Tighter Bounds on the Log Marginal Likelihood of Gaussian Process Regression Using Conjugate Gradients

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Abstract

We propose a lower bound on the log marginal likelihood of Gaussian process regression models that can be computed without matrix factorisation of the full kernel matrix. We show that approximate maximum likelihood learning of model parameters by maximising our lower bound retains many of the sparse variational approach benefits while reducing the bias introduced into parameter learning. The basis of our bound is a more careful analysis of the log-determinant term appearing in the log marginal likelihood, as well as using the method of conjugate gradients to derive tight lower bounds on the term involving a quadratic form. Our approach is a step forward in unifying methods relying on lower bound maximisation (e.g. variational methods) and iterative approaches based on conjugate gradients for training Gaussian processes. In experiments, we show improved predictive performance with our model for a comparable amount of training time compared to other conjugate gradient based approaches.

1. Introduction

Scaling models involving Gaussian process priors to large datasets is an important and well-researched problem in Bayesian statistics and machine learning. In order for a method to succeed in this task it should provide high-quality approximations to 1) the posterior mean and (co-)variance over functions, 2) the log marginal likelihood (LML). While only the former is needed for making predictions, the latter is a useful tool for model selection; when the kernel is differentiable with respect to hyperparameters, the LML or an approximation to it can be optimised using gradient based methods in order to automatically select model hyperparameters.

We derive a lower bound on the LML of regression with a Gaussian process prior and a Gaussian likelihood. We refer to this bound as CGLB. Parameter learning with CGLB combines many of the strengths of sparse variational Gaussian process regression (SGPR) (Titsias, 2009) with the strengths of conjugate gradient (CG) methods (Gibbs and Mackay, 1997) for GP inference. We use an improved bound on the log-determinant of the covariance matrix as well as CG to tighten the SGPR evidence lower bound (ELBO). We show empirically that this leads to less bias in parameter selection than maximisation of the ELBO. This reduced bias leads to improved performance on several benchmark tasks involving large datasets.

Wang et al. (2019) showed conjugate gradient based approaches to GP inference perform excellently on many regression tasks and argued that these methods should be considered ‘exact’. The latter claim has two caveats. First, gradient estimates provided by these methods are biased if conjugate gradients is stopped too early; while this bias can be reduced by running more iterations of CG, this comes at an additional computational cost. Second, the estimates of the LML are stochastic. The variance of the estimator provided can be reduced at the cost of needing to solve more systems of equations. Following Davies (2015), we refer to these approaches as ‘Iterative GPs’, to contrast them with implementations using deterministic, direct methods for computing the LML.

Building on work in Gibbs and Mackay (1997) and Davies (2015) we derive a stopping criterion for our application of CG that ensures more iterations of CG would not improve the bound on the LML significantly. We also exploit old solutions to

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We assume \( k \) is parameterised, and denote these hyperparameters together with \( \sigma_\text{f} \) by \( \theta \). The choice of \( \theta \) has a significant impact on the generalisation properties of the posterior (Rasmussen and Williams, 2006, Chapter 5).

Type-II maximum likelihood is a heuristic that automates selection of \( \theta \) by maximising the LML, defined as the log density of the prior probability distribution over \( Y \) evaluated at \( Y = y \), with respect to the hyperparameters \( \theta \). For this model the LML is

\[
\log p_Y(y; \theta) = c - \frac{1}{2} y^\top K^{-1} y - \frac{1}{2} \log |K| ,
\]

with \( c = -\frac{n}{2} \log 2\pi \). Here and elsewhere, we suppress the dependence of kernel matrices on \( \theta \). Common implementations of Gaussian process inference and hyperparameter selection rely on a Cholesky factorisation of \( K \) in order to evaluate \( \log |K| \) and \( K^{-1} y \). The Cholesky decomposition is usually implemented in a way that requires roughly \( n^3/3 \) floating point operations and stores a matrix with \( n(n+1)/2 \) distinct entries in memory. This can be a prohibitive cost for regression problems with many observations.

2.2. Conjugate Gradients

The conjugate gradient algorithm (Hestenes and Stiefel, 1952) is a method for solving systems of equations using only matrix-vector multiplication and elementary vector operations. Given a symmetric positive definite matrix \( K \) and a vector \( y \) the goal of conjugate gradients is to find an vector \( v \) satisfying \( K v = y \). Starting with an initial guess for \( v \), each iteration of conjugate gradient chooses a search direction and updates the current guess for \( v \) by adding a vector in the chosen direction. In exact arithmetic, CG is guaranteed to solve an \( n \times n \) system of equations in \( n \) iterations, each of which involves a \( O(n^2) \) matrix-vector multiplication, viewed as an iterative algorithm CG has strong guarantees on the rate at which the error decreases, at least for well-conditioned matrices (Hackbusch, 1994, Section 10.2.3). The convergence of conjugate gradient is often practically assessed by examining the residual \( r = y - K v \), which can be evaluated with a matrix-vector
multiplication. If the residual is 0, then the algorithm has converged. Often CG is stopped when the residual has a sufficiently small Euclidean norm.

2.3. Gaussian Process Regression with Conjugate Gradient Methods

Conjugate gradients have been suggested as a method to directly approximate the gradient of eq. (1) (Gibbs and Mackay, 1997). An obstacle to this approach is the evaluation of the gradient of the log-determinant, \( \partial \log |K| = \text{tr}(K^{-1} \partial K) \). Evaluating this trace directly is computationally expensive, as it requires solving \( n, n \times n \) systems of linear equations. Hutchinson’s trace estimator (Hutchinson, 1989) provides a stochastic estimate of this gradient. The estimator is formed by first noting that for any \( \mathbb{R}^n \)-valued random variable \( p \) such that \( \mathbb{E}_p [pp^\top] = I, \text{tr}(K^{-1} \partial K) = \mathbb{E}_p [p^\top K^{-1} \partial K p] \). The expectation can be estimated with Monte Carlo, using CG to approximate \( K^{-1} p_i \), where \( p_i \) is a sample of \( p \).

This results in a biased, stochastic estimate of the gradient. The bias in this estimator can be decreased, and practically removed, at the cost of increasing the number of iterations of CG. The variance can be reduced by increasing the number of \( p_i \) samples, at the cost of needing to solve more systems of equation. The variance of this estimator for various distributions of \( p \) as well as high probability bounds on the relative error are known (Avron and Toledo, 2011).

In cases when the objective function itself is of interest, for example if model comparison is performed with discrete hyperparameters, approximations to the LML using CG and related ideas have also been proposed (Ubaru et al., 2017). Iterative GPs have been shown to be highly scalable with modern computational architectures (Gardner et al., 2018; Wang et al., 2019).

2.4. Gaussian Process Regression with Sparse Methods

An alternative approach, which avoids the computation of \( K \) entirely, relies on sparsity assumptions in the data-domain that lead to a low-rank approximation of \( K \) (e.g. Williams and Seeger, 2001; Snelson and Ghahramani, 2005). This approach reduces the computational requirement to \( O(nm^2) \) where \( m \) is a parameter that controls the rank of the approximation to \( K \). Titsias (2009) proposed an interpretation of sparse methods as variational inference with a structured family of posterior distributions. This framework defines an evidence lower bound (ELBO), \( L(y; \theta) \leq \log p(y; \theta) \), where

\[
L(y; \theta) = c - \frac{1}{2} \mathbb{E}_p \left[ Q^{-1} y \right] \frac{1}{2} \left( \log |Q| + \frac{\text{tr}(K_{uf} - Q_{uf})}{\sigma^2} \right) \tag{2}
\]

with \( Q = Q_{uf} + \sigma^2 I \), with \( Q_{uf} = K_{uf}^T K_{uu} K_{uf} \), \( K_{uu} \) an \( m \times m \) matrix with \( K_{uu} = k(z_i, z_j) \), \( K_{uf} \) an \( m \times n \) matrix with \( (K_{uf})_{ij} = k(z_i, x_j) \), and the \( z_i \in \mathcal{X} \) are variational parameters. The ELBO can be evaluated in \( O(nm^2) \), and is frequently jointly maximised with respect to variational parameters \( \{z_i\}_{i=1}^m \) and hyperparameters \( \theta \) as a form of approximate maximum likelihood learning. The variational posterior is then used for prediction. This is a Gaussian process, with mean and covariance,

\[
\hat{m}(x) = k_{us}^T k_{us}^{-1} Q^{-1} y \quad \text{and} \quad \hat{k}(x, x') = k(x, x') - k_{us}^T k_{us}^{-1} Q^{-1} k_{us}' \tag{3}
\]

where \( k_{us}, k_{us}' \in \mathbb{R}^m \) have entries \( k_{us,i} = k(z_i, x) \) and \( k_{us,i}' = k(z_i, x') \). When the number of training examples is large, the kernel is sufficiently smooth, and the data is not too spread out \( \log p\gamma(y; \theta) - L(y; \theta) \) is small for some \( m \ll n \) (Burt et al., 2020), in which case one expects that similar hyperparameters would be selected by maximising the ELBO as would be selected by maximising the LML. However, certain settings of \( \theta \), for example those for which \( \sigma^2 \) is very small, lead to large discrepancies between the LML and ELBO, which results in significant bias in parameter selection and underfitting (Bauer et al., 2016).

3. Lower Bounds on the Log Marginal Likelihood

In this section we present our lower bound on the log marginal likelihood that can be computed in \( O(nm^2 + (t + 1)n^2) \), where \( t \) is the number of steps of CG run. We also present a mean function that can be used for prediction in conjunction with this bound. We additionally derive lower bounds on the LML that are tighter than the evidence lower bound eq. (2) and can
be computed in $O(nm^2)$. While we focus on the CG version of our bounds, which we refer to as CGLB, these bounds may be of independent interest.

3.1. Conjugate Gradient Lower Bound

We now state the lower bound, we refer to as CGLB:

**Lemma 1.** Let $K$ as in eq. (1), $Q$ as in eq. (2), $c = -\frac{n}{2} \log 2\pi$ and for any $v \in \mathbb{R}^n$

$$\log p(y; \theta) \geq c - \frac{1}{2} (r^T Q^{-1} r + 2 y^T v - v^T K v) - \frac{1}{2} \left( \log |Q| + n \log \left( 1 + \frac{\text{tr}(K - Q)}{n \sigma^2} \right) \right),$$  \hspace{1cm} (5)

where $r = y - K v$.

The right hand side of eq. (5) can be maximised with respect to $\{\theta, v, \{z_i\}_{i=1}^m\}$ for parameter learning. For fixed $v$, the right hand side can be computed in $O(n^2 + nm^2)$ using similar computations to eq. (2) but with an additional $n \times n$ matrix-vector product to compute $K v$. If $v = K^{-1} y$, then $r = 0$, and the first term in the bound becomes $-\frac{1}{2} y^T K^{-1} y$. This choice of $v$ maximises the lower bound (CGLB) for any choice of $\{\theta, \{z_i\}_{i=1}^m\}$, and is independent of $\{z_i\}_{i=1}^m$, and can be approximated by running conjugate gradients on the system of equation $K v = y$.

In order to derive this lower bound on the log marginal likelihood, it suffices to upper bound the quadratic term and the log-determinant term from eq. (1).

3.2. Bounds on the Log-Determinant Term

Unlike previous Iterative GPs (Gibbs and Mackay, 1997; Gardner et al., 2018), we aim for a deterministic estimate of the LML and its gradient. A simple approach is to combine estimates of the term $y^T K^{-1} y$ based on CG with the bound $\log |K| \leq \log |Q| + \frac{1}{2} \text{tr}(K - Q)$ from SGPR. This bound is tight when $\text{tr}(K - Q) \approx 0$, but is loose otherwise. We derive a tighter bound on $\log |K|$ using properties of $Q$.

We recall several matrix properties.

**Proposition 1** (Horn and Johnson, 2012, page 51). Let $A \in \mathbb{R}^{k \times k}$ and $\{\lambda_i\}_{i=1}^k$ denote the eigenvalues of $A$ (counted with multiplicity). Then $|A| = \prod_{i=1}^k \lambda_i$ and $\text{tr}(A) = \sum_{i=1}^k \lambda_i$.

We say a symmetric matrix $A \in \mathbb{R}^{k \times k}$ is positive semi-definite (PSD) if for all $z \in \mathbb{R}^k$, $z^T A z \geq 0$. For any PSD matrix, we have $\lambda_i \geq 0$ where $\lambda_i$ denotes an eigenvalue of $A$.

**Proposition 2** (Horn and Johnson, 2012, page 495). Let $H$ be a symmetric real matrix with $H = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}$ with $A$ non-singular. Then $H$ is PSD if and only if $A$ and $C - B^T A^{-1} B$ are both PSD.

Applying this lemma to the block matrix $H = \begin{bmatrix} K_{ff} & K_{fu} \\ K_{uf} & K_{uu} \end{bmatrix}$, which is PSD since the kernel is PSD, leads to the conclusion $K_{ff} - Q_{ff}$ is PSD.

**Proposition 3** (Horn and Johnson, 2012, Corollary 7.7.4). Let $A_1, A_2 \in \mathbb{R}^{k \times k}$ such that $A_1 - A_2$ is PSD. Let $\lambda_i(A_j), 1 \leq i \leq k, j \in \{1, 2\}$ denote the $i$th largest eigenvalue of $A_j$. Then,

1. If $A_1$ and $A_2$ are invertible, $A_2^{-1} - A_1^{-1}$ is PSD,
2. $\lambda_i(A_1) \geq \lambda_i(A_2)$ for $1 \leq i \leq k$.

We now derive the SGPR bound $\log |K| \leq \log |Q| + \frac{1}{2} \text{tr}(K_{ff} - Q_{ff})$; the bound on the log-determinant term used in lemma 1 is derived by a modification of this argument and the arithmetic-geometric mean inequality.

Let $\lambda_i$ denote the eigenvalues of $K$ and $\ell_i$ denote the eigenvalues of $Q$, both sorted in descending order. Adding zero and using proposition 1,

$$\log |K| = \log |Q| + \log |K| - \log |Q| = \log |Q| + \sum_{i=1}^n \log \left( 1 + \frac{\lambda_i - \ell_i}{\ell_i} \right).$$ \hspace{1cm} (6)
Since $Q - \sigma^2 I = Q_{ff}$ is PSD, we may apply proposition 3 to conclude,

$$
\sum_{i=1}^{n} \log \left( 1 + \frac{\lambda_i - \ell_i}{\ell_i} \right) \leq \sum_{i=1}^{n} \log \left( 1 + \frac{\lambda_i - \ell_i}{\sigma^2} \right). 
$$

(7)

Applying the inequality $\log(1 + x) \leq x$ for $x > -1$ to each summand,

$$
\sum_{i=1}^{n} \log \left( 1 + \frac{\lambda_i - \ell_i}{\sigma^2} \right) \leq \frac{1}{\sigma^2} \left( \sum_{i=1}^{n} \lambda_i - \sum_{i=1}^{n} \ell_i \right) 
= \frac{1}{\sigma^2} \text{tr}(K - Q). 
$$

(8)

Note that the bound $\log(1 + x) \leq x$ is only tight for $x = 0$. Applying this elementwise can lead to loose bounds in cases when $\text{tr}(K_{ff} - Q_{ff})$ is large. We would like to replace the inequality in eq. (8) with a tighter inequality. We recall the arithmetic-geometric mean inequality.

**Proposition 4** (AM-GM inequality; Horn and Johnson, 2012, page 559). Let $a_1, \ldots, a_n \geq 0$, then

$$
\left( \prod_{i=1}^{n} a_i \right)^{1/n} \leq \frac{1}{n} \sum_{i=1}^{n} a_i. 
$$

(10)

We now state the bound on the log-determinant.

**Lemma 2.** For $K, Q \in \mathbb{R}^{n \times n}$ PSD such that $K - Q$ is PSD and $Q - \sigma^2 I$ is PSD,

$$
\log |K| \leq \log |Q| + n \log \left( 1 + \frac{\text{tr}(K - Q)}{n\sigma^2} \right) 
\leq \log |Q| + \frac{1}{\sigma^2} \text{tr}(K - Q). 
$$

(11)

(12)

A related result to lemma 2 was proven concurrently to this work in (Vakili et al., 2020), and used in deriving a bound on the information gain of Gaussian process models.

**Proof of lemma 2.** By proposition 2 and proposition 3, $\lambda_i - \ell_i$ is non-negative for all $i$. We can therefore apply proposition 4 to the left hand side of eq. (8),

$$
\sum_{i=1}^{n} \log \left( 1 + \frac{\lambda_i - \ell_i}{\sigma^2} \right) \leq n \log \left( 1 + \frac{\sum_{i=1}^{n} \lambda_i - \ell_i}{n\sigma^2} \right) = n \log \left( 1 + \frac{\text{tr}(K - Q)}{n\sigma^2} \right). 
$$

Equation (12) follows from $\log(1 + x) \leq x$ for all $x > -1$.

Like the SGPR bound on the log-determinant term, we only need to compute $\log |Q|$ and $\text{tr}(K_{ff} - Q_{ff})$. We could use lemma 2 together with the bound on the quadratic form from SGPR, giving a lower bound on the LML that can be computed in $O(nm^2)$, with only minor modifications to standard implementations of SGPR.

We show in the appendix that this bound can be further improved using a similar approach, by phrasing the problem of upper bounding the log-determinant of $K$ as a constrained convex optimisation problem, subject to the constraints that $K - Q$ is PSD, and $\text{tr}(K)$ as well as the eigenvalues of $Q$ are known. For simplicity, we run experiments using lemma 2.

### 3.3. Bounds on the Quadratic Term

We now turn our attention to an upper bound on the quadratic form $y^T K^{-1} y$. In order to combine the benefits of SGPR and iterative methods derive an upper bound on $y^T K^{-1} y$ that is tight if either: 1) $Q_{ff} \approx K_{ff}$ 2) we are able to find a $v \in \mathbb{R}^n$ such that $v \approx K^{-1} y$. 

Lemma 3. Let $K, Q \in \mathbb{R}^{k \times k}$ be PD such that $K - Q$ is PSD. Then, for any $v, y \in \mathbb{R}^{k}$,
\[ 2y^T v - v^T Q v \leq y^T (K - Q) y \leq r^T Q^{-1} r + 2y^T v - v^T K v, \]
where $r = y - Kv$.

Remark 1. The lower bound is standard, and yields the popular interpretation of CG as optimisation of a quadratic function, (e.g. Hackbusch, 1994, Section 9.1.1)

Choosing $v = 0$ results in the upper bound $y^T K^{-1} y \leq y^T Q^{-1} y$, which corresponds to the quadratic term in the SGPR bound. If we have $m = 0$ so that $Q = \sigma^2 I$, after some rearranging we recover the upper bound considered in Gibbs and Mackay (1997, eqn. 50) for monitoring the convergence of CG.

Proof of lemma 3. We begin by expanding out the quadratic form,
\[ y^T K^{-1} y = (r + Kv)^T K^{-1} (r + Kv) = r^T K^{-1} r + 2r^T v + v^T K v. \]

Let $w = K^{-1} y$. Then $r^T K^{-1} r = w^T Kw \geq 0$. This proves the lower bounds in lemma 3.

Adding 0 to the term involving an inverse,
\[ r^T K^{-1} r = r^T Q^{-1} r - r^T (Q^{-1} - K^{-1}) r. \]

From proposition 3 and the assumption that $K - Q$ is PSD $Q^{-1} - K^{-1}$ is PSD. Hence, $r^T K^{-1} r \leq r^T Q^{-1} r$.

3.4. Approximate Predictive Posterior

After selecting model hyperparameters, we must compute a mean and (co-)variance at test points. We use the same covariance calculation as in SGPR (eq. (4)). For the mean, we would like to recover the exact GP mean if $K = Q$ or $v = K^{-1} y$, as in both cases our bound estimates $y^T K^{-1} y$ exactly. We propose the estimator
\[ m(x) = k_{fs}^T v + k_{us}^T K_{uu}^{-1} K_{uf} Q^{-1} (y - Kv), \]
where $k_{us}$ is as in eq. (4) and $k_{fs} \in \mathbb{R}^{n}$ with $k_{fs} = k(x_t, x)$. The first term is the estimate given by running conjugate gradient and replacing $K^{-1} y$ with its approximation. The second term is a correction that is equivalent to the mean of SGPR, but replacing $y$ with the residual of the CG computation. The mean predictor eq. (16) is not sparse, but the covariance we use is induced in the same way as in the sparse variational framework. The CGLB predictive posterior closely resembles ‘decoupled’ variational Gaussian process inference Cheng and Boots (2017), with the inducing points used to determine the mean function $Z' = \{X, Z\}$ and the inducing points used to determine the covariance function $Z$.

A worthwhile question is whether CGLB has a variational interpretation, i.e. whether the gap between CGLB and the LML is a Kullback-Leibler divergence between an approximate posterior and the posterior. Variationally formulated bounds would mean that the implicit approximate posterior provides an alternative predictive distribution to the predictive distribution we describe in section 3.4.

3.5. Implementation with Conjugate Gradient

The vector $v \in \mathbb{R}^{n \times n}$ is an auxiliary parameter in our lower bound on the LML. From lemma 3, for fixed $\theta$, CGLB is maximized by $v = K^{-1} y$. A simple approach is to treat $v$ as an additional parameter, and optimise the bound jointly with respect to $\{\theta, v, \{z_i\}_{i=1}^m\}$. However, this introduces $n$ additional dimensions to the optimisation problem, and we find it leads to slow parameter learning.

We instead select $v$ by running conjugate gradient on the system of equations $Kv = y$ each time we evaluate the lower bound on the LML. We make several design choices when running conjugate gradients to improve and assess convergence of the approximation.

Preconditioner We use $Q$ as a preconditioner. This preconditioner has been used previously in kernel methods (Cutajar et al., 2016). In our case, this has computational advantages: we can reuse some of the calculations used in bounding the log-determinant.
Tighter Bounds on the LML of GPR Using CG

Figure 1. The number of CG iterations spent in CGLB and Iterative GP to achieve a pre-set residual error (note the stopping criteria for the methods is different) on the protein dataset. For CGLB this number goes to zero (the plot uses log(x + 1) scaling for the CG step axis), and CGLB reuses the vector v in the subsequent iterations. The figure shows the average number of steps (shaded lines) spent per function evaluation during optimisation for five experiments on a different data splits; solid lines are the smoothing applied to the average number of steps for each model. The inner box-whisker plot depicts IQRs of CG steps that CGLB and Iterative GP models ran throughout 1500 iterations. The whiskers set to 95 percentile. The initial flat line for Iterative GP at 10 iterations is due to a hard-coded constraint in the GPytorch code.

Initializing CG We initialize CG using the value of v found in the previous evaluation of the lower bound. As the optimiser often evaluates similar settings of kernel hyperparameters in sequence, as long as $\sigma^2$ is not very close to zero, similar parameter settings generally result in similar optimal values for v this is often a good guess for the the solution to $K^{-1}y$. We show in section 4 for many datasets, after the first handful of optimisation steps the old solution for v is good enough and no iterations of CG are needed during most steps of parameter optimisation.

Stopping Criterion We monitor upper and lower bounds on $y^T K^{-1} y$ in order to decide when to terminate CG, as advocated in Gibbs and Mackay (1997). Subtracting the upper and lower bounds in lemma 3, we derive the stopping criteria $r^T Q^{-1} r \leq 2\epsilon$. This ensures that the slack in our bound introduced from not exactly computing the quadratic term is at most $\epsilon$. Because of our choice of preconditioner, $r^T Q^{-1} r$ is computed in every iteration, so this stopping criterion requires only a single extra matrix-vector multiplication with the preconditioner in the final iteration.

Although stopping criteria based on $\|r\|_2$ are a popular heuristic and often practical, they can lead to significant biases in parameter selection in this application. In particular, the bias in the lower bound (the gradient of which corresponds to the gradient estimate used in Gardner et al. (2018)) in lemma 3 is $r^T K^{-1} r$. In the worst-case the bias introduced into the LML can be as large as $\|r\|_2^2/(2\sigma^2)$. A similar argument shows that in the worst case and when $m = 0$, the upper bound in lemma 3 could have the same bias in the opposite direction. By instead ensuring $r^T Q^{-1} r \leq 2\epsilon$, we ensure the bias we introduce through this term in CGLB is uniformly bounded by $\epsilon$ over all parameter settings. We therefore expect this bias to have a smaller impact on the estimation of hyperparameters, in particular $\sigma^2$.

3.6. Selecting Optimization Parameters with CGLB versus Iterative Methods

An advantage of our approach compared to existing iterative methods is that the quality of design and optimization choices can be assessed directly through the approximation to the log marginal likelihood, as is done in Cholesky-based implementations of GPR and SGPR. Good choices of the parameters v, $\{z_i\}_{i=1}^m$ result in tighter lower bounds on the log marginal likelihood.

In contrast, when using Iterative GP any bias introduced due to an insufficient number of iterations of CG may lead to either over or under estimation of the log marginal likelihood. In this case, changes to optimization parameters that increase the estimated log marginal likelihood could be indicative of additional bias instead of improved hyperparameter selection. Additionally, as the estimate is stochastic, without many evaluations of the LML or many vectors used in Hutchinson’s trace estimator, it may be difficult to tell which of two models is preferred by the estimate of the LML.
While methods considered in Gibbs and Mackay (1997); Ubaru et al. (2017); Gardner et al. (2018); Wang et al. (2019) are capable of having less bias when estimating the LML than our method (at least for fixed $m, \theta$), any bias introduced is harder to assess. In the next section, we find empirically this makes achieving good performance with these methods more challenging.

4. Experiments

We now compare hyperparameter selection with CGLB (lemma 1), with sparse methods (SGPR) as well as the conjugate gradient method considered in Wang et al. (2019) (Iterative GP). We would like to determine which method finds better hyperparameters, and how these hyperparameters effect predictive performance. We consider several regression UCI datasets, and compare the methods on the basis of root mean square error (RMSE) and negative log predictive density (NLPD) on held-out data to assess predictive performance. In order to assess the quality of the hyperparameters found by the methods, for datasets where it is computationally feasible, we compare the LML of the model with the hyperparameters selected by each method, computed directly with Cholesky decomposition.

4.1. Data Preparation

We randomly split each dataset into a training set consisting of $2/3$ of examples, and a test set consisting of the remaining $1/3$. We run 5 seeds in all experiments, with each seed corresponding to a different random split of the dataset. Each input dimension is normalised to have mean 0 and variance 1 within the training set. Similarly, the training outputs are normalised to have 0 mean and variance 1. We apply the same normalisation to test data when making predictions, using the statistics computed on the training data. All metrics reported are on the standardised data, so that we would expect a model predicting a constant mean function to have RMSE near 1.0. Dataset are downloaded using the Bayesian benchmarks package (Salimbeni, 2019).

4.2. Model Class and Initialisation of Parameters

We run experiments with a Matérn 3/2 kernel, with independently learned lengthscales along each input dimension (i.e. automatic relevance detection). While in the derivations we have assume the prior mean is 0, in experiments we take the prior mean to be a constant function that is learned as a hyperparameter. The changes to the predictive distribution and lower bound presented in the previous section to account for this are straightforward. This is the same experimental setup considered in Wang et al. (2019).

All kernel lengthscales, the kernel variance and the likelihood variance are initialised at $1.0$. The prior mean is initialised at 0. We use soft-plus constraints on the lengthscales and likelihood, lower bounding them at $1e^{-6}$ for SGPR and CGLB and $1e^{-4}$ for iterative GP, as we found this was necessary for numerical stability. Experiments are run using double precision.
4.3. Training Procedure

For CGLB and SGPR we vary the number of inducing points between 512 and 4096. We train CGLB and SGPR with the L-BFGS optimiser (Liu and Nocedal, 1989) for either 2000 steps or until the optimiser stops due to a small projected gradient norm or being unable to find a point that improves upon the current value during line-search. We initialise \( \{z_i\}_{i=1}^{m} \) using the ‘Greedy’ method advocated for in Burt et al. (2020), then optimise them jointly with hyperparameters. Alternatives to joint optimisation, such as reinitialisation of inducing points as suggested in Burt et al. (2020) may lead to further improvements in the training procedure, though we do not explore those here. For CGLB we stop CG when the residual \( r \) satisfied \( \frac{1}{2}r^T Q^{-1}r \leq \epsilon = 1.0 \) when selecting \( v \) for use in predictions. The criteria \( \epsilon = 1.0 \) used during training ensures that the additional slack introduced into CGLB from estimating the quadratic term is at most 1.0, regardless of the current value of \( \theta \).

We follow the procedure described in Wang et al. (2019) to train Iterative GP. We first pre-train the model on a subset of 10000 observations with 10 iterations of L-BFGS. Then we run 10 iterations of Adam optimiser (Kingma and Ba, 2015) on the same subset, followed by 2000 iterations of Adam with 0.1 learning rate on the full dataset. For forming Hutchinson’s trace estimation, 10 vectors \( \{p_i\}_{i=1}^{10} \) are sampled. In order to run L-BFGS, the vectors \( \{p_i\}_{i=1}^{10} \) are fixed along each line search, as suggested in the documentation for GPytorch (Gardner et al., 2018).

For experiments with SGPR we use GPflow (Matthews et al., 2017). For small datasets \((n < 20000)\), we use a GPflow implementation of CGLB as we found this to be faster than our GPytorch implementation. However, for larger datasets we use GPytorch kernel abstractions with KeOps (Charlier et al., 2020) to perform matrix-vector operations to reduce memory requirements. For Iterative GPs we use the GPytorch implementation (Gardner et al., 2018). Following Wang et al. (2019), we use the Lanczos variance estimator (without kernel interpolation) introduced in Pleiss et al. (2018) for computing the predictive NLPD for Iterative GPs. We run all experiments on a single Tesla V100-32GB GPU.

4.4. Results

| Dataset | LML | NLPD | RMSE |
|---------|-----|------|------|
| bike n=17379, d=17 | Iterative GP 30992.8 | 31319.1 | -2.016 | -3.257 | 0.014 | 0.020 |
| SGPR-4096 30502.5 | 32814.2 | -3.280 | -3.336 | 0.010 | 0.010 |
| CGLB-4096 37732.7 | **42023.0** | **-4.216** | **-4.329** | 0.004 | 0.004 |
| CGLB-2048 34102.8 | 38936.7 | -3.811 | -3.972 | **0.003** | **0.003** |
| CGLB-1024 30493.9 | 35351.8 | -3.403 | -3.615 | 0.005 | 0.005 |
| elevators n=16599, d=18 | Iterative GP -4709.0 | -4705.1 | 0.407 | 0.384 | **0.353** | **0.353** |
| SGPR-4096 -4675.3 | **-4653.3** | **0.386** | **0.386** | 0.354 | 0.354 |
| CGLB-4096 -4669.8 | -4639.1 | **0.386** | **0.386** | 0.354 | 0.354 |
| CGLB-2048 -4677.9 | -4656.4 | 0.387 | 0.387 | 0.355 | 0.355 |
| CGLB-1024 -4712.0 | -4670.0 | 0.392 | 0.391 | 0.356 | 0.356 |
| poletele n=15000, d=26 | Iterative GP 13552.5 | -7641.5 | -0.935 | 1.217 | 0.079 | 0.078 |
| SGPR-4096 9057.7 | 9624.0 | -1.172 | -1.180 | 0.078 | 0.078 |
| CGLB-4096 9377.1 | **9862.2** | **-1.201** | **-1.203** | **0.077** | **0.077** |
| CGLB-2048 8248.6 | 9248.0 | -1.126 | -1.145 | 0.080 | 0.080 |
| CGLB-1024 7250.7 | 8694.2 | -1.057 | -1.098 | 0.083 | 0.083 |
| kin40k n=40000, d=8 | Iterative GP 23859.0 | — | -0.454 | — | 0.087 | — |
| SGPR-4096 7486.0 | — | -0.705 | — | 0.107 | — |
| CGLB-4096 9057.7 | — | **-0.919** | — | **0.086** | — |
| CGLB-2048 8248.6 | — | -0.826 | — | 0.088 | — |
| CGLB-1024 7250.7 | — | -0.714 | — | 0.093 | — |
| protein n=45730, d=9 | Iterative GP -25703.9 | — | — | — | 0.531 | — |
| SGPR-4096 -27714.6 | — | — | — | 0.541 | — |
| CGLB-4096 -26570.7 | — | **0.749** | — | **0.522** | — |
| CGLB-2048 -27442.0 | — | — | — | 0.529 | — |
| CGLB-1024 -28243.7 | — | — | — | 0.535 | — |
In fig. 1, we show that CGLB typically only needs a single matrix-vector multiply with the kernel matrix, and reuses v in most training steps. Adding more inducing points, which results in a better preconditioner, decreases the number of steps of optimisation before we use zero CG steps in most subsequent parameter updates. Iterative GP requires a considerably greater number of CG steps, particularly in later training steps.

In fig. 2, we demonstrate the predictive performance of CGLB during training and compare it with Iterative GP and SGPR on the ‘protein’ UCI dataset (Dua and Graff, 2017). After splitting, the ‘protein’ dataset has 29267 training examples, 16463 testing examples and input dimensionality 9. The predictive RMSE of CGLB is either better or equal to Iterative GP and consistently outperforms SGPR. Moreover, CGLB shows improved predictive uncertainty estimations as measured by NLPD compared to Iterative GP and SGPR. For CGLB and SGPR, increasing the number of inducing points leads to large performance gains. SGPR is faster per iteration than CGLB for a fixed m; however, achieving comparable performance to CGLB requires many more inducing points with SGPR on several datasets (bike, kin40k, protein).

Results for other datasets are shown in table 1. For small datasets where we can compute the log marginal likelihood using Cholesky-based methods, we see that CGLB often finds settings of hyperparameters with higher LML than competing methods, suggesting that the gains in predictive performance are attributable to improved hyperparameter selection. We also note that on some datasets, Iterative GP significantly overestimates the LML. We hypothesise this is due to the interaction between bias and optimisation that can occur when maximising an estimate that is not a lower bound. The supplementary material shows model performance over time for several more regression datasets.

For several datasets, we found that Iterative GP achieved good test performance as measured by RMSE after a handful of iterations, but that continuing to optimise the objective lead to a small dropoff in performance, e.g. fig. 2. We initially thought this might be due to a high learning rate. However, in the supplement, we show that even if the learning rate for Adam is reduced from 0.1 to 0.01 the same phenomena occurs, but convergence is slower. In contrast, we do not see this behaviour for SGPR or CGLB.

Further, we observed unusual behaviour of the Iterative GP method on some datasets when the positive constraint of likelihood noise is set to a low number. In Iterative GP experiments, we used the GPytorch default noise value $1e^{-4}$. We attempted to lower this constraint to $1e-6$ as the noise variance on several datasets selected by other methods, particularly bike was generally below $1e-4$, and this low noise variance led to improved predictive performance. However, Iterative GP training and predictive performance became unstable in later optimisation steps. Neither CGLB nor SGPR exhibited degradation in predictive performance during optimisation, even in cases where the noise level was near the lower bound of $1e-6$. We hypothesise this is further evidence that lower bound maximisation is more robust as an optimisation procedure than other biased estimates of the LML, and results from optimising an objective that can overestimate the LML in ways that are non-uniform in $\theta$ (c.f. discussion of stopping criteria in section 3.5).

5. Conclusion

CGLB combines benefits from sparse variational methods with iterative approaches for hyperparameter selection. Maximising CGLB alleviates some of the hyperparameter bias that results from ELBO maximisation with sparse methods. As CGLB is deterministic, optimisation is frequently easier than using the stochastic approximations to the LML given by existing Iterative GP methods. Additionally, as the bias in CGLB results in a lower bound on the LML, we can assess choices made regarding optimisation choices using only training data, as higher lower bounds correlate well with better hyperparameter selection.

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A. Additional bounds on the Log marginal likelihood of Gaussian process regression

In this section, we discuss additional bounds on the log marginal likelihood of GPR regression that can be computed efficiently. We focus on the case when we have access to a rank-$m$-plus-diagonal approximate $Q \prec K$. We also assume we can efficiently compute the trace of $K$. We can then think of finding the optimal lower bound on $\log p_Y(y; \theta)$ as a
We now consider each term separately, we can then apply an element-wise bound,
\[ \log p_Y(y; \theta) = c - \frac{1}{2} y^T K^{-1} y - \frac{1}{2} \log |K| \geq c + \inf_{A \succ Q} \left( -\frac{1}{2} y^T A^{-1} y - \frac{1}{2} \log |A| \right). \]  
We define \( A = Q + EE \), where \( E \) is the PSD square root of \( A - Q \). Then applying Woodbury’s Lemma,
\[ y^T A^{-1} y = y^T Q^{-1} y - y^T Q^{-1} I (E + Q^{-1} E)^{-1} E Q^{-1} y. \]  
The second term is non-negative, but can be 0; in particular if \( K = Q + tz z^T \), where \( z \) is a unit vector orthogonal to \( Q^{-1} y \). Hence,
\[ \inf_{A \succ Q} \frac{1}{2} y^T A^{-1} y = -\frac{1}{2} y^T Q^{-1} y. \]  
\[ A.1. \text{ Quadratic term} \]
Since \( A \prec Q \), we may write \( A = Q + EE \), where \( E \) is the PSD square root of \( A - Q \). Then applying Woodbury’s Lemma,
\[ y^T A^{-1} y = y^T Q^{-1} y - y^T Q^{-1} I (E + Q^{-1} E)^{-1} E Q^{-1} y. \]  
The second term is non-negative, but can be 0; in particular if \( K = Q + tz z^T \), where \( z \) is a unit vector orthogonal to \( Q^{-1} y \). Hence,
\[ \inf_{A \succ Q} \frac{1}{2} y^T A^{-1} y = -\frac{1}{2} y^T Q^{-1} y. \]  
\[ A.2. \text{ Log-determinant term} \]
We write
\[ \log |A| = \sum_{i=1}^{n} \log(a_i) = \sum \log(\ell_i + e_i), \]  
where \( a_i \) are the eigenvalues of \( A \), \( \ell_i \) are the eigenvalues of \( Q \), both sorted in descending order, and \( e_i := a_i - \ell_i \). We can then translate the constraints of \( K \) as \( e_i \geq 0 \) and \( \sum_i (e_i + \ell_i) = t \). The \( e_i \) are eigenvalues of \( Q \), which can be computed in \( O(nm^2) \) by noting that \( n - m \) of them are \( \sigma^2 \), and the remaining eigenvalues coincide with the eigenvalues of \( M M^T + \sigma^2 I \), where \( M = K^{-1/2} K_{cr} \).
We define \( t' = t - \text{tr}(Q) \) and consider
\[ \sup_{A \succ Q} \log |A| = \sup_{A \succ Q} \sum_{e_i > 0} \log(e_i + \ell_i). \]  
This coincides with a problem in information theory related to power-allocation over channels. It is a convex optimization which can be solved using Lagrange multiplier and the KKT conditions. The solution of this equation is,
\[ e_i = \max(0, t'/\nu - t'\ell_i), \]  
where \( \nu \) is chosen such that, \( \sum_{i=1}^{n} \max(0, 1/\nu - \ell_i) = 1 \). See Example 5.2 in Boyd and Vandenberghe (2004) for details of this maximization.
The eigenvalues of \( Q \) can be computed in \( O(nm^2) \) and the Lagrange multiplier can be found in \( O(n) \) as it is the solution to a piecewise linear problem.
\[ A.2.1. \text{ LOWER BOUNDING THE LOG DETERMINANT} \]
In some cases upper bounds on the log marginal likelihood are of interest (Titsias, 2014; Kim and Teh, 2018). We therefore turn to the problem of lower bounding the log determinant of \( A \). Improvements in this bound can be used in conjunction with either of the bounds on the quadratic term given in Titsias (2014) or Kim and Teh (2018). We have,
\[ \log(A) = \sum \log(\ell_i + e_i) = \log |Q| + \sum \log(1 + e_i/\ell_i). \]
Rewriting the second term on the right hand side as the log of a product, expanding the product and using that $e_i \geq 0$,

$$
\sum_{i=1}^{n} \log \left( 1 + \frac{e_i}{\ell_i} \right) = \log \prod_{i=1}^{n} \left( 1 + \frac{e_i}{\ell_i} \right) \geq \log \left( 1 + \sum_{i=1}^{n} \frac{e_i}{\ell_i} \right).
$$

(25)

Using that $\ell_i \leq \ell_1$,

$$
\log |A| \geq \log |Q| + \log \left( 1 + \frac{\text{tr}(K - Q)}{\ell_1} \right).
$$

(26)

We now show that this is the greatest upper bound given the constraints on $A$ by constructing an $A$ satisfying this bound. Consider $A = Q + \text{tr}(K - Q)ww^T$, where $w$ is the eigenvector of $Q$ corresponding to $\ell_1$. Then all of the eigenvalues of $K$ coincide with the eigenvalues of $Q$, except that largest, which is $\ell_1 + \text{tr}(K - Q))$. Rearranging the formula for the log determinant, we see that this recovers the bound given above.

### B. Additional Experiments

We performed Iterative GP experiments with all combinations of Adam learning rates ($0.1$, $0.01$) and minimum likelihood noise constraints ($\sigma^2_{\min} = 1e^{-4}$, $\sigma^2_{\min} = 1e^{-6}$) for poletele, kin40k, elevators, bike and protein datasets. The experiments displayed instability and sensitivity to some settings (fig. 7, fig. 9, and fig. 10). In particular, we found that the setting with $\sigma^2_{\min} = 1e^{-6}$ and Adam learning rate $0.1$ (Wang et al. (2019) uses $\sigma^2_{\min} = 1e^{-4}$ and Adam learning rate $0.1$), causes severe predictive performance degradation in poletele, bike, and kin40k datasets after 2000 iterations. Lowering the learning rate to $0.01$ facilitates smoother, but much slower convergence. However, datasets such as poletele (fig. 10) and protein (fig. 11) still exhibit a decrease in the predictive performance during training.

![Figure 3](image-url)  
*Figure 3.* Test root mean square error (RMSE) and negative log predictive density (NLPD) metrics of CGGP, SGPR and Iterative GP models computed on bike dataset. The shaded area is IQR region, and the line is a median over five experiment trials with different dataset splits.
Figure 4. Test root mean square error (RMSE) and negative log predictive density (NLPD) metrics of CGGP, SGPR and Iterative GP models computed on elevators dataset. The shaded area is IQR region, and the line is a median over five experiment trials with different dataset splits.

Figure 5. Test root mean square error (RMSE) and negative log predictive density (NLPD) metrics of CGGP, SGPR and Iterative GP models computed on kin40k dataset. The shaded area is IQR region, and the line is a median over five experiment trials with different dataset splits.

Figure 6. Test root mean square error (RMSE) and negative log predictive density (NLPD) metrics of CGGP, SGPR and Iterative GP models computed on poletele dataset. The shaded area is IQR region, and the line is a median over five experiment trials with different dataset splits.
Figure 7. Test RMSE and NLPD for the Iterative GP method with learning rates 0.01 and 0.1 and minimum likelihood noise constrained at $10^{-4}$ and $10^{-6}$ on the bike dataset.

Figure 8. Test RMSE and NLPD for the Iterative GP method with learning rates 0.01 and 0.1 and minimum likelihood noise constrained at $10^{-4}$ and $10^{-6}$ on the elevators dataset.

Figure 9. Test RMSE and NLPD for the Iterative GP method with learning rates 0.01 and 0.1 and minimum likelihood noise constrained at $10^{-4}$ and $10^{-6}$ on the kin40k dataset.
Figure 10. Test RMSE and NLPD for the Iterative GP method with learning rates 0.01 and 0.1 and minimum likelihood noise constrained at $1e^{-4}$ and $1e^{-6}$ on the poletele dataset.

Figure 11. Test RMSE and NLPD for the Iterative GP method with learning rates 0.01 and 0.1 and minimum likelihood noise constrained at $1e^{-4}$ and $1e^{-6}$ on the protein dataset.
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