11 ± 0.18 | 1.19 ± 0.25 | −1.33 ± 0.01 | −4.94 ± 0.20 | 2.76 ± 0.02 | 2.79 ± 0.01 | 2.47 ± 2.34 | |
| IPVI GP 5    | 2.51 ± 0.20 | 3.08 ± 0.17 | 1.15 ± 0.22 | −1.29 ± 0.02 | −5.09 ± 0.49 | 2.72 ± 0.04 | 2.80 ± 0.01 | 2.84 ± 3.64 | |
| SGHMC GP     | 2.82 ± 0.33 | 3.13 ± 0.09 | 1.08 ± 0.28 | −1.08 ± 0.01 | −6.23 ± 0.14 | 2.76 ± 0.05 | 2.81 ± 0.01 | −0.31 ± 0.28 | |
| SGHMC GP 2   | 2.77 ± 0.37 | 2.99 ± 0.07 | 0.91 ± 0.15 | −1.32 ± 0.01 | −6.57 ± 0.11 | 2.72 ± 0.04 | 2.71 ± 0.02 | −0.52 ± 0.14 | |
| SGHMC GP 3   | 2.78 ± 0.28 | 3.02 ± 0.16 | 0.91 ± 0.14 | −1.37 ± 0.02 | −6.56 ± 0.09 | 2.68 ± 0.02 | 2.66 ± 0.03 | −0.57 ± 0.19 | |
| SGHMC GP 4   | 2.75 ± 0.34 | 2.98 ± 0.13 | 0.69 ± 0.22 | −1.38 ± 0.02 | −6.42 ± 0.08 | 2.67 ± 0.04 | 2.62 ± 0.02 | −0.69 ± 0.12 | |
| SGHMC GP 5   | 3.75 ± 1.91 | 3.11 ± 0.21 | 1.00 ± 0.22 | −1.39 ± 0.02 | −6.55 ± 0.09 | 2.65 ± 0.04 | 2.59 ± 0.02 | −0.53 ± 0.18 | |
| SVGP         | 2.53 ± 0.25 | 3.18 ± 0.05 | 1.75 ± 0.06 | −1.01 ± 0.01 | −6.67 ± 0.09 | 2.79 ± 0.02 | 2.92 ± 0.01 | 0.78 ± 0.13 | |

Table 7: Tabular version of Figure 7 in the main paper.

| DATASET PRIOR TYPE | BOSTON | CONCRETE | ENERGY | KINSNM | NAVAL | POWERPLANT | PROTEIN | YACHT |
|--------------------|--------|----------|--------|--------|-------|------------|---------|-------|
| DETERMINANTAL      | 2.59 ± 0.06 | 3.30 ± 0.15 | 1.28 ± 0.10 | −1.08 ± 0.01 | −7.93 ± 0.32 | 2.73 ± 0.02 | 2.79 ± 0.01 | 0.78 ± 0.21 | |
| NORMAL             | 2.54 ± 0.07 | 3.12 ± 0.04 | 0.95 ± 0.08 | −1.13 ± 0.01 | −8.38 ± 0.05 | 2.70 ± 0.02 | 2.77 ± 0.01 | −0.32 ± 0.14 | |
| UNIFORM            | 2.65 ± 0.23 | 3.21 ± 0.04 | 1.04 ± 0.07 | −1.09 ± 0.01 | −8.47 ± 0.04 | 2.73 ± 0.03 | 2.79 ± 0.01 | 0.21 ± 0.09 | |