Regularized Sparse Gaussian Processes

Rui Meng and Herbert Lee
University of California
Santa Cruz, CA, US, 95060

Soper Braden and Priyadip Ray
Lawrence Livermore National Laboratory
Livermore, CA, US, 94550

Abstract

Gaussian processes are a flexible Bayesian nonparametric modelling approach that has been widely applied to learning tasks such as facial expression recognition, image reconstruction, and human pose estimation. To address the issues of poor scaling from exact inference methods, approximation methods based on sparse Gaussian processes (SGP) and variational inference (VI) are necessary for the inference on large datasets. However, one of the problems involved in SGP, especially in latent variable models, is that the distribution of the inducing inputs may fail to capture the distribution of training inputs, which may lead to inefficient inference and poor model prediction. Hence, we propose a regularization approach for sparse Gaussian processes. We also extend this regularization approach into latent sparse Gaussian processes in a unified view, considering the balance of the distribution of inducing inputs and embedding inputs. Furthermore, we justify that performing VI on a sparse latent Gaussian process with this regularization term is equivalent to performing VI on a related empirical Bayes model with a prior on the inducing inputs. Also stochastic variational inference is available for our regularization approach. Finally, the feasibility of our proposed regularization method is demonstrated on three real-world datasets.

Introduction

A Gaussian process (GP) is a generalization of a multivariate Gaussian distribution that can be seen as a stochastic random process in the space of general continuous functions. Due to its flexibility, it is widely applied in various fields such as geostatistics (Haining 1993), multistask-learning (Banerjee et al. 2008) and reinforcement learning (Rasmussen and Kuss 2004). A standard textbook for Gaussian process regression and classification is (Rasmussen and Williams 2005).

Although the GP is flexible, exact inference is expensive with time complexity $O(n^3)$, where $n$ is the number of data points. This renders GP inference infeasible for large real-world datasets. Approximations based on inducing points, named sparse Gaussian process (SGP) methods, have been proposed to avoid the computational issue. The predictive process (PP/DTC) is proposed by Seeger (Seeger 2003) to approximate a GP by introducing inducing variables. It reduces the time complexity from $O(n^3)$ to $O(nm^2)$ where $m$ is the number of inducing variables. Snelson and Ghahramani (2006) proposes a fully independent training conditional (FITC) approximation as one of most efficient approximation methods. Its corresponding Bayesian approach is proposed as the modified predictive process (MPP), which corrects the bias brought from the PP in Finley et al. (2009). Moreover, Snelson and Ghahramani (2007) proposes a partially independent training conditional (PITC) approximation and Csato and Opper (2002) proposes an expectation propagation pseudo-point approximation. In most approximation approaches, the locations of inducing points are optimized via a gradient-based optimization. From a Bayesian perspective, Guhaniyogi et al. (2011) discusses inducing input selection using MCMC sampling. On the other hand, Titsias (2009) applies variational inference to SGP, marginalizing the optimal variational distribution of inducing variables. Hensman, Rattray, and Lawrence (2012); Hensman, Fusi, and Lawrence (2013) directly optimize the variational distribution of the inducing variables and embedding inputs to gain computational benefits.

The Gaussian process latent variable model (GPLVM) (Lawrence 2004) is proposed by Lawrence as a probabilistic dimensionality reduction method. This method extends the linear mappings from the embedding space in dual probabilistic principal component analysis (DPPCA) to nonlinear mappings (Lawrence 2004, 2005). Lawrence (2005) also discusses its relationship with other dimensionality reduction methods such as Multidimensional Scaling (Mardia, Kent, and Bibby 1979) and Kernel PCA (Bernhard, Alexander, and Klaus-Robert 1998). Due to the poor scaling properties, Titsias and Lawrence (2010) proposes Bayesian GPLVM using variational inference on a SGP in Titsias (2009). And Hensman, Fusi, and Lawrence (2013) proposes stochastic variational inference on a latent SGP. Many variants of GPLVM are studied in Lawrence and Moore (2007); Lawrence and Quinonero Candela (2006); Urtasun and Darrell (2007).

The main contribution of this work is to propose a regularization approach for the latent SGP of Hensman, Fusi, and Lawrence (2013), balancing the distribution of inducing inputs and embedding inputs, and leading to better model pre-
Regularization for Sparse Gaussian Processes

In this section, we show the importance of regularization for inducing inputs in a SGP. From a variational inference perspective, there are two efficient approaches named sparse Gaussian process regression (SGPR) (Titsias 2009) and stochastic variational Gaussian process (SVGP) (Hensman, Fusi, and Lawrence 2013). SGPR marginalizes the optimal variational distribution of inducing variables while SVGP directly models and optimizes the variational distribution of inducing variables. Assuming we have $N$ observations and $M$ inducing points, the lower bound of computational complexity in SGPR is $O(M^2N)$ while that in SVGP is $O(M^3)$. Titsias (2009) optimizes inducing inputs by selecting them from training set. Hensman, Fusi, and Lawrence (2013) optimizes inducing inputs by maximizing the corresponding variational bound with initialized inducing inputs via K-means method. Moreover, Guhaniyogi et al. (2011) shows that the distribution of inducing inputs should capture the distribution of the covariate inputs for better model prediction. We illustrate that the better model prediction should balance that maximizing the variational bound and increasing the similarity of distributions between inducing inputs and covariate inputs. We illustrate this on 1-D synthetic data, where we uniformly generate 100 inputs $x$ on the unit interval $[0, 1]$. Then the corresponding observations are generated from

$$y \mid f \sim \mathcal{N}(y \mid f, 0.1)$$

$$f = \sin(2\pi x) + 0.2 \cos(22\pi x).$$

We take 100 evenly spaced inputs on $[0, 1]$ and generate corresponding outputs without noise as their ground-truth for testing. We use a linear combination of a Matern kernel and a linear kernel as the covariance function and take three different models with respect to 10 inducing points. The first model $M_1$ initializes inducing inputs using K-means and optimizes them through maximizing the variational bound in SVGP. The second model $M_2$ fixes the inducing points as evenly spaced inputs on $[0, 1]$ in optimization and the last model $M_3$ maximizes the variational bound while maintaining the similarity of distributions between inducing inputs and training inputs. A unified view of the three approaches is to maximize the sum of a lower bound of $\log p(y \mid x)$ and a regularization term.

$$L_2 \triangleq L_1 + \lambda D(x, z)$$

where $L_1 = \left( \langle \log p(y \mid f) \rangle_{p(f \mid u)} + \log p(u) - \log q(u) \rangle_{q(u)} \right)$ is a variational bound of log likelihood, $\lambda$ is regularization weight and $D$ is a measurement for the distributions of training inputs $x$ and inducing inputs $z$. $M_1$ fixes $\lambda = 0$, $M_2$ fixes $z$ and $M_3$ is the generalized version of $M_1$ and $M_2$, which considers the balance of $L_1$ and $D$. Specifically, in the toy example, we set $\lambda = 1$ and $D(x, z) = \min \sum_{n=1}^{N} (\lvert x_n - z_{n(s)} \rvert)$ where $s$ is an index mapping from $1, \ldots, N$ to $1, \ldots, M$. The smaller the $D(x, z)$ is, the more similar the distributions between $x$ and $z$ are.

All predictive posterior processes are shown in Figure[1] and the predictive likelihood and predictive root mean square error are summarized in Table[1] illustrating that the model has best predictive performance when the distribution of the inducing inputs balance maximizing the variational bound and capturing the distribution of actual inputs.

Figure 1: Stochastic variational Gaussian process on 1D synthetic data with different schedules for inducing inputs.

| $M_1$          | $M_2$          | $M_3$          |
|----------------|----------------|----------------|
| $\ell$         | 1.2987         | 1.5792         | 1.7508         |
| RMSE           | 0.0687         | 0.0504         | 0.0420         |

Table 1: Predictive log likelihood ($\ell$) and predictive root mean square error (RMSE) on 1-D synthetic data with different schedules with respect to inducing points.

Regularization for Latent Sparse Gaussian Processes

The Gaussian process latent variable model (GPLVM) is a powerful dimensionality reduction approach (Lawrence 2004; Ek, Torr, and Lawrence 2007) and it is a base model for many sophisticated models (Lawrence and Moore 2007; Urtasun and Darrell 2007; Damianou, Titsias, and Lawrence 2016). However, Two main drawbacks exist. One is the poor scaling property. The sparse Gaussian process is introduced in Titsias and Lawrence (2010), Hensman, Fusi, and Lawrence (2013). The other is that model fitting is sensitive to initialization for both inducing inputs and embedding inputs. Principal component analysis (PCA) initialization for embedding inputs and K-means initialization for inducing inputs are standard procedures. Lawrence and Quinonero Candela (2006) proposes a back-constraint approach to maintain similar manifold between embedding inputs and observations.
We next propose a regularized sparse Gaussian process in latent Gaussian process to balance maximizing the marginal likelihood lower bound and maintaining the similarity between the inducing inputs and embedding inputs.

A Unified View of Sparse Latent Gaussian Processes

Suppose $Y \in \mathbb{R}^{N \times D}$ is the observed data with latent variables $F \in \mathbb{R}^{N \times D}$, where $N$ is the number of observations and $D$ the dimension of the observations. Let the observations have corresponding latent variables $X \in \mathbb{R}^{N \times Q}$ where $Q$ is the dimension of the latent space. Assuming independence across features, the GPLVM is

$$
Y \mid F \sim \mathcal{N}(F, \sigma^2 = \beta^{-1})
$$

$$
f \mid X \sim \mathcal{F}_d(x_n) \quad \mathcal{F}_d \overset{iid}{\sim} \mathcal{GP}(0, C(\theta))
$$

with a normal prior for the latent variables $X$, $p(X) = \prod_{n=1}^N \mathcal{N}(x_n | \mu_n, \Sigma_n)$ where $x_n$ is the $n$th row of $X$. Usually we take $\mu_n = 0$ and $\Sigma_n = I_q$. Titsias and Lawrence (2010) use a variational sparse GP formulation by introducing $D$ separate sets of $M$ inducing variables $U \in \mathbb{R}^{M \times D}$ evaluated at a set of inducing inputs $Z \in \mathbb{R}^{M \times Q}$.

Then Titsias and Lawrence (2010); Hensman, Fusi, and Lawrence (2013) propose the same variational structure

$$
q(U, X) = \prod_{d=1}^D (p(f_d | u_d, X)q(u_d)) q(X),
$$

where $f_d$ is the $d$th column of $F$ and $u_d$ is the $d$th column of $U$. Specifically, $X$ has variational distribution $q(X) = \prod_{n=1}^N \mathcal{N}(x_n | \mu_n, \Sigma_n)$. Then the evidence lower bound (ELBO) is

$$
\text{ELBO} = \sum_{d=1}^D E_{q(F \mid U, X)} \log p(y_d | f_d) - \text{KL}(q(U) || p(U)) - \text{KL}(q(X) || p(X)).
$$

Titsias and Lawrence (2010) derives the variational bound by marginalizing the optimal $q(U)$ based on the SGPR in Titsias (2009). After the marginalization, the ELBO is derived as

$$
\text{ELBO}_1 = \sum_{d=1}^D E_{q(X)} \left( \log \mathcal{N}(y_d | 0, \Sigma_{NM} \Sigma_{MN}^{-1} \Sigma_{NMM}^{-1} \Sigma_{MM} + \beta^{-1} I) - \beta \frac{1}{2} \text{tr}(\Sigma) \right) - \text{KL}(q(X) || p(X))
$$

where $Q = K_{NN} - K_{NM} \Sigma_{M}^{-1} K_{NN}$. On the other hand, directly employing variational distributions $q(u) = \prod_{d=1}^D \mathcal{N}(u_d | m_d, S_d)$, we extend the univariate latent Gaussian process in Hensman, Fusi, and Lawrence (2013) to multivariate latent Gaussian processes. We call the variational lower bound as ELBO2 with the expectation term derived as:

$$
\begin{align*}
E_{q(F \mid U, X)} \log p(y_d | f_d) &= E_{q(X)} \left( \log \mathcal{N}(y_d | 0, \Sigma_{NM} \Sigma_{MN}^{-1} \Sigma_{MM} + \beta^{-1} I) \\
&- \beta \frac{1}{2} \text{tr}(\Sigma) \right) \frac{1}{2} \text{tr}(S_d A) 
\end{align*}
$$

where $A = \Sigma_{MM}^{-1} \Sigma_{MN}^{-1} \Sigma_{MM}$. With sufficient statistics $\Psi_0 = \text{tr}(K_{NN} q(U))$, $\Psi_1 = \langle K_{NM} \theta \rangle$ and $\Psi_2 = \langle K_{MM} \theta \rangle$, the expectation term becomes tractable and model fitting and prediction are easy to derive as the same in [Titsias and Lawrence (2010)].

Comparing ELBO1 with ELBO2, ELBO2 is scalable for large datasets via introducing the parametric distribution $q(U)$, while it is more difficult to optimize because that more parameters required to optimize without marginalization.

For some larger and complicated datasets, variational inference may fail to capture the distribution of the embedding inputs. We will illustrate the benefits of regularization with different latent dimension settings and different ELBOs using the two real datasets in the experiments section. To address this concern, we next propose an innovative regularization approach.

Regularization

In order to ensure the inducing inputs capture the distribution of the embedding inputs, it is necessary to propose a way to quantify the difference between the distribution of the inducing inputs and the distribution of the embedding inputs, and penalize this difference in the objective function. We define the modified evidence lower bound as

$$
\text{MELBO} = \text{ELBO} - \lambda R
$$

where $\lambda$ is a regularization weight and $R$ is a regularization term which measures the difference between the distribution of the embedding inputs $X$ and the distribution of the inducing inputs $Z$. As $\lambda$ increases, the optimization emphasizes more similarity in the distributions.

Specifically, we build a global model for the variational mean of $X$ such that every $\mu_n$ has an independent identical Gaussian distribution $p_\mu(\mu_n) = \mathcal{N}(\mu_n | \mu, \Sigma_{\mu})$, and build another global model for the inducing points $Z$ such that every $z_m$ has an independent identical distribution $p_Z(z_m) = \mathcal{N}(z_m | \mu, \Sigma_{Z})$. Then given $\mu$ and $Z$, we derive the maximum likelihood estimates $\hat{\mu}, \hat{\Sigma}_{\mu}, \hat{\mu}_Z$ and $\hat{\Sigma}_Z$ using the mean and covariance matrix of $\{\mu_n\}$ and $\{z_m\}$. We derive $q_X = \mathcal{N}(\mu, \Sigma)$ to summarize the global distribution of the embedding inputs and derive $q_Z = \mathcal{N}(\hat{\mu}_Z, \hat{\Sigma}_Z)$ to summarize the global distribution of the inducing inputs $Z$.

We define the regularization term $R$ by the Kullback-Leibler divergence between $q_X$ and $q_Z$:

$$
R = \text{KL}(q_Z || q_X).
$$

In (7), $\lambda$ can be chosen by cross validation or be set as the number of inducing points as a rule of thumb. As $\lambda = M$, we justify that performing VI on the sparse GPLVM with regularization is equivalent to performing VI on a related empirical Bayesian model with a prior on inducing inputs in the next section.

If we choose $\text{ELBO} = \text{ELBO}_2$, stochastic variational inference is available to employ. Specifically, the modified
lower bound can be written as

\[
\text{MELBO} = \sum_{n=1}^{N} \left[ \sum_{d=1}^{D} E_{q(x_n)} \log N(y_{nd}|k_{nm}K^{-1}_{MM}m_d, \beta^{-1}) 
- E_{q(x_n)} \frac{\beta}{2} Q_{nn} - E_{q(x_n)} \frac{\beta}{2} \text{tr}(S_d \Lambda_m) - \frac{\lambda}{N} \KL(q_Z||q_Y) \right]
\]

where \(\Lambda_m = K^{-1}_{MM}k_{nm}K^{-1}_{MM}\).

**Regularization Theory**

This section discusses the underlying relationship between regularization in a sparse GPLVM and an empirical Bayesian model. First, we display a related empirical Bayesian model with a prior on its inducing inputs \(Z\) and derive its variational lower bound. Then we illustrate that maximizing the MELBO is equivalent to maximizing a variational lower bound in the empirical Bayesian model.

The related empirical Bayesian model is extended from (1) and (2). We put an informative prior on the inducing inputs and propose a variational distribution on them as

\[
z_m \sim N(z_m|\tilde{\mu}_m, \tilde{\Sigma}_m)
q(z_m) = N(z_m|\nu_m, \Upsilon_m)
\]

where \(\tilde{\mu}_m, \tilde{\Sigma}_m\) are mean and covariance matrix of \(\{\mu_n\}\).

The empirical Bayesian model is displayed using a probability graph in Figure 2. The prior of inducing points borrow the information from the variational mean of embedding inputs \(\mu\).

The variational joint distribution is defined as 

\[
q(F, U, X, Z) = q(Z)q(X|q(U)p(F|Z,X,U). \text{ Then variational lower bound is derived as }
\]

\[
\log p(Y) \geq E_{q(F, U, X, Z)} \log p(Y|F) - KL(q(Z)||p(Z)) - KL(q(X)||p(X)) - KL(q(U)||p(U))
\]

\[
\triangleq \text{ELBO}_E
\]

(10)

We define \(\tilde{\nu}_m\) and \(\tilde{\Sigma}_m\) as the mean and covariance matrix of \(\{\nu_m\}\) and define a distribution family for \(q(Z)\) such that \(\Upsilon_m = \epsilon I\) for \(m = 1, \ldots, M\). We justify that under the assumption that the covariance of \(\{\nu_m\}\) is finite, implying \(\tilde{\Sigma}_m < K\), we have following three lemmas and one theorem. The proof of Lemma 3 is provided in the supplementary materials.

**Lemma 1** Assume \(q(z_m) = N(z_m|\nu_m, \Upsilon_m), \text{ as } \epsilon \to 0, z_m \overset{p}{\to} \nu_m\

**Proof 1** Since \(\forall \epsilon_0 > 0, \)

\[
\lim_{\epsilon \to 0} p(|z_m - \nu_m| > \epsilon_0) = \lim_{\epsilon \to 0} p\left(\frac{|z_m - \nu_m|}{\epsilon} > \frac{\epsilon_0}{\epsilon}\right)
= 2 \lim_{\epsilon \to 0} (1 - \Phi\left(\frac{\epsilon_0}{\epsilon}\right))^{\epsilon_0}\]

\[
= 0,
\]

we conclude that \(z_m \overset{p}{\to} \nu_m\).

**Lemma 2** In the variational lower bound (10), \(\text{KL}(q(Z)||p(Z)) \leq A - B - C\)

(11)

where

\[
A = \frac{M}{2} \left( \log|\tilde{\mu}\rangle + \log|\tilde{\Sigma}\rangle + \mathcal{O} \right)
+ \frac{1}{2} \left( \sum_{m=1}^{M} (\nu_m - \tilde{\mu})^T \tilde{\Sigma}_m^{-1} (\nu_m - \tilde{\mu}) \right).
B = \frac{M}{2} (Q \log \epsilon - \log K),
C = \frac{2\epsilon}{\text{Mitr}(\tilde{\Sigma}_m^{-1})}.
\]

**Proof 2**

\[
\text{KL}(q(Z)||p(Z)) = A - \frac{M}{2} (Q \log \epsilon - \log |\tilde{\Sigma}\rangle - C \leq A - B - C
\]

because of the finite variance assumption that \(\tilde{\Sigma}_m < K\).

**Lemma 3**

\[
\text{MKL}(q(Z)||q_X) = \frac{M}{2} (\log|\tilde{\mu}\rangle + \log|\tilde{\Sigma}\rangle + \mathcal{O})
+ \frac{1}{2} \left( \sum_{m=1}^{M} (z_m - \tilde{\mu}_m)^T \tilde{\Sigma}_m^{-1} (z_m - \tilde{\mu}_m) \right).
\]

**Proof 3 In the appendix**

**Theorem 1** Given Lemma 1, Lemma 2 and Lemma 3, as \(\epsilon \to 0, \text{ maximizing the variational lower bound in empirical Bayesian model is equivalent to maximizing the MELBO in the sparse GPLVM with respect to } Z, q(X) \text{ and } q(U).\)

**Proof 4** In the empirical Bayesian model, denote all parameters as \(\Theta = \{\mu, \Sigma, m, s, \nu, h\}, \text{ } h \text{ denote all hyper-parameters in GP kernels.}\)

Because of Lemma 1,

\[
\lim_{\epsilon \to 0} E_{q(F, U, X, Z)} \log p(Y|F) = E_{q(F, U, X)} \log p(Y|F, Z = \nu).
\]

Moreover, \(\lim_{\epsilon \to 0} C = \frac{2}{\text{Mitr}(\tilde{\Sigma}_m^{-1})}, \lim_{\epsilon \to 0} \epsilon = 0\). Then because of Lemma 2, we have a loose lower bound as \(\text{ELBO}_E \geq \text{ELBO}_E + \text{MKL}(q(Z)||q_X) - A + B + C \overset{\epsilon \to 0}{=} \text{ELBO}_E\). Instead of directly maximizing \(\text{ELBO}_E\), we maximizing the loose lower bound that

\[
\hat{\Theta} = \arg \max_{\Theta} \text{ELBO}_E
\]

\[
= \arg \max_{\Theta} \text{ELBO}_E
= \arg \max_{\Theta} E_{q(F, U, X)} \log p(Y|F) - KL(q(X)||p(X)) - KL(q(U)||p(U)) - A + B + C
\]

Due to Lemma 3, this optimization is equivalent to maximize \(\text{ELBO} - \text{MKL}(q_Z||q_X)\) which is the exactly MELBO. Finally, due to Lemma 1, the \(q(Z)\) in empirical Bayesian model will converges to the same optimized \(Z\) in the regularized sparse GPLVM.
Experiments

We illustrate our regularization on three datasets. First, we show that regularization is necessary in sparse latent Gaussian process for a moderate dataset. Taking the Anuran Calls dataset for instance, we explore the regularization for two different lower bounds and also explore the regularization approach for different latent dimension sizes. Second, we illustrate the regularization approach for a large dataset with different number of inducing points, using the Flight dataset. Finally, we take Driver Face dataset as an example for an application for high dimensional datasets. All optimizations employ the Limited-memory BFGS approach with maximum iteration number 1000.

Anuran Calls Example

We show that regularization improves inference on the Anuran Call dataset. This dataset is available from the UCI repository at [https://archive.ics.uci.edu/ml/datasets/Anuran+Calls+(MFCCs)](https://archive.ics.uci.edu/ml/datasets/Anuran+Calls+(MFCCs)) where there are 7195 instances, and each instance has 22 attributes. We model all instances using a sparse latent Gaussian process and perform inference with and without regularization.

Specifically, we set the latent dimension size $Q = 5$ and use $M = 20$ inducing points in the multivariate latent Gaussian process model. We choose independent standard Gaussian distributions as the prior distributions of the inducing points. We employ the PCA approach for initialization of the embedding inputs and employ the K-means algorithm for initialization of the inducing inputs.

Regularization with ELBO$_1$ This section considers the optimal variational distribution of inducing variables, exploring three schedules with respect to the inducing inputs. The first schedule is to fix the inducing inputs as the initial K-means’ centroids. The second schedule is to treat the inducing inputs as trainable parameters in optimization. And the last schedule is to consider our proposed regularization approach, where $\lambda$ is searched in $[1, 10, 100, 1000]$. After model training, we estimate embedding inputs as their variational mean $\hat{X} = \hat{\mu}$ and reconstruct all observations given the estimated embedding inputs. Then we compare the root mean square errors (RMSE) for the fitting results.

We also compare the similarity of distributions between embedding inputs $X$ and inducing inputs $Z$ by introducing averaged symmetric KL divergence criteria (ASKL). It is defined as

$$\text{ASKL} = \frac{1}{Q} \sum_{q=1}^{Q} \left( 0.5 \text{KL}(\hat{p}(X_q) | \hat{p}(Z_q)) + 0.5 \text{KL}(\hat{p}(Z_q) | \hat{p}(X_q)) \right),$$

where $\hat{p}(X)$ is a Gaussian distribution fitted by $X$. Both RMSE and ASKL are summarized in Table 2. It demonstrates that our regularization approach is significantly better on both model fitting and latent input deployment.

| Schedule 1 | Schedule 2 | Schedule 3 |
|------------|------------|------------|
| RMSE       | 0.0575     | 0.0438     | 0.0434     |
| ASKL       | 2.5330     | 0.4213     | 0.0111     |

Table 2: Root mean square errors (RMSE) and averaged symmetric KL divergence (ASKL) for three different schedules with respect to inducing inputs under ELBO$_1$ setting. (Anuran Calls Example)

Regularization with ELBO$_2$ This section considers the parameterized variational distribution of inducing variables. Using the same model evaluation rules in the last section, we show RMSEs and ASKLs in Table 2 and the empirical distributions of estimated embedding inputs and inducing inputs for each dimension are shown in Figure 3. It is obvious that our regularization approach achieves the best model fitting and the best latent input deployment. Also, it is clear to see that schedule 2 using ELBO$_2$ has a significantly larger ASKL compared with the same schedule using ELBO$_1$. This is because without marginalization, objective function ELBO$_2$ is more non-convex and thus more difficult
Table 3: Root mean square errors (RMSE) and averaged symmetric KL divergence (ASKL) for three different schedules with respect to inducing inputs under ELBO2 setting. (Anuran Calls Example)

| Schedule 1 | Schedule 2 | Schedule 3 |
|------------|------------|------------|
| RMSE       | 0.0690     | 0.0521     | **0.0453** |
| ASKL       | 2.6125     | 31.9826    | **0.0766** |

Table 4: Root mean square errors (RMSE) and averaged symmetric KL divergence (ASKL) for model with regularization (R) and without regularization (N) under different latent dimension sizes $Q = 2, 5, 10$. (Anuran Calls Example)

| $Q$ | RMSE(N) | RMSE(R) | ASKL(N) | ASKL(R) |
|-----|---------|---------|---------|---------|
| 2   | 0.0851  | 0.0492  | 1022.3650 | 162.4201 |
| 5   | 0.0692  | 0.0457  | 38.8489  | 0.0143  |
| 10  | 1.2367  | 0.1403  | 162.4201 | **0.0147** |

Regularization with different latent dimension sizes

We explore the benefits of regularization with respect to different latent dimension sizes under ELBO2 setting in the section. Specifically, because of output dimension size $D = 22$, we consider $Q = 2, 5, 10$ and set $\lambda = 1000$. The RMSEs and ASKLs are displayed in Table 4. The relative ratio of RMSEs, defined by $(\text{RMSE}(N)-\text{RMSE}(R))/\text{RMSE}(N)$ as model improvement statistics, for $Q = 2, 5, 10$ are 18.7%, 7.1% and 9.9%. It shows that regularization is always contributing to better model fitting, especially when latent dimension size is significantly smaller than the output dimension size.

Table 5: Root mean square errors (RMSE) of training data/reconstruction data (T/R) for baseline model/regularized model (B/R). Training time (T) are available for both models. (Flight Example)

| $M$ | RMSE (TB) | RMSE (TR) | RMSE (RR) |
|-----|-----------|-----------|-----------|
| 10  | 0.77      | 0.66      | 0.66      |
| 20  | 0.65      | 0.64      | 0.61      |
| 50  | 0.82      | 0.67      | 0.68      |
| 100 | 0.67      | 0.66      | 0.63      |

Driver Face Example

This section illustrates regularized sparse latent Gaussian processes for high dimensional data such as image data. We show regularization on the Driver Face dataset, which is available from the UCI repository at https://archive.ics.uci.edu/ml/datasets/DrivFace. It includes 606 instances and each instance is an image with $80 \times 80$ pixels. Each pixel’s value is in a unit interval $[0, 1]$. Specifically, This dataset contain three driver’s face images with different head poses. We use $2 \times 2$ max-pooling to reduce the original image size $80 \times 80$ to $40 \times 40$ as pre-processing.

Model Fitting

We employ a sparse latent Gaussian process with ELBO2 as a baseline model and set latent dimension size $Q = 5$. We consider different inducing point sizes $M = 10, 20, 50, 100$ and different regularization weights $\lambda = 10, 100, 1000, 10000$. To compare the model with and without regularization, we employ RMSEs for the model evaluation and AKLs to show the balance between inducing inputs and embedding inputs. Results are shown in Figure 4. It shows that as $\lambda$ increases, inducing inputs capture embedding points better. More importantly, with proper regularization, our model fitting results are always better than the baseline model for all cases of $M$.

Image Denoising

We apply our regularized latent sparse Gaussian process for the image denoising task in this section. First, we randomly select six images, in which we randomly select 50 pixels to add white noise and clip them into a unit interval $[0, 1]$. Three images of them with and without noise are displayed in Figure 5. We train the whole dataset and reconstruct the six images under different settings with respect to the number of inducing points $M = 10, 20, 50, 100$. The regularization weight is selected in the set $(10, 100, 1000, 10000)$. The predictive RMSEs are displayed in Table 5. It shows that our regularized model performs better than the corresponding baseline model for model prediction in all cases of $M = 10, 20, 50, 100$. We displayed the best regularized model predictive result in Figure 5.
Figure 3: Empirical distributions of estimated embedding inputs and inducing inputs under ELBO$_2$ setting. Schedule 1 to 3 are shown by row and latent dimension 1 to Q are shown by column. (Anuran Calls Example)

Figure 4: Root mean square errors and averaged symmetric KL divergence for the Driver Face dataset with different number of inducing points $M = 10, 20, 50, 100$ and with different regularization weights $\lambda = 10, 100, 1000, 10000$. Baseline model results are also provided. (Driver Face Example)

| $M$ | 10  | 20  | 50  | 100 |
|-----|-----|-----|-----|-----|
| Baseline model | 0.1221 | 0.1085 | 0.1033 | 0.0982 |
| Regularized model | **0.1195** | **0.1079** | **0.1024** | **0.0976** |

Table 6: Predictive root mean square errors for the six noisy images under different number of inducing points $M$s. (Driver Face Example)

**Conclusion**

Regularization is necessary for both sparse Gaussian processes and sparse latent Gaussian processes. Our regularization approach improves global optimization in model fitting and achieves better model prediction. In the case of sparse latent Gaussian processes, the use of regularization is also justified by proving that performing VI on a sparse latent Gaussian process with this regularization is equivalent to performing VI on a related empirical Bayes model. Generally, the regularization weight $\lambda$ is selected via cross validation. When cross validation is not available, we give a rule of thumb for the selection of regularization by setting $\lambda = M$ as a corresponding empirical Bayes model. We illustrate that our regularized model performs better model fitting under both ELBO$_1$ and ELBO$_2$ settings using the Anuran Calls dataset. We demonstrate the better model fitting under different latent dimension sizes $Q$. Moreover, we demonstrate the necessity of regularization for large datasets in noisy fea-
ture reconstruction tasks, using the Flight data. Finally, we illustrate our regularized model also has good performance for high dimensional data such as image data. We take the Driver Face dataset for example, in which our model has better model fitting and better prediction results for the noisy image reconstruction task.

References

Banerjee, S.; Gelfand, A. E.; Finley, A. O.; and Sang, H. 2008. Gaussian predictive process models for large spatial data sets. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 70(4):825–848.

Bernhard, S.; Alexander, S.; and Klaus-Robert, M. 1998. Kernel principle component analysis. Advances in Kernel Methods - Support Vector Learning 327–352.

Csato, L., and Opper, M. 2002. Sparse online gaussian processes. Neural Computation 641–669.

Damianou, A. C.; Titsias, M. K.; and Lawrence, N. D. 2016. Variational inference for latent variables and uncertain inputs in gaussian processes. Journal of Machine Learning Research 17(42):1–62.

Ek, C. H.; Torr, P. H. S.; and Lawrence, N. D. 2007. Gaussian process latent variable models for human pose estimation. In MLMI.

Finley, A.; Sang, H.; Banerjee, S.; and Gelfand, A. 2009. Improving the performance of predictive process modeling for large datasets. Computational statistics and data analysis.

Guhaniyogi, R.; Finley, A.; Banerjee, S.; and Gelfand, A. 2011. Adaptive gaussian predictive process models for large spatial datasets. Environmetrics.

Haining, R. 1993. Statistics for spatial data. Computers and Geosciences 19:615–616.

Hensman, J.; Fusi, N.; and Lawrence, N. D. 2013. Gaussian processes for big data. In Proceedings of the Twenty-Ninth Conference on Uncertainty in Artificial Intelligence, UAI’13, 282–290. Arlington, Virginia, United States: AUAI Press.

Hensman, J.; Rattray, M.; and Lawrence, N. D. 2012. Fast variational inference in the conjugate exponential family. In Advances in neural information processing systems, 2888–2896.

Lawrence, N. D., and Moore, A. J. 2007. Hierarchical gaussian process latent variable models. In Proceedings of the 24th International Conference on Machine Learning, ICML ’07, 481–488. New York, NY, USA: ACM.

Lawrence, N. D., and Quinonero Candela, J. 2006. Local distance preservation in the gp-lvm through back constraints. In Proceedings of the 23rd International Conference on Machine Learning, ICML ’06, 513–520. New York, NY, USA: ACM.

Lawrence, N. D. 2004. Gaussian process latent variable models for visualisation of high dimensional data. In Advances in neural information processing systems, 329–336.

Lawrence, N. 2005. Probabilistic non-linear principal component analysis with gaussian process latent variable models. J. Mach. Learn. Res. 6:1783–1816.

Mardia, K. V.; Kent, J. T.; and Bibby, J. M. 1979. Multivariate analysis. Academic Press, London.

Rasmussen, C., and Rasmussen, C. E. 2004. Gaussian processes in reinforcement learning. In Advances in Neural Information Processing Systems 16, 751–759. Cambridge, MA, USA: Max-Planck-Gesellschaft.

Rasmussen, C. E., and Williams, C. K. I. 2005. Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning). The MIT Press.

Seeger, M. 2003. Pac-bayesian generalisation error bounds for gaussian process classification. J. Mach. Learn. Res. 3:233–269.

Snellson, E., and Ghahramani, Z. 2006. Sparse gaussian processes using pseudo-inputs. In Weiss, Y.; Schölkopf, B.; and Platt, J. C., eds., Advances in Neural Information Processing Systems 18. MIT Press. 1257–1264.

Snellson, E., and Ghahramani, Z. 2007. Local and global sparse gaussian process approximations. In Meila, M., and Shen, X., eds., Proceedings of the Eleventh International Conference on Artificial Intelligence and Statistics, volume 2 of Proceedings of Machine Learning Research, 524–531. San Juan, Puerto Rico: PMLR.

Titsias, M., and Lawrence, N. D. 2010. Bayesian gaussian process latent variable model. In Teh, Y. W., and Titterington, M., eds., Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, volume 9 of Proceedings of Machine Learning Research, 844–851. Chia Laguna Resort, Sardinia, Italy: PMLR.

Titsias, M. 2009. Variational learning of inducing variables in sparse gaussian processes. In van Dyk, D., and Welling, M., eds., Proceedings of the Twelfth International Conference on Artificial Intelligence and Statistics, volume 5 of Proceedings of Machine Learning Research, 567–574. Hilton Clearwater Beach Resort, Clearwater Beach, Florida USA: PMLR.

Urtasun, R., and Darrell, T. 2007. Discriminative gaussian process latent variable model for classification. In ICML.