Scalable Cross Validation Losses for Gaussian Process Models

Martin Jankowiak
Broad Institute

Geoff Pleiss
Columbia University

Abstract

We introduce a simple and scalable method for training Gaussian process (GP) models that exploits cross-validation and nearest neighbor truncation. To accommodate binary and multi-class classification we leverage Polya-Gamma auxiliary variables and variational inference. In an extensive empirical comparison with a number of alternative methods for scalable GP regression and classification, we find that our method offers fast training and excellent predictive performance. We argue that the good predictive performance can be traced to the non-parametric nature of the resulting predictive distributions as well as to the cross-validation loss, which provides robustness against model mis-specification.

1 Introduction

As machine learning becomes more widely used, it is increasingly being deployed in applications where autonomous decisions are guided by predictive models. For example, supply forecasts can determine the prices charged by retailers, expected demand for transportation can be used to optimize bus schedules, and data-driven algorithms can guide load balancing in critical electrical subsystems. For these and many other applications of machine learning, it is essential that models are well-calibrated, thus enabling downstream decisions to factor in uncertainty and risk.

Gaussian processes are a general-purpose modeling component that offer excellent uncertainty quantification in a variety of predictive tasks, including regression, classification, and beyond (Rasmussen 2003). Despite their many attractive features, wider use of Gaussian process (GP) models is hindered by computational requirements that can be prohibitive. For example, classic methods for training GP regressors using the marginal log likelihood (MLL) scale cubically with the number of data points. This bottleneck has motivated extensive research into approximate GP inference schemes with more favorable computational properties (Liu et al. 2020).

A particularly popular and fruitful approach has centered on inducing point methods and variational inference (Snelson and Ghahramani 2006; Titsias 2009; Hensman et al. 2013). These methods rely on the ELBO, which is a lower bound to the MLL, for training and trade cubic complexity in the size of the dataset $N$ for cubic complexity in the number of inducing points $M$. Since $M$ is a hyperparameter controlled by the user, inducing point methods can lead to substantial speed-ups. One disadvantage of inducing point methods—as we will see explicitly in our empirical evaluation—is that some datasets may require prohibitively large values of $M$ to ensure good model fit.

Instead of targeting the MLL directly or via a lower bound, we investigate the suitability of training objectives based on cross-validation (CV). In this work we argue that CV is attractive in the context of GP models for three reasons in particular: i) it can provide robustness against model mis-specification; ii) it opens the door to simple approximation schemes based on nearest neighbor truncation; and iii) nearest neighbor truncation enables non-parametric predictive distributions that avoid some of the disadvantages of inducing point methods. To put it differently, although nearest neighbors are a natural starting point for scalable GP methods, their combination with MLL-based objectives is typically made awkward by the need to specify an ordering of the data (Vecchia 1988; Datta et al. 2016). In contrast, CV-based objectives are free of any such requirement, resulting in an attractive synergy between cross-validation and nearest neighbor approximations. To exploit this synergy we make the following contributions:

1. We introduce the $k$-nearest-neighbor leave-one-out (LOO-$k$) objective, which can be used to train GP models on large datasets.
2. We introduce a Pólya-Gamma auxiliary variable construction that extends this approach to binary and multi-class classification.

3. We perform an extensive empirical comparison with a number of alternative methods for scalable GP regression and classification and demonstrate the excellent predictive performance of our approach.

Before we describe our approach in Sec. 3 we first review some basic background on Gaussian processes, which also gives us the opportunity to establish some of the notation we will use throughout.

2 Background on Gaussian processes

A GP on the input space \( D \subset \mathbb{R}^D \) is specified by a covariance function or kernel \( K : D \times D \to \mathbb{R} \) (Rasmussen, 2003). A common choice is the RBF or squared exponential kernel, which is given by

\[
K(x, z) = \sigma_K^2 \exp\left(-\frac{1}{2} \sum_i (x_i - z_i)^2 / \rho_i^2 \right) \tag{1}
\]

where \( \{\rho_i\} \) are length scales and \( \sigma_K \) is the kernel scale. For scalar regression \( f : D \to \mathbb{R} \) the joint density of a GP regressor takes the form

\[
p(y, f|X) = N(y|f, \sigma_{\text{obs}}^{-2} I_N) N(f|0, K_{N,N}) \tag{2}
\]

where \( y \) are the real-valued targets, \( f \) are the latent function values, \( X = \{x_i\}_{i=1}^N \) are the \( N \) inputs with \( x_i \in D \), \( \sigma_{\text{obs}}^2 \) is the variance of the Normal likelihood, and \( K_{N,N} \) is the \( N \times N \) kernel matrix. The marginal log likelihood (MLL) \( \log p(y|X) = \log \int p(y, f|X) \) of the observed data can be computed in closed form:

\[
\log p(y|X) = \log N(y, K_{N,N} + \sigma_{\text{obs}}^2 I_N) \tag{3}
\]

Computing \( \log p(y|X) \) has cost \( \mathcal{O}(N^3) \), which has motivated the great variety of approximate methods for scalable training of GP models (Liu et al., 2020). The posterior predictive distribution \( p(y|y, X, x_*) \) of the GP at a test point \( x_* \in D \) is the Normal distribution \( N(\mu_f(x_*), \sigma_f(x_*)^2 + \sigma_{\text{obs}}^2) \) where \( \mu_f(\cdot) \) and \( \sigma_f(\cdot)^2 \) are given by

\[
\mu_f(x_*) = K_{*,N}^T(K_{N,N} + \sigma_{\text{obs}}^2 I_N)^{-1} y \tag{4}
\]

\[
\sigma_f(x_*)^2 = K_{*,*} - K_{*,N}^T(K_{N,N} + \sigma_{\text{obs}}^2 I_N)^{-1} K_{*,N} \tag{5}
\]

Here \( K_{*,*} = K(x_*, x_*) \) and \( K_{*,N} \) is the column vector with elements \( (K_{*,N})_n = K(x_*, x_n) \).

3 Nearest neighbor cross-validation losses

The marginal log likelihood of a GP can be written as a sum of logs of univariate posterior conditionals, where for a fixed, arbitrary ordering \( \{1, \ldots, N\} \) we have

\[
\mathcal{L}_{\text{MLL}} \equiv \log p(y|X) = \sum_{n=1}^N \log p(y_n|y_{<n}, x_{\leq n}) \tag{6}
\]

and where \( y_{<n} \equiv \{y_1, \ldots, y_{n-1}\} \) and \( x_{\leq n} \equiv \{x_1, \ldots, x_n\} \). Summing over all \( N! \) permutations \( \tau \in S^N \) we obtain

\[
\mathcal{L}_{\text{MLL}} = \frac{1}{N!} \sum_{\tau \in S^N} \sum_{n=1}^N \log p(y_n|y_{<n}^\tau, x_{\leq n}^\tau) \equiv \sum_{n=0}^{N-1} \mathcal{L}_{\text{CV}}^n \tag{7}
\]

where \( \tau \) superscripts denote application of the permutation \( \tau \). Additionally on the RHS of Eqn. 7 we have grouped the \( N \times N! \) terms in the sum w.r.t. the number of data points that each term conditions on, i.e. each term in \( \mathcal{L}_{\text{CV}}^n \) conditions on exactly \( n \) data points and is implicitly defined by Eqn. 7. For example we have

\[
\mathcal{L}_{\text{CV}}^{N-1} = \frac{1}{N} \sum_{n=1}^N \log p(y_n|y_{<n}, X) \tag{8}
\]

\[
\mathcal{L}_{\text{CV}}^0 = \frac{1}{N} \sum_{n=1}^N \log p(y_n|x_n) \tag{9}
\]

where \( y_{<n} \equiv \{y_1, \ldots, y_{n-1}, y_{n+1}, \ldots, y_N\} \). This decomposition makes a number of properties of the marginal log likelihood apparent. First, the MLL is directly linked to the average posterior predictive performance conditioned on all possible training data sets, including the empty set (Fong and Holmes, 2020). Second, the inclusion of conditioning sets that are only a small fraction of the full dataset—in the extreme case empty conditioning sets as in \( \mathcal{L}_{\text{CV}}^0 \)—means that \( \mathcal{L}_{\text{MLL}} \) can exhibit substantial dependence on the prior. Indeed the term \( \mathcal{L}_{\text{CV}}^0 \) scores the model exclusively with respect to the prior predictive. Conversely, \( \mathcal{L}_{\text{CV}}^{N-1} \) exhibits the least dependence on the prior.

In the following we will use \( \mathcal{L}_{\text{CV}}^{N-1} \) as the basis for our training objective, in particular using it to learn the hyperparameters of the kernel. This choice is motivated by two observations. First, as we have just argued, we expect \( \mathcal{L}_{\text{CV}}^{N-1} \) to provide robustness against prior misspecification due to its reduced dependence on the prior. Indeed it is well known that conventional Bayesian inference can be suboptimal when the model is misspecified: see (Masegosa, 2019) and references therein for recent discussion. Second, while \( \mathcal{L}_{\text{CV}}^{N-1} \) depends on

\footnotetext{Unless otherwise noted we assume that the prior mean is uniformly zero.}

\footnotetext{We define \( y_{<1} \equiv \emptyset \). Note that here and elsewhere we suppress dependence on the kernel hyperparameters.}

\footnotetext{For example \( y^*_n \equiv y_T(n) \) and \( y^*_{<n} \equiv \{y_T(1), \ldots, y_T(n-1)\} \)
the entire dataset, individual predictive distributions $p(y_n|y_{-n}, X)$ in the sum typically exhibit non-negligible dependence on only a small subset of the conditioning data. This latter observation opens the door to nearest neighbor truncation, which we describe next.

### 3.1 Nearest neighbor truncation

In the regression case (see Eqn. 45) computing $\mathcal{L}_{CV}^{-1}$ in Eqn. 8 has $O(N^4)$ cost if done naively, which is very expensive for $N \gtrsim 10^3$. While this can be reduced to $O(N^3)$ for a stochastic estimate or if care is taken with the algebra (Petit et al., 2020; Ginsbourger and Schäfer, 2021), this still precludes a training algorithm that scales to large datasets with millions of data points.

To enable scalability, we apply a $k$-nearest-neighbor truncation to $\mathcal{L}_{CV}$ to obtain the $k$-truncated leave-one-out (LOO-k) objective

$$\mathcal{L}_{LOO}^k = \frac{1}{N} \sum_{n=1}^{N} \log p(y_n|y_{-n}, X_{-n}, x_n)$$

where we use $k = \infty$ to denote the non-truncated objective. Here the pair $(y_{n}, X_{n}, x_n)$ denotes the $k$-nearest-neighbors of $x_n$ (and the corresponding targets) as determined using the Euclidean metric defined with kernel length scales $\rho_e$. For univariate regression computing Eqn. 9 has a $O(Nk^3)$ cost. Utilizing data subsampling to obtain a stochastic estimate $\hat{\mathcal{L}}_{LOO}^k$, this cost becomes $O(Bk^3)$ for mini-batch size $B$. Notably, the bottleneck in computing $\hat{\mathcal{L}}_{LOO}^k$ involves a batch Cholesky decomposition of a $B \times k \times k$ tensor, which can be done extremely efficiently on a GPU for $k \lesssim 500$ even for $B \sim 100$. The nearest neighbor search takes $O(N \log N)$ time using standard algorithms like k-d trees (Bentley, 1975), though for $N \lesssim 10^7$ it is often faster to use $O(N^2)$ brute force algorithms that make use of GPU parallelism. In practice we recompute the nearest neighbor index somewhat infrequently, e.g. after every 50th gradient update. See Algorithm 1 in the supplement for a summary of the training procedure. Note that since there are no inducing points, the sole purpose of the training step is to identify good kernels.

### 3.2 Binary classification

Above we implicitly assume that the LOO posterior probability $p(y_n|y_{-n}, X_{-n}, x_n)$ can be computed analytically. What if this is not the case, as happens in classification? In this section we briefly describe how we define a LOO training objective for binary classification. The basic strategy is to introduce auxiliary variables that restore Gaussianity and thus enable closed form (conditional) posterior distributions. Let $D = \{(x_n, y_n)\}_{n=1}^{N}$ with $y_n \in \{-1, 1\}$ and consider a GP classifier with likelihood $p(y_n|f(x_n)) = [1 + \exp(-y_n f(x_n))]^{-1}$ governed by a logistic function. We introduce a $N$-dimensional vector of Polya-Gamma (Polson et al., 2013) auxiliary variables $\omega$ and exploit the identity $[1 + e^\psi]^{-1} = \frac{1}{2} \E_{p(\omega|1, 0)} \exp \{-\frac{1}{2} \omega^2 - \frac{1}{2} \psi\}$ to massage the likelihood terms into Gaussian form and end up with a joint density $p(y, f, \omega|X)$ proportional to

$$p(\omega)p(f|K, N)\exp \left\{ \frac{1}{2} y^T f - \frac{1}{2} f^T \Omega f \right\}$$

where $\Omega = \text{diag}(\omega)$ is a diagonal $N \times N$ matrix. Note that this augmentation is exact. We proceed to integrate out $f$ and perform variational inference w.r.t. $\omega$.

This results in the variational objective

$$\mathcal{L}_{ELBO} = \E_{q(\omega)} [\log p(y|X, \omega) - \text{KL}(q(\omega)|p(\omega))]$$

where we take $q(\omega)$ to be a mean-field log-Normal variational distribution and KL denotes the Kullback-Leibler divergence. We then replace $\log p(y|X, \omega)$ with its LOO approximation to obtain

$$\mathcal{L}_{LOO} \equiv \frac{1}{N} \sum_{n=1}^{N} \E_{q(\omega)} [\log p(y_n|y_{-n}, X_{-n}, \omega_{-n})]$$

$$- \text{KL}(q(\omega)|p(\omega))$$

where the (conditional) posterior predictive distribution $p(y_n|y_{-n}, X_{-n}, \omega_{-n})$ is given by

$$p(y_n|y_{-n}, X_{-n}, \omega_{-n}) = \int df_n p(y_n|f_n)p(f_n|y_{-n}, X_{-n}, \omega_{-n})$$

Here the (conditional) posterior over the latent function value $f_n$, namely $p(f_n|y_{-n}, X_{-n}, \omega_{-n})$, is given by

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4. At least for approximately compactly-supported kernels like RBF or Matérn. Our method is not immediately applicable to, e.g., periodic kernels as are commonly used in time-series applications.

5. That is we compute nearest neighbors w.r.t. the distance function $d(x, z) = \sqrt{\sum_i (x_i - z_i)^2 / \rho_i^2}$. Note that by definition $X_{-n,k}$ does not contain $x_n$.

6. Modern nearest neighbor libraries, e.g. FAISS [Johnson et al., 2019], perform nearest neighbor searches in a map-reduce fashion. This yields an $O(N)$ memory requirement, which is feasible on a single GPU for $N \lesssim 10^7$. For larger datasets it is possible to achieve speed-ups with quantization, trading off speed for accuracy.
the Normal distribution $N(f_n|\mu_n, \sigma_n^2)$ with mean and variance equal to

$$\begin{align*}
\mu_n &= \frac{1}{2} K_{n,n}^T (K_{n,n} + \Omega_n^{-1})^{-1} \Omega_n^{-1} y_n \\
\sigma_n^2 &= K_{n,n} - K_{n,n}^T (K_{n,n} + \Omega_n^{-1})^{-1} K_{n,n} \\
K_{n,n} &\equiv K(X_n, x_n) \in \mathbb{R}^{n \times 1, 1} \\
K_{n,n} &\equiv K(X_n, X_n) \in \mathbb{R}^{n \times 1, n-1}.
\end{align*}$$

We approximate the univariate integral in Eqn. 13 with Gauss-Hermite quadrature. Our final objective function is obtained by applying a $k$-nearest-neighbor truncation to Eqn. 12. To maximize this objective function we use standard techniques from stochastic variational inference, including data subsampling and reparameterized gradients of $\omega$. At test time predictions can be obtained by computing Eqn. 13 after conditioning on a sample $\omega \sim q(\omega)$. Note that in practice we use a single sample, since we found negligible gains from averaging over multiple samples. The computational cost of a training iteration is $O(Bk^3 + BQ)$, where $Q$ is the number of points in the quadrature rule. For a more comprehensive derivation and additional details on binary classification see Sec. A.7.

### 3.3 Multi-class classification

The Pólya-Gamma auxiliary variable construction used in Sec. 3.2 can be generalized to the multi-class setting with $K$ classes using a stick-breaking construction \cite{Linderman2015}. Among other disadvantages, this construction requires choosing a class ordering. To avoid this, and to obtain linear computational scaling in the number of classes $K$, we instead opt for a one-against-all construction, which results in a $O(BKk^3 + BKQ)$ computational cost per training iteration. We refer the reader to Sec. A.8 for details and Sec. 5.9 for empirical results.

### 3.4 Other likelihoods

The auxiliary variable construction in Sec. 3.2, 3.3 can be extended to a number of other likelihoods, including binomial and negative binomial likelihoods as well as Student’s t likelihood. See Sec. A.9 for more details.

### 4 Related work

Our work is related to various research directions in machine learning and statistics. Here we limit ourselves to an abbreviated account and refer the reader to Sec. A.2 for a more detailed discussion.

Nearest neighbor constructions in the GP context have been explored by several authors. \cite{Datta2016} define a Nearest Neighbor Gaussian Process, which is a valid stochastic process, derive a custom Gibbs inference scheme, and illustrate their approach on geospatial data. Vecchia approximations \cite{Vecchia1988} and \cite{Katzfuss2021} exploit a nearest neighbor approximation to the MLL. Both these approaches can...
work well in 2 or 3 dimensions but tend to struggle in higher dimensions due to the need to choose a fixed ordering of the data. Tran et al. (2021) introduce a variational scheme for GP inference (SWSGP) that leverages nearest neighbor truncation within an inducing point construction. Gramacy and Apley (2015) introduce a ‘Local Gaussian Process Approximation’ for regression that iteratively constructs a nearest neighbor conditioning set at test time; in contrast to our approach there is no training phase.

Cross-validation (CV) in the GP (or rather kriging) context was explored as early as 1983 by Dubrule (1983). Bachoc (2013) compares predictive performance of GPs fit with MLL and CV and concludes that CV is more robust to model mis-specification. Smith et al. (2016) consider CV losses in the context of differentially private GPs. Recent work explores how the CV score can be efficiently computed for GP regressors (Ginsbourger and Schäfer, 2021; Petit et al., 2020). Jankowiak et al. (2020) introduce an approximate inference scheme for binary and multi-class classification that exploits inducing points, Pólya-Gamma auxiliary variables, and variational inference.

5 Experiments

In this section we present an empirical evaluation of GPs trained with the LOO-\(k\) objective Eqn. 9. In Sec. 5.1, we explore general characteristics of our method and in Sec. 5.6-5.9 we compare our method to a variety of baseline methods for GP regression and classification.

5.1 Model mis-specification

We explore whether the LOO-\(k\) objective in Eqn. 9 is robust to model mis-specification, as we would expect following the discussion in Sec. 3. Since models can be mis-specified in a great variety of ways, it is difficult to make quantitative statements about mis-specification in general terms. Instead we choose a simple controlled setting where we can toggle the degree of mis-specification. First we sample 8096 data points \(x_i\) uniformly from the cube \([-1, 1]^4 \subset \mathbb{R}^4\). Next we generate targets \(y\) using a GP prior specified by an isotropic stationary RBF kernel with observation noise \(\sigma_{\text{obs}} = 0.1\). We then apply a coordinatewise warping to each \(x_n\), where the warping is given by the identity...
mapping for $x_i \geq 0$ and $x_i \rightarrow (1 + \gamma)x_i$ for $x_i < 0$. We use half the data points for training and the remainder for testing predictive performance. The results can be seen in Fig. 1. We see that as $\gamma$ increases and the dataset becomes more non-stationary, the LOO-$k$ GP exhibits superior predictive performance. We note that the degraded test log likelihood of the MLL GP for large $\gamma$ stems in part from severely underestimating the observation noise $\sigma_{\text{obs}}$. Fig. 1 confirms our expectation that using a CV-based objective can be more robust to model mis-specification, especially as the latter becomes more severe.

5.2 Objective function comparison

In Fig. 2 we compare how the MLL, SVGP, and LOO-$k$ objective functions depend on the kernel hyperparameters $\sigma_K$ and $\sigma_{\text{obs}}$. First we subsample the UCI Bike dataset to $N = 2000$ datapoints. We then train a GP using MLL on this dataset and keep all the hyperparameters fixed to their MLL values except for the one hyperparameter that is varied. Fig. 2 makes apparent the well-known tendency of SVGP to overestimate the observation noise $\sigma_{\text{obs}}$ and, consequently, prefer a smaller value of $\sigma_K$ (Bauer et al., 2016). This overestimation of $\sigma_{\text{obs}}$ can lead to severe overestimation of uncertainty at test time. Since $\sigma_K$ and $\sigma_{\text{obs}}$ appear symmetrically in Eqn. 5 and likewise in $E^k_{\text{LOO}}$, the LOO-$k$ GP does not exhibit the same tendency (as argued in (Jankowiak et al., 2020b)).

5.3 Dependence on number of nearest neighbors $k$

In Fig. 3 we explore how predictive performance of a LOO-$k$ GP depends on the number of nearest neighbors $k$. As expected, we generally find that performance improves as $k$ increases, although the degree of improvement depends on the particular dataset. In addition the marginal gains of increasing $k$ past $k \sim 128$ are small on most datasets. This finding is advantageous for our method with respect to computational cost, whereas inducing point methods often require $M \gtrsim 500$ to achieve good model fit. This tendency is easy to understand, since the $M$ inducing points need to ‘compress’ the entire dataset, while the $k$ nearest neighbors only need to model the vicinity of a given test point.

5.4 Runtime performance

In Fig. 4 we compare the runtime performance of LOO-$k$ to SVGP on datasets from $N = 1000$ to $N = 5$ million. As discussed further in Sec. A.3, we can take these two methods’ runtimes as representative of other nearest neighbor (e.g. Vecchia) and inducing point (e.g. PPGPR) methods, respectively. Thanks to highly parallel GPU-accelerated nearest neighbor algorithms (Johnson et al., 2019), only a small fraction of LOO-$k$ training time is devoted to nearest neighbors queries up to $N \sim 10^6$. Though these queries become more costly as $N$ approaches 10 million, LOO-$k$ is comparable to SVGP in this regime, and search time can be improved by sharding or other approximations. Since a LOO-$k$ regressor is fully parameterized by a handful of kernel hyperparameters and does not make use of variational parameters, it requires substantially fewer gradient steps to converge. For example on the Kegg-undirected dataset with $N = 47706$ considered in the next section we find that LOO-256 trains $\sim 4x$ faster than SVGP with $M = 1024$ inducing points.

5.5 Degenerate data regime

To better understand the limitations of LOO-$k$ we run an experiment in which we create artificially ‘degenerate’ datasets by adding a noisy replicate of each data point in the training set (adding $N(0, 10^{-4})$ noise both to inputs $x$ and responses $y$). We expect that a potential failure mode of nearest neighbor methods like LOO-$k$ is a reduced ability to model long-distance correlations. Indeed we expect better performance from a global inducing point method like SVGP in this regime. As expected—see Table 6 in the supplement for complete results—the performance of SVGP-512 is not much affected by the addition of severe degeneracy, while LOO-64 exhibits a large loss in performance on 3/4 datasets (although LOO still exhibits better predictive performance than SVGP on 2/4 degenerate datasets). Ultimately this loss in performance in LOO-64 can be traced to a systematic preference for smaller kernel lengthscales. While the good empirical results on most datasets in subsequent sections suggest that many datasets do not exhibit such degeneracy, this limitation of LOO-$k$ should be kept in mind.

5.6 Univariate regression

We compare the performance of GP regressors trained with the LOO-$k$ objective in Eqn. 9 to six scalable baseline methods. SVGP (Hensman et al., 2013) and PPGPR (Jankowiak et al., 2020b) are both inducing point methods; SVGP targets the MLL via an ELBO lower bound, while PPGPR uses a regularized cross-validation loss. The remaining baselines, MLL-$k$, Vecchia, SWSGP, and ALC, exploit nearest neighbors. MLL-$k$ uses a biased $k$-nearest-neighbor truncation of the MLL for training (Chen et al., 2020). Vecchia (Vecchia, 1988) uses a different $k$-nearest-neighbor approximation of the MLL that requires specifying a fixed ordering of the data. SWSGP (Tran et al., 2021) combines nearest neighbor approximations and inducing point methods, where each data point only depends...
on a subset of inducing points. ALC (Gramacy and Apley 2015) iteratively constructs a nearest neighbor conditioning set at test time using a variance reduction criterion and chooses hyperparameters using the ‘local’ MLL. See Sec. A.3 in the supplemental materials for a conceptual framing of these different approaches. We also include a comparison to GPs trained with MLL using the methodology in Wang et al. (2019). See Sec. A.10 for additional experimental details.

The results are depicted in Fig. 5 and summarized in Table 1. We find that LOO-k exhibits the best predictive performance overall, both w.r.t. log likelihood and RMSE, followed by MLL-k. ALC performs well on some datasets but poorly on others; indeed we are unable to obtain reasonable results on the Kegg-directed dataset. Vecchia does poorly overall, presumably due to the need to use a strict ordering of the data. SVGP also does poorly overall; as argued by Bauer et al. (2016) and Jankowiak et al. (2020b), degraded performance w.r.t. log likelihood can be traced to a tendency to overestimate the observation noise and consequently underestimate function uncertainty. PPGPR exhibits good log likelihoods but poor RMSE performance due to the priority it places on uncertainty quantification.

The nearest neighbor methods can perform well in high-dimensional input spaces; e.g. the Slice dataset is 380-dimensional.

### 5.7 Multivariate regression

We continue our empirical evaluation by considering four multivariate regression datasets. In each dataset the input and output dimensions correspond to various joint positions/velocities/etc. of a robot. Each GP regressor employs the structure of the linear model of coregionalization (LMC) (Alvarez et al. 2012). We compare against three baseline methods: SVGP, PPGPR, and MLL-k. The results are depicted in Fig. 6 and...
Table 2: We summarize the performance ranking of various GP methods on the multivariate regression experiments in Fig. 6 averaged over all dataset splits. We compare the predictive performance of the LOO- \(k \) and MLL- \(k \) with the two inducing point methods, SVGP and PPGPR, with LOO- \(k \) and MLL- \(k \) performing the best w.r.t. NLL and RMSE, respectively. Strikingly, for 3/4 datasets the RMSEs for the nearest neighbor methods are much smaller than for the inducing point methods, even though we use no more than \( k = 32 \) nearest neighbors. We hypothesize that it is difficult to capture the complex non-linear dynamics underlying these datasets using a limited number of inducing points. In addition, training objectives that depend on large numbers of inducing points can be challenging to optimize, potentially resulting in suboptimal solutions. This highlights one of the advantages of methods like LOO- \(k \) and MLL- \(k \), which avoid optimization in input space and result in flexible non-parametric nearest neighbor predictive distributions.

Table 3: We summarize the performance ranking of various GP methods for binary classification averaged over all dataset splits. We find that the two nearest neighbor methods, LOO- \(k \) and MLL- \(k \), outperform the two inducing point methods, SVGP and PPGPR, with LOO- \(k \) and MLL- \(k \) performing the best w.r.t. NLL and RMSE, respectively. Strikingly, for 3/4 datasets the RMSEs for the nearest neighbor methods are much smaller than for the inducing point methods, even though we use no more than \( k = 32 \) nearest neighbors. We hypothesize that it is difficult to capture the complex non-linear dynamics underlying these datasets using a limited number of inducing points. In addition, training objectives that depend on large numbers of inducing points can be challenging to optimize, potentially resulting in suboptimal solutions. This highlights one of the advantages of methods like LOO- \(k \) and MLL- \(k \), which avoid optimization in input space and result in flexible non-parametric nearest neighbor predictive distributions.

5.8 Binary classification

Next we compare the predictive performance of the LOO- \(k \) objective for binary classification, Eqn. [12] to two scalable GP baselines. Both SVGP [Hensman et al., 2015] and PGVI [Wenzel et al., 2019] are inducing point methods that utilize variational inference; PGVI also makes use of natural gradients and Polya-Gamma augmentation. The results are depicted in Fig. 7 and summarized in Table 3. The predictive performance is broadly comparable for most datasets. Most striking is the superior performance of LOO- \(k \) on the two Covtype datasets, which exhibit (geospatial) decision boundaries with complex topologies that are difficult to capture with a limited number of inducing points.

5.9 Multi-class classification

We compare the predictive performance of the LOO- \(k \) objective for multi-class classification to a SVGP baseline. We consider 13 datasets with 5 splits per dataset for a total of 65 splits. We find that LOO- \(k \) outperforms SVGP on 41/65 and 42/65 splits w.r.t. log likelihood and error, respectively. See Sec. A.11 for complete results and Sec. A.8 for details on the method.

6 Discussion

Most scalable methods for fitting Gaussian process models target the marginal log likelihood. As we have shown, the fusion of cross-validation and nearest neighbor truncation provides an alternative path to scalability. The resulting method is simple to implement and offers fast training and excellent predictive performance, both for regression and classification. We note three limitations of our approach. First, non-Gaussian likelihoods that do not admit suitable auxiliary variables may be difficult to accommodate. Second, as discussed in Sec. 5.5, LOO- \(k \) GPs may be inappropriate for highly degenerate datasets. Third, nearest neighbor queries may be prohibitively slow for datasets with tens of millions of data points. Modifications to our basic approach may be required to support this regime, including for example approximate nearest neighbor queries or dataset sharding.
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A Appendix

Algorithm 1: We outline the main steps in learning a LOO-k GP in the case of univariate regression.

**Input:** Dataset $D = \{y, X\}$ with $N$ data points; number of nearest neighbors $k$; optimizer $\text{optim}$; mini-batch size $B$; number of iterations $T$; nearest neighbor index update frequency $T_{nn}$; initial kernel hyperparameters $\{\rho_i^0, \sigma_K^0, \sigma_{obs}^0\}$

**Output:** Learned kernel hyperparameters $\{\rho_i^T, \sigma_K^T, \sigma_{obs}^T\}$

1. \textbf{for} $t = 1, ..., T$ \textbf{do}
2. \hspace{1em} If $(t-1) \mod T_{nn} = 0$, (re)compute the nearest neighbor index using $\{\rho_i^{t-1}\}$
3. \hspace{1em} Choose a random mini-batch of indices of size $B$: $\mathcal{I} \subset \{1, ..., N\}$ with $|\mathcal{I}| = B$
4. \hspace{1em} For each $i \in \mathcal{I}$ form the $k$-nearest-neighbor tuple $(y_{i,k}, X_{i,k})$
5. \hspace{1em} Compute a stochastic estimate $\mathcal{L}_{\text{LOO}}^k$ of Eqn. 9 using Eqn. 4-5, $\{(y_{i,k}, X_{i,k})\}_{i=1}^B$ and $\{\rho_i^{t-1}, \sigma_{K}^{t-1}, \sigma_{obs}^{t-1}\}$
6. \hspace{1em} Let $\{\rho_i^t, \sigma_K^t, \sigma_{obs}^t\} = \text{optim}(\mathcal{L}_{\text{LOO}}^k)$
7. \textbf{return} $\{\rho_i^T, \sigma_K^T, \sigma_{obs}^T\}$

A.1 Societal impact

We do not anticipate any negative societal impact from the methods described in this work, although we note that they inherit the risks that are inherent to any predictive algorithm. In more detail there is the possibility of the following risks. First, predictive algorithms can be deployed in ways that disadvantage vulnerable groups in a population. Even if these effects are unintended, they can still arise if deployed algorithms are poorly vetted with respect to their fairness implications. Second, algorithms that offer uncertainty quantification may be misused by users who place unwarranted confidence in the uncertainties produced by the algorithm. This can arise, for example, in the presence of undetected covariate shift. Third, since our algorithm makes use of non-parametric predictive distributions, it is necessary to retain the training data to make predictions. This is in contrast to fully parametric models where the training data can be discarded. As such, nearest neighbor methods may be more vulnerable to data breaches, although standard security practices should mitigate any such risk. That said, for these reasons nearest neighbor methods may be inappropriate for use with sensitive datasets, e.g. those that contain personally identifiable information.

A.2 Related work (extended)

Nearest neighbor constructions in the GP context have been explored by several authors. Vecchia approximations (Vecchia, 1988; Katzfuss and Guinness, 2021) exploit a nearest neighbor approximation to the MLL. This approach can work well in 2 or 3 dimensions but tends to struggle in higher dimensions due to the need to choose a fixed ordering of the data. Dutta et al. (2016) extend the Vecchia approach to the Nearest Neighbor Gaussian Process, which is a valid stochastic process, deriving a custom Gibbs inference scheme, and illustrating their approach on geospatial data. Chen et al. (2020) explore a different biased approximation to the MLL, which does not require specifying an ordering of the data and which we refer to as MLL-k. For more details on Vecchia approximations and MLL-k see the next section, Sec. A.3. Tran et al. (2021) introduce a variational scheme for GP inference (SWSGP) that leverages nearest neighbor truncation within an inducing point construction. Specifically, they introduce a masking latent variable that selects a subset of inducing points for every given data point. This makes it possible to use many inducing points (unlike conventional inducing point methods like SVGP): which consequentially introduces many new variational parameters that make optimization more challenging. Gramacy and Apley (2015); Gramacy (2016), addressing the computer simulation community, introduce a ‘Local Gaussian Process Approximation’ for regression that iteratively constructs a nearest neighbor conditioning set at test time; in contrast to our approach there is no training phase. Somewhat related to nearest neighbors, several authors have explored the computational advantages of compactly-supported kernels (Melkumyan and Ramos, 2009; Barber, 2020).

Cross-validation (CV) in the GP (or rather kriging) context was explored as early as 1983 by Dubrule (1983), with follow-up work including Emery (2009), Zhang and Wang (2010), and Le Gratiet and Cannamela (2015). Bachoc (2013) compares predictive performance of GPs fit with MLL and CV and concludes that CV is more robust to model mis-specification. The classic GP textbook (Rasmussen, 2003, Sec. 5.3) also briefly touches on CV in the
**Table 4**: We summarize the conceptual differences between seven of the methods for GP regression benchmarked in Sec. 5.6.

GP setting. Smith et al. (2016) consider CV losses in the context of differentially private GPs. Recent work explores how the CV score can be efficiently computed for GP regressors (Ginsbourger and Schäfer, 2021; Petit et al., 2020). Vehtari et al. (2016) investigate approximate leave-one-out approaches for gaussian latent variable models. Jankowiak et al. (2020b) introduce an inducing point approach for GP regression, PPGPR, that like our approach uses a loss function that is defined in terms of the predictive distribution. Indeed our approach can be seen as a non-parametric analog of PPGPR, and Eqn. 7 provides a novel conceptual framing for that approach. PPGPR and LOO-\(k\) are also related to Direct Loss Minimization, which emerges from a view of approximate inference as regularized loss minimization (Sheth and Khardon, 2020; Wei et al., 2021). Fong and Holmes (2020) explore the connection between MLL and CV in the context of model evaluation and consider a decomposition like that in Eqn. 7 specialized to the case of exchangeable data. They also advocate using a Bayesian cumulative leave-P-out CV score for fitting models, although the computational cost limits this approach to small datasets.

Various approaches to approximate GP inference are reviewed in Liu et al. (2020). An early application of inducing points is described in Snelson and Ghahramani (2006), which motivated various extensions to variational inference (Titsias, 2009; Hensman et al., 2013, 2015). Wenzel et al. (2019); Galy-Fajou et al. (2020) introduce an approximate inference scheme for binary and multi-class classification that exploits inducing points, Polya-Gamma auxiliary variables, and variational inference.

### A.3 Objective function summary

In Table 4 we provide a conceptual summary of how the different methods for scalable GP regression benchmarked in Sec. 5.6 are formulated. We note that Vecchia and MLL-\(k\) are quite similar, as both utilize nearest neighbor truncation to target the MLL. The Vecchia approximation does this using a fixed ordering in a decomposition of the MLL into a product of univariate conditionals, while MLL-\(k\) ignores the restrictions that are imposed by a specific ordering. Both approximations result in biased approximations of the MLL, and for both methods we utilize mini-batch training. In particular for Vecchia the objective function is of the form

\[
L_{\text{Vecchia}} = \frac{1}{N} \sum_{n=1}^{N} \log p(y_n | X_{n,k}^{\text{Vecchia}}, y_{n,k}^{\text{Vecchia}}, x_n)
\]

where \(X_{n,k}^{\text{Vecchia}}\) and \(y_{n,k}^{\text{Vecchia}}\) are the \(k\) nearest neighbors of \(x_n\) that respect a given ordering of the data. For example, for \(n' \geq n\) we necessarily have that \(y_{n'} \notin y_{n,k}\). Since the Vecchia approximation respects a fixed ordering of a data, it can be understood as a nearest neighbor approximation to a particular decomposition of the MLL. Conversely for MLL-\(k\) the objective function takes the form

\[
L_{k}^{\text{MLL}} = \frac{1}{N} \sum_{n=1}^{N} \log p(y_{n,k}^{\text{MLL}} | X_{n,k}^{\text{MLL}})
\]

where, for example, \(X_{n,k}^{\text{MLL}}\) consists of the \(k - 1\) nearest neighbors of \(x_n\) together with \(x_n\) itself.

### A.4 A pragmatic view of Bayesian methods

Gaussian processes are often seen from a Bayesian perspective. This is of course very natural since a Gaussian process makes for a powerful and flexible prior over functions. However, Gaussian processes can be utilized in a...
wide variety of applications, and we conceptualize these as occurring along a spectrum. At one end of the spectrum we can imagine a practitioner we might call the ‘Bayesian Statistician’. Typically, this statistician is particularly interested in obtaining high-fidelity posterior approximations. For example, we might imagine constructing a semi-mechanistic model of air pollution in a city that uses Gaussian processes to model concentrations of different pollutants. Here it might be of particular interest to compute a posterior probability that a pollutant concentration exceeds a given threshold in a particular area. On the other end of the spectrum there is a practitioner we might call the ‘Probabilistic Machine Learner’. This individual is typically interested in making high quality predictions with well-calibrated uncertainties. Accurate posterior marginals over various latent variables in the model may be of secondary interest, as the focus is on prediction. We primarily see LOO-k GPs as being of interest to this second group of practitioners. That is, while one could certainly use a LOO-k approximation within a typical Bayesian workflow, this choice may be inappropriate for a statistician whose primary concern is with high-fidelity posterior approximations. For the probabilistic ML practitioner, however, LOO-k GPs have a lot to offer as they represent a simple and robust method for making well-calibrated predictions on common regression and classification tasks. We expect LOO-k GPs to be particularly useful in the regime with \( N \sim 10^4 - 10^5 \) datapoints, a regime in which there may be too little data to train e.g. a neural network but too much data to train a GP using the exact MLL.

A.5 Computational complexity

We provide a brief discussion of the computational complexity of LOO-k as compared to other scalable GP methods. For simplicity we limit our discussion to the case of univariate regression. Let \( M \) be the number of inducing points, \( k \) be the number of nearest neighbors, and \( B \) be the size of the mini-batch. The computational complexity of SVGP and PPGPR are identical. In particular the time complexity of a training step is \( \mathcal{O}(BM^2 + M^3) \) and the space complexity is \( \mathcal{O}(M^2 + BM) \), while the time and space complexity at test time (for a single input) are both \( \mathcal{O}(M^2) \). The computational complexity of Vecchia, MLL-k, and LOO-k are identical. During training, we must compute the set of \( k \)-nearest neighbors for each training data point, which takes \( \mathcal{O}(N \log N) \) time (or \( \mathcal{O}(N^2) \) time with a brute-force approach). Once the nearest neighbors are computed, the time complexity of a training step is \( \mathcal{O}(Bk^3) \) and the space complexity is \( \mathcal{O}(Bk^2) \). During testing, the time and space complexity (for a single input) are \( \mathcal{O}(\log N + k^3) \) and \( \mathcal{O}(k^2) \), respectively. The \( \mathcal{O}(\log N) \) factor is the time to compute the test input’s nearest neighbors (\( \mathcal{O}(N) \) with a brute-force approach), and the \( \mathcal{O}(k^3) \) factor is the cost of computing the posterior mean and variance.

A.6 Pólya-Gamma density

The probability density function of the Pólya-Gamma distribution \( p(\omega|1, 0) \), which has support on the positive real line, is given by the alternating series (Polson et al., 2013):

\[
p(\omega|1, 0) = \sum_{n=0}^{\infty} (-1)^n \frac{2n + 1}{\sqrt{2\pi\omega^3}} \exp\left(-\frac{(2n+1)^2}{8\omega}\right)
\]

(16)

The mean of this distribution is given by \( \frac{1}{\pi} \) and the vast majority of the probability mass is located in the interval \( \omega \in (0, 2.5) \). To perform variational inference w.r.t. \( p(\omega|1, 0) \) we need to be able to compute this density. We leverage the implementation in Pyro (Bingham et al., 2019), which is formulated as follows. Estimating Eqn. [16] accurately requires computing increasingly many terms in the alternating sum as \( \omega \) increases. To address this issue we truncate the distribution to the interval \((0, 2.5)\). We then retain the leading 7 terms in Eqn. [16]. This is accurate to about 6 decimal places over the entire truncated domain. We find that this approximation is sufficient for our purposes. We note that as a consequence of the truncation our variational distribution is properly speaking a truncated log-Normal distribution, although given the large truncation point and given that most of the posterior mass concentrates in \( \omega \in (0, 0.5) \) the truncation of \( q(\omega) \) plays a negligible role numerically and can be safely ignored.
A.7 Binary classification

We expand on our method for binary GP classification discussed in Sec. 3.2. We consider a dataset \( \mathcal{D} = \{(x_n, y_n)\}_{n=1}^{N} \) with \( y_n \in \{-1, 1\} \) and a GP with joint density given by

\[
p(f|K_{N,N}) \prod_{n=1}^{N} p(y_n|f(x_n))
\]

(17)

where \( p(f|K_{N,N}) \) is the GP prior, and \( p(y_n|f(x_n)) = [1 + \exp(-y_n f(x_n))]^{-1} \) is a Bernoulli probability governed by a logistic link function. We introduce a \( N \)-dimensional vector of Pólya-Gamma auxiliary variables \( \omega \) and exploit the identity (Polson et al., 2013)

\[
e^\psi = \frac{1}{1 + e^{\psi}} = \frac{1}{2} e^\psi \mathbb{E}_{p(\psi|1,0)} \left[ e^{-\frac{1}{2} \psi^2} \right]
\]

(18)

and the shorthand \( f_n = f(x_n) \) to write

\[
\prod_{n=1}^{N} p(y_n|f_n) = \prod_{n=1}^{N} \frac{1}{1 + \exp(-y_n f_n)} = \prod_{n=1}^{N} \exp(y_n f_n) / (1 + \exp(y_n f_n)) = 2^{-N} \prod_{n=1}^{N} \exp(\frac{1}{2} y_n f_n - \frac{1}{2} \omega_n y_n^2 f_n^2)
\]

\[
= 2^{-N} \prod_{n=1}^{N} \exp(\frac{1}{2} y_n f_n - \frac{1}{2} \omega_n y_n^2 f_n^2) \propto \mathbb{E}_{p(\omega)} \left[ \prod_{n=1}^{N} \exp \left( \frac{1}{2} y^T f - \frac{1}{2} f^T \Omega f \right) \right]
\]

(19)

(20)

where \( \Omega = \text{diag}(\omega) \) is a diagonal \( N \times N \) matrix. Crucially, thanks to the Pólya-Gamma augmentation \( f \) is now conditionally gaussian when we condition on \( y \) and \( \omega \). We emphasize that this augmentation is exact. Next we integrate out \( f \). This is made easy if we recycle familiar formulae from the GP regression case. In particular write

\[
\frac{1}{2} y^T f - \frac{1}{2} f^T \Omega f = \frac{1}{2} \sum_{n} \omega_n \left( f_n - \frac{y_n}{2 \omega_n} \right)^2 + \sum_{n} \frac{1}{8 \omega_n}
\]

(22)

and observe that (apart from the last term which is independent of \( f \)) this takes the form of a Normal likelihood with ‘pseudo-observations’ \( \frac{y_n}{2 \omega_n} \) and data point dependent observation variances \( \omega_n^{-1} \). From this we can immediately write down the marginal log likelihood:

\[
\log p(y|X) = \log \mathbb{E}_{p(\omega)} p(y|X, \omega) \quad \text{with}
\]

\[
p(y|X, \omega) = \mathcal{N} \left( \frac{1}{2} \Omega^{-1} y, K_{N,N} + \Omega^{-1} \right) \times \exp \left( \frac{\Sigma_n}{8 \omega_n} \right)
\]

(23)

(24)

Next we introduce a variational distribution \( q(\omega) \) and apply Jensen’s inequality to obtain

\[
\log p(y|X) \geq \mathbb{E}_{q(\omega)} [\log p(y|X, \omega)] - \text{KL}(q(\omega)||p(\omega)) + \frac{1}{8} \mathbb{E}_{q(\omega)} \left[ \Sigma_n \omega_n^{-1} \right]
\]

(25)

where we choose \( q(\omega) \) to be a (truncated) mean-field log-Normal distribution (see the discussion in Sec. A.6). We note that if \( q(\omega) \) is parameterized with location and scale parameters \( m \) and \( s \) then \( \mathbb{E}_{q(\omega)}[\omega^{-1}] = \exp(-m + \frac{1}{2} s^2) \). This expectation is unbounded from above as \( s \to \infty \) or \( m \to -\infty \), corresponding to putting lots of posterior mass near \( \omega = 0 \). This is potentially an issue for our variational procedure, since it can potentially lead to undesired run-away solutions. One way to address this issue is to limit ourselves to variational distributions that are sufficiently well-behaved at \( \omega = 0 \). For example, we could truncate the log-Normal distribution at some finite \( \omega_{\text{min}} \). Here we take a simpler approach and omit the \( \mathbb{E}_{q(\omega)}[\omega^{-1}] \) term from our variational objective, noting that this term is always positive so that our modified variational objective is still guaranteed to be a lower bound to the log evidence. In practice we find that this approach works well. A different approach would lead to slightly different regularization of \( \omega \) but we do not expect this to be an important effect. Indeed what’s most important
We are given a dataset \( \Omega \) where \( K \) data points are represented as a one-against-all encoding where \( \omega \) goes into computing the predictive distribution. In practice we take a batch of test points of size \( B \). The computational cost of a training iteration is \( \mathcal{O}(Bk^3 + BQ) \), where \( B \) is the mini-batch size. Note that (excluding the cost of finding the nearest neighbors) the cost at test time for a batch of test points of size \( B \) is also \( \mathcal{O}(Bk^3 + BQ) \), since the main cost of computing the objective function goes into computing the predictive distribution. In practice we take \( Q = 16 \) so that the cost of Gauss-Hermite quadrature is negligible. Consequently the main determinants of computational cost are \( B \) and \( k \).

### A.8 Multi-class classification

We are given a dataset \( \mathcal{D} = \{ (\mathbf{x}_n, y_n) \} \), where each \( y_n \) encodes one of \( K \) discrete labels and we suppose that \( y_n \) is represented as a one-against-all encoding where \( y_n \in \{-1, 1\}^K \) and \( y_{n,k} = 1 \) for exactly one of \( k \in \{1, \ldots, K\} \). In the following we will effectively learn \( K \) one-against-all GP classifiers constructed as in Sec. A.7 with the difference that we will aggregate the \( K \) one-against-all classification probabilities and form a single multi-class likelihood.

In more detail we introduce a \( N \times K \) matrix of Pólya-Gamma auxiliary variables \( \omega_{n,k} \). As in Eqn. 13 for each data point \( n \) we can form \( K \) Bernoulli distributions

\[
\tilde{p}(y_{n,k} \mid y_{-n,k}, \mathbf{X}, \omega_{-n,k}) = \int df_{n,k} p(y_{n,k} \mid f_{n,k}) p(f_{n,k} \mid y_{-n,k}, \mathbf{X}, \omega_{-n,k})
\]

where each of the \( K \) univariate integrals can be numerically approximated with Gauss-Hermite quadrature. We use a tilde in Eqn. 32 to indicate that \( \tilde{p}(y_{n,k} \mid \cdot) \) is an intermediate quantity that serves as an ingredient in computing a joint predictive distribution. In particular we form a joint predictive distribution by jointly normalizing all of the Bernoulli probabilities:

\[
p(y_{n,k} = 1 \mid y_{-n}, \mathbf{X}, \omega_{-n}) = \frac{\tilde{p}(y_{n,k} = 1 \mid \cdot)}{\sum_{k'} \tilde{p}(y_{n,k'} = 1 \mid \cdot)}
\]
Given the matrix of Pólya-Gamma variates $\omega_{n,k}$, $p(y_{n,k} = 1 | \cdot)$ in Eqn. 33 is a normalized distribution over the label $k \in \{1, ..., K\}$ that can be computed in closed form thanks to Gauss-Hermite quadrature. To train the kernel hyperparameters and Pólya-Gamma mean-field variational distribution we use an objective function that is a direct generalization of Eqn. 12:

$$L_{\text{multi LOO}} \equiv \frac{1}{N} \sum_{n=1}^{N} \mathbb{E}_{q(\omega)} \left[ \log p(y_{n,k} | y_{-n}, x_{-n}, \omega_{-n}) \right] - \text{KL}(q(\omega) || p(\omega))$$

(34)

The final objective function is obtained by applying a $k$-nearest-neighbors truncation to Eqn. 34. During test time we sample $\omega \sim q(\omega)$ and use Eqn. 33.

A.9 Other likelihoods

The auxiliary variable construction in Sec. 3.2-3.3 can be extended to a number of other likelihoods. For example, Pólya-Gamma auxiliary variables can also be used to accomodate binomial and negative binomial likelihoods (Polson et al., 2013). Additionally, gamma auxiliary variables can be used to accomodate a Student’s t likelihood, which is useful for modeling heavy-tailed noise.

A.10 Experimental details

All the datasets we use, apart from those used in the multivariate regression experiments, can be obtained from the UCI depository (Dua and Graff, 2017). The Fw.-Kuka, Fw.-Baxter, and Rythmic-Baxter multivariate regression datasets are available from https://bitbucket.org/athapoly/datasets/src/master/, and the Sarcos dataset is available from http://www.gaussianprocess.org/gpml/data/.

A.10.1 General training details

For all experiments the GP model we fit uses a Matérn 5/2 kernel with individual length scales for each input dimension. For all regression experiments the prior GP mean is a learnable constant; otherwise it is fixed to zero. For all experiments we use the Adam optimizer (Kingma and Ba, 2014). When training a GP with MLL we set Adam’s momentum hyperparameter $\beta_1$ to $\beta_1 = 0.5$; otherwise we set $\beta_1 = 0.90$. We use a stepwise learning rate schedule in which the learning rate starts high (0.03) and is reduced by a factor of 5 after 25%, 50%, and 75% of optimization. Our default batch size is $B = 128$, although we use $B = 64$ when the computational demands are higher (e.g. for multi-class classification). We use FAISS for nearest neighbor queries (Johnson et al., 2019). During training we update nearest neighbor indices every 50 gradient steps, although we note that a smaller update frequency also works well.

To run our experiments we used a small number of GPUs, including a GeForce RTX 2080 GPU, a Quadro RTX 5000, and a GeForce GTX 1080 Ti. We estimate that we used ~200 GPU hours running pilot and final experiments.

A.10.2 Details for particular experiments

Model mis-specification The GP prior we use to generate synthetic data has length scale $\rho = \frac{1}{2}$. Note we generate a single data set and then apply different warpings to it; i.e. results for different $\gamma$ differ only in the warping applied to the inputs.

Objective function comparison Inducing point locations are set using k-means clustering. We retrain SVGP variational parameters for each hyperparameter setting, while keeping the $M = 100$ inducing point locations fixed.

Dependence on number of nearest neighbors $k$ Fig. 3 uses the results reported in Sec. 5.6 with the difference that additional runs with smaller/larger $k$ are included.

Runtime performance To define a regression task we use the Slice UCI dataset and downsample the input dimension to $D = 25$. To accommodate large $N$ we also enlarge the dataset by repeating individual data points and adding noise (both to inputs and targets). We use a mini-batch size of $B = 128$ and run on a GeForce RTX 2080 GPU. As in our other experiments, we update the nearest neighbor index every 50 gradient steps.
Degenerate data regime. For each (univariate regression) dataset we duplicate each data point in the training set and add zero mean gaussian noise (with variance given by $10^{-4}$) to each input $x_n$ and each response $y_n$. Other details are as in the next section.

Univariate regression. Since we reproduce some of the baseline results from (Jankowiak et al., 2020b), we follow the experimental procedure detailed there. In particular regression datasets are centered and normalized so that the trivial zero prediction has a mean squared error of unity. All the experiments in Sec. 5.6-5.9 use training/test/validation splits with proportions 15:3:2. For LOO-k we vary $k \in \{32, 64, 128, 256\}$ and use the validation set LL to choose the best $k$. SVGP uses $M = 1000$ inducing points with $\beta_{\text{reg}} \in \{0.1, 0.3, 0.5, 1.0\}$ where $\beta_{\text{reg}}$ is a scaling term in front of the KL divergence. PPGPR (specifically the MFD variant, see (Jankowiak et al., 2020b)) uses $M = 1000$ inducing points with $\beta_{\text{reg}} \in \{0.01, 0.05, 0.2, 1.0\}$. Both SVGP and PPGPR results are reproduced from (Jankowiak et al., 2020b). In both cases inducing point locations are initialized with $k$-means.

For Vecchia and MLL-k we also vary $k \in \{32, 64, 128, 256\}$. For the Vecchia baseline, the data are ordered according to the first PCA vector. For SWSGP, we use $M = 10000$ inducing points (a order of magnitude more than SVGP) since this method scales linearly with $M$. Following Tran et al. (2021), we parameterize the variational distribution $q(u_1, \ldots, u_M)$ to be independent Gaussians. We vary $k \in \{32, 64, 128, 256\}$, and we jointly optimize the variational parameters and hyperparameters for 6400 iterations. For ALC we use the software described in (Gramacy, 2016). Since prediction is slow, both because the implementation is CPU only and because the iterative procedure is inherently expensive, we use a fixed number of $k = 64$ nearest neighbors. For ALC we use an isotropic kernel on Kegg-undirected because we were unable to obtain reasonable results with a kernel with per-dimension length scales on this particular dataset.

Multivariate regression. Since we reproduce some of the baseline results from (Jankowiak et al., 2020a), we follow the experimental procedure detailed there. In particular regression datasets are centered and normalized so that the trivial zero prediction has a mean RMSE of unity (i.e. the RMSE averaged across all output dimensions). For LOO-k we vary $k \in \{16, 32\}$ and use the validation set LL to choose the best $k$. For MLL-k we vary $k \in \{16, 32\}$. SVGP and PPGPR both use $M = 300$ inducing points with $\beta_{\text{reg}} \in \{0.1, 0.3, 0.5, 1.0\}$.

Binary classification. For LOO-k we vary $k \in \{32, 64, 128, 256\}$ and use the validation set LL to choose the best $k$. For the SVGP and the Polya-Gamma PGVI baseline we use $M = 1024$ inducing points and vary $\beta_{\text{reg}} \in \{0.1, 0.3, 0.5, 1.0\}$. We subsample the SUSY and Higgs datasets down to $N = 2 \times 10^5$ data points for simplicity. The Covtype dataset is inherently a multi-class dataset with $K = 7$ datasets. We convert it into two binary classification datasets by combining the two Pine and Fir classes, respectively, in a two-against-five fashion to obtain two derived datasets, Covtype-Pine and Covtype-Fir, respectively. We use $Q = 16$ Gauss-Hermite quadrature points.

Multi-class classification. For LOO-k we vary $k \in \{32, 64, 128, 256\}$ and use the validation set LL to choose the best $k$. For SVGP we use $M = 512$ inducing points and vary $\beta_{\text{reg}} \in \{0.1, 0.3, 0.5, 1.0\}$. We use $Q = 16$ Gauss-Hermite quadrature points.

A.11 Additional figures

In Fig. 8 we replicate the experiment described in Sec. 5.1 for two additional warping functions. In Fig. 9 we depict the results for the multi-class classification experiment in Sec. 5.9.

A.12 Results tables

Tables 7, 8, and 9 report results for the principal regression and classification experiments from Section 5. See Table 6 for complete results for the experiment in Sec. 5.5.
Figure 8: These two figures are companions to Fig. 1 in the main text. We compare predictive performance of a GP trained with a LOO-\(k\) objective to a GP trained via MLL, where the GP regressor is mis-specified due to non-stationarity in the dataset introduced by a warping function controlled by \(\gamma\). **Top:** The coordinatewise warping function is the identity for \(x_i \leq 0\) and \(x_i \rightarrow x_i^{1+\gamma}\) otherwise. **Bottom:** The coordinatewise warping function is \(x_i \rightarrow x_i + \gamma x_i^3\). In both cases as \(\gamma\) increases and the dataset becomes more non-stationary, the LOO-\(k\) GP exhibits superior predictive performance, both w.r.t. log likelihood (LL) and root mean squared error (RMSE).

Figure 9: We depict predictive negative log likelihoods (NLL, top) and predictive error (bottom) for 13 multi-class classification datasets using LOO-\(k\) and SVGP. Results are averaged over 5 dataset splits. Lower numbers are better.

Table 5: We summarize the performance ranking of LOO-\(k\) and SVGP on the multi-class classification datasets in Figure 9, averaged over all splits.
Table 6: We summarize the results for the experiment in Sec. 5.5 exploring the performance of LOO-64 and SVGP-512 on degenerate datasets. We report both test log likelihood and RMSE on held out test data.

| Dataset   | Method   | Original Log Likelihood | Degenerate Log Likelihood |
|-----------|----------|-------------------------|---------------------------|
| Bike      | SVGP-512 | 0.859                   | 0.553                     |
| Bike      | LOO-64   | 2.498                   | −0.912                    |
| Elevators | SVGP-512 | −1.111                  | −1.107                    |
| Elevators | LOO-64   | −0.414                  | −3.783                    |
| Pol       | SVGP-512 | −1.040                  | −1.054                    |
| Pol       | LOO-64   | 1.162                   | 0.689                     |
| Slice     | SVGP-512 | 0.611                   | 0.726                     |
| Slice     | LOO-64   | 2.723                   | 2.787                     |

Table 7: A compilation of all univariate regression results from Section 5.6. Numbers are averages ± standard errors over dataset splits.

| Metric | Dataset | SVGP | PPGPR | MLL-k | LOO-k |
|--------|---------|------|-------|-------|-------|
| CRPS   | Pol     | 0.051 | 0.061 | 0.119 | 0.116 |
| Bike   | 0.019   | 0.049 | 0.037 | 0.018 | 0.026 |
| Bin60K | 0.093   | 0.082 | 0.077 | 0.063 | 0.066 |
| Protein| 0.293   | 0.326 | 0.310 | 0.333 | 0.285 |
| Keggdir| 0.046   | 0.037 | 0.031 | 0.038 | 0.038 |
| Slice  | 0.029   | 0.031 | 0.032 | 0.019 | 0.012 |
| Keggdir| 0.056   | 0.051 | 0.050 | 0.051 | 0.050 |

Table 8: A compilation of all multivariate regression results from Section 5.7. Numbers are averages ± standard errors over dataset splits.

| Metric | Dataset | MLL-k | LOO-k |
|--------|---------|-------|-------|
| RMSE   | Rt.-Baxter | 0.583 | 0.106 |
|        | Fw.-Baxter | 0.043 | 0.035 |
|        | Fw.-Kuka   | 0.089 | 0.115 |
|        | Sarcos     | 0.105 | 0.076 |

standard
Table 9: A compilation of all binary (left) and multi-class (right) classification results from Sections 5.8 and 5.9. Numbers are averages ± standard errors over dataset splits.