EigenGP: Gaussian process models with adaptive eigenfunctions

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Abstract
Gaussian processes (GPs) provide a nonparametric representation of functions. However, classical GP inference suffers from high computational cost for big data and it is difficult to design nonstationary GP priors in practice. In this paper, we propose a sparse Gaussian process model, EigenGP, based on data-dependent eigenfunctions of a GP prior. The data-dependent eigenfunctions make the Gaussian process nonstationary and can be viewed as dictionary elements. We learn these dictionary elements in an empirical Bayesian framework; more specifically, we learn all hyperparameters associated with these elements—including basis points and lengthscales—from data by maximizing the model marginal likelihood. We explore computational linear algebra to simplify the gradient computation significantly. Our experimental results demonstrate improved predictive performance of EigenGP over alternative sparse GP methods such as the Nyström method and sparse spectrum Gaussian process regression.

1 Introduction
Gaussian processes (GPs) are powerful nonparametric Bayesian models with numerous applications in machine learning and statistics. However, GP models have two limitations. First, simple stationary covariance functions (e.g., Gaussian covariance) are often used and it can be difficult to model nonstationary data by GPs. The difficulty of constructing nonstationary GPs is associated with the statistical and computational challenges of parameterizing positive definite covariance matrices. Second, and perhaps more importantly in practice, GP inference is costly. Training the exact GP regression model with \( N \) samples demands an \( O(N^3) \) space cost to save the whole covariance matrix and an \( O(N^3) \) time cost for inverting this matrix. For big data with large \( N \), the cost of GP inference will be prohibitively high. To reduce the computational cost, a variety of approximate GP inference approaches have been developed [Williams and Seeger, 2001, Csató and Opper, 2002, Snelson and Ghahramani, 2006, Qi et al., 2010]. An elegant unifying view for various approximate sparse GP regression models is given by Quiñonero-Candela and Rasmussen [2005].

Among all sparse GP regression methods, a state-of-the-art approach is to represent a function as a sparse Bayesian linear combination of pairs of trigonometric basis functions, a sine and a cosine for each spectral point; thus this approach is called sparse spectrum Gaussian process (SSGP) [Lázaro-Gredilla et al., 2010]. SSGP integrates out both weights and phases of the trigonometric functions and learns all hyperparameters of the model (frequencies and amplitudes) by maximizing the marginal likelihood. Using global trigonometric functions as basis functions, SSGP has the capability of approximating any stationary Gaussian process model and been shown to outperform alternative sparse GP methods—including fully independent training conditional (FITC) approximation [Snelson and Ghahramani, 2006]—on benchmark datasets.

In this paper, we propose a new Bayesian approach, EigenGP, that uses eigenfunctions—instead of sine and a cosine functions—as basis functions. It is well known that, among all orthogonal basis functions including trigonometric basis functions, eigenfunctions can provide the most compact representation. Furthermore, we marginalize out weights of eigenfunctions and estimate all hyperparameters—including basis points for eigenfunctions, lengthscales, and precision of the weight prior—by maximizing the model marginal likelihood (also known as evidence). To do so, we explore computational linear algebra and greatly simplify the gradient computation for optimization. As a result of this optimization, our eigenfunctions are data dependent and, thus, make EigenGP capable of accurately modeling nonstationary data. From the dictionary learning perspective, EigenGP integrates out weights over dictionary elements to avoid overfitting and learns dictionary elements—eigenfunctions—from data.

EigenGP is computationally efficient. It takes \( O(NM) \) space and \( O(NM^2) \) time for training on \( N \) samples with
$M$ estimated eigenfunctions. Note that similar to FITC and SSGP, EigenGP focuses on predictive accuracy at low computational cost, rather than on faithfully converging towards the full GP as the number of basis functions grows (For the latter case, see the approach by Yan and Qi [2010], which explicitly minimizes the KL divergence between exact and approximate GP posterior processes.)

The rest of the paper is organized as follows. Section 2 describes the background of GPs. Section 3 presents the EigenGP model and an illustrative example. Section 4 outlines the marginal likelihood maximization over all the hyperparameters, such as lengthscales and basis points. In Section 5, we discuss related works—in particular, the difference between EigenGP and the Nyström method [Williams and Seeger, 2001] and relevance vector machine (RVM) [Tipping, 2000]. Section 6 shows regression results on multiple benchmark regression datasets, demonstrating improved performance of EigenGP over the Nyström method, RVM, FITC, and SSGP.

2 Background of Gaussian processes

We denote $N$ independent and identically distributed samples as $D = \{(x_1, y_1), \ldots, (x_n, y_n)\}_n$, where $x_i$ is a $D$ dimensional input (i.e., explanatory variables) and $y_i$ is a scalar output (i.e., a response), which we assume is the noisy realization of a latent function $f$ at $x_i$.

A Gaussian process places a prior distribution over the latent function $f$. Its projection $f_x$ at $x_i$ defines a joint Gaussian distribution $p(f_x) = \mathcal{N}(f|m^0, K)$, where, without any prior preference, the mean $m^0$ are set to 0 and the covariance function $k(x_i, x_j) \equiv K(x_i, x_j)$ encodes the prior notion of smoothness. A popular choice is the anisotropic squared exponential covariance function:

$$k(x, x') = a_0 \exp \left( - (x - x')^T \text{diag}(\eta)(x - x') \right)$$ (1)

where the hyperparameters include the signal variance $a_0$ and the lengthscales $\eta = \{\eta_d\}_{d=1}^D$, controlling how fast the covariance decays with the distance between inputs. Using this covariance function, we can prune input dimensions by shrinking the corresponding lengthscales based on the data (when $\eta_d = 0$, the $d$-th dimension becomes totally irrelevant to the covariance function value). This pruning is known as Automatic Relevance Determination (ARD) and therefore this covariance is also called the ARD squared exponential. Note that the covariance function value remains the same when $(x' - x)$ is the same — regardless where $x'$ and $x$ are. This thus leads to a stationary GP model. For nonstationary data, however, a stationary GP model is a misfit. Although nonstationary GP models have been developed and applied to real world applications, they are often limited to low-dimensional problems, such as applications in spatial statistics [Paciorek and Schervish, 2004]. Constructing general nonstationary GP models remains a challenging task.

For regression, we use a Gaussian likelihood function

$$p(y_i|f) = \mathcal{N}(y_i|f(x_i), \sigma^2),$$ (2)

where $\sigma^2$ is the observation noise.

Given the Gaussian process prior over $f$ and the data likelihood, the exact posterior process is

$$p(f|D, y) \propto GP(f|0, K) \prod_{i=1}^N p(y_i|f)$$ (3)

Although the posterior process for GP regression has an analytical form, we need to store and invert an $N \times N$ matrix, which has the computational complexity $O(N^3)$, rendering GP unfeasible for big data analytics.

3 Model of EigenGP

To enable fast inference and obtain a nonstationary covariance function, our new model EigenGP projects the GP prior in an eigensubspace. Specifically, we set the latent function $f$

$$f(x) = \sum_{j=1}^M \alpha_j \phi^j(x)$$ (4)

where $M \ll N$ and $\{\phi^j(x)\}$ are eigenfunctions of the GP prior. We assign a Gaussian prior over $\alpha = [\alpha_1, \ldots, \alpha_M]$. $\alpha \sim \mathcal{N}(0, \text{diag}(w))$, (5)

so that $f$ follows a GP prior with zero mean and the following covariance function

$$\tilde{k}(x, x') = \sum_{j=1}^M w_j \phi^j(x) \phi^j(x').$$ (6)

To compute the eigenfunctions $\{\phi^j(x)\}$, we can use the Galerkin projection to approximate them by Hermite polynomials [Marzouk and Najm, 2009]. For high dimensional problems, however, this approach requires a tensor product of univariate Hermite polynomials that dramatically increases the number of parameters.

To avoid this problem, we use the Nyström method [Williams and Seeger, 2001] that allows us to obtain an approximation to the eigenfunctions in a high dimensional space efficiently. Specifically, assuming we have inducing variables (i.e. basis points $B = [b_1, \ldots, b_M]$, we replace

$$\int k(x, x') \phi^j(x) p(x) \text{d}x = \lambda_j \phi^j(x')$$ (7)

by its Monte Carlo approximation

$$\frac{1}{M} \sum_{i=1}^M k(x, b_i) \phi^j(b_i) \approx \lambda_j \phi^j(x)$$ (8)
Then, with simple derivations, we obtain the $j$-th eigenfunction $\phi^j(x)$ as follows
\[
\phi^j(x) = \sqrt{\frac{M}{\lambda_j^{(M)}}} k(x)\hat{u}_j = k(x)u_j
\]
where $k(x) \triangleq [k(x, b_1), \ldots, k(x, b_M)]$, $\lambda_j^{(M)}$ and $\hat{u}_j$ are the $j$-th eigenvalue and eigenvector of the covariance function evaluated at $B$, and $u_j = \sqrt{\frac{M}{\lambda_j^{(M)}}} \hat{u}_j$. Note that, for simplicity, we have chosen the number of the inducing variables to be the same as the number of the eigenfunctions; in practice, we can use more inducing variables while computing only the top $M$ eigenvectors.

Inserting (9) into (4) we obtain
\[
f(x) = \sum_{j=1}^{M} \alpha_j \sum_{i=1}^{M} u_{ij} k(x, b_i) \tag{10}
\]
This equation reveals a two-layer structure of EigenGP. The first layer linearly combines multiple kernel functions to generate each eigenfunction $\phi^j$. The second layer takes these eigenfunctions as the basis functions to generate the function value $f$. Note that $f$ is a Bayesian linear combination of $\{\phi^j\}$ where the weights $\alpha$ are integrated out to avoid overfitting. Thus EigenGP can be viewed as a deep Bayesian kernel machine.

All the model hyperparameters are learned from data. Specifically, for the first layer, to learn the eigenfunctions $\{\phi_i\}$, we estimate the inducing variables $B$ and the kernel hyperparameters (such as lengthscales $\eta$ for the ARD kernel) by maximizing the model marginal likelihood. For the second layer, we marginalize out $\alpha$ to avoid overfitting and maximize the model marginal likelihood to learn the hyperparameter $w$ of the prior in (5).

With the estimated hyperparameters, the prior over $f$ is nonstationary because its covariance function in (6) varies at different regions of $x$. This comes at no surprise since the eigenfunctions are tied with $p(x)$ in (7). This nonstationarity reflects the fact that our model is adaptive to the distribution of the explanatory variables $x$.

Note that to recover the full uncertainty captured by the kernel function $k$, we can add the following term into the kernel function of EigenGP:
\[
\delta(x - x')(k(x, x') - \bar{k}(x, x')) \tag{11}
\]
where $\delta(a) = 1$ if and only if $a = 0$. Compared to the original EigenGP model, which has a finite degree of freedom, this modified model has the infinite number of basis functions (assuming $k$ has an infinite number of basis functions as the ARD kernel). Thus, this model can accurately model the uncertainty of a test point even when it is far from the training set. We derive the optimization updates of all the hyperparameters for both the original and modified EigenGP models. But according to our experiments, the modified model does not improve the prediction accuracy over the original EigenGP (it even reduces the accuracy sometimes). Therefore, we will focus on the original EigenGP model in our presentation for its simplicity. But before we present details about hyperparameter optimization, let us first look at an illustrative example on the effect of hyperparameter optimization, in particular, the optimization of the inducing variables $B$.

### 3.1 Illustrative example

For this example, we consider a toy dataset used by the FITC algorithm (http://www.gatsby.ucl.ac.uk/~snelson/SPGP_dist.zip). It contains one-dimensional data with 200 training samples. We use 5 basis points ($M = 5$) and choose the ARD kernel. We then compare the basis functions $\{\phi^j\}$ and the corresponding predictive distributions in two cases. For the first case, we use the kernel width $\eta$ learned from the full GP model as the kernel width for EigenGP, and apply K-means to set the basis points $B$ as cluster centers. The idea of using K-means to set the basis points has been suggested by Zhang et al. [2008] to minimize an error bound for the Nyström approximation. For the second case, we optimize $\eta$, $B$ and $w$ by maximizing the marginal likelihood of EigenGP.

The results are shown in Figure 1. The first row of 1 demonstrates that, by optimizing the hyperparameters,
4 Learning hyperparameters

In this section we describe how we optimize all the hyperparameters, denoted by \( \theta \), which include \( B \), \( w \) in the covariance function (6), and all the kernel hyperparameters (e.g., the signal power \( a_0 \) and the lengthscales \( \eta \)).

To optimize the hyperparameters, we maximize the marginal likelihood (i.e., evidence) based on a conjugate Newton method\(^1\). The key computation is the evaluation of the log marginal likelihood and its gradient in the vector or matrix form. A naive calculation would be very costly. We apply identities from computational linear algebra [Minka, 2001, de Leeuw, 2007] to simplify the needed computation dramatically. Note that the log marginal likelihood and its gradient have the following form:

\[
\ln p(t; \theta) = -\frac{1}{2} \ln |C_N| - \frac{1}{2} t^T C_N^{-1} t - \frac{N}{2} \ln(2\pi) \tag{12}
\]

\[
d\ln p(t; \theta) = -\frac{1}{2} \left[ \text{tr}(C_N^{-1} dC_N) - \text{tr}(C_N^{-1} t^T C_N^{-1} dC_N) \right] \tag{13}
\]

where \( C_N = K + \sigma^2 I \), \( K = \Phi \text{diag}(w) \Phi^T \), and \( \Phi = \{ \phi^m(x_n) \} \) is a \( N \times M \) matrix. Because of the rank of \( K \) is \( M \ll N \), we can compute \( \ln |C_N| \) and \( C_N^{-1} \) efficiently with the cost of \( M^2 N \) (instead of \( N^3 \)) via the matrix inversion and determinant lemmas.

We explore two strategies for evidence maximization. The first one is sequential optimization, which first fixes \( w \) while updating all the other hyperparameters, and then optimizes \( w \) while fixing the other hyperparameters. The second strategy is to optimize all the hyperparameter jointly. In practice, the sequential optimization is computationally more efficient and less prone to bad local optima than the joint optimization.

\(^1\) we use minimize.m in the GPML package: www.gaussianprocess.org/gpml/code/matlab/doc

4.1 Sequential optimization

4.1.1 Gradient over \( w \)

To compute the gradient over \( w \), we apply the following formula for arbitrary matrices \( P \) and \( Q \) with appropriate sizes: \( \text{tr}(PQ) = \text{tr}(QP) \) and \( \text{tr}(P \text{diag}(w)Q) = 1^T (Q^T \circ P) w \), where \( 1 \) is a column vector of all ones, and \( \circ \) represents the Hadamard product. We can then obtain the two trace terms in the gradient (11) as follows:

\[
\frac{\text{d}(C_N^{-1} dC_N)}{d(w)} = 1^T(\Phi \circ (C_N^{-1} \Phi)) \tag{14}
\]

\[
\frac{\text{d}(C_N^{-1} t^T C_N^{-1} dC_N)}{d(w)} = 1^T(\Phi \circ (C_N^{-1} t^T C_N^{-1} \Phi)) \tag{15}
\]

where both \( C_N^{-1} \Phi \) and \( C_N^{-1} \) can be computed efficiently via low-rank operations.

4.1.2 Gradient over \( B \)

To compute the gradient over \( B \) in the sequential optimization, we first notice that, when \( w \) is fixed, we have

\[
C_N = K + \sigma^2 I = K_{XB} K_{BB}^{-1} K_{BX} + \sigma^2 I \tag{16}
\]

where \( K_{XB} \) is the cross-covariance matrix between the training data \( X \) and the inducing variables \( B \), and \( K_{BB} \) is the covariance matrix on \( B \).

Based on (16), the first trace term in the gradient of the log marginal likelihood (13) becomes:

\[
\text{tr}(C_N^{-1} dC_N) = 2\text{tr}(C_N^{-1} K_{XB} K_{BB}^{-1} dK_{BX}) + \text{tr}(K_{BX} C_N^{-1} K_{XB} d(K_{BB}^{-1})) \tag{17}
\]

where both \( C_N^{-1} \) and \( C_N^{-1} K_{XB} \) can be computed efficiently via low-rank operations with the cost of \( O(M^2) \). We can compute the second trace term, \( \text{tr}(C_N^{-1} t^T C_N^{-1} dC_N) \), in (13) similarly by replacing \( C_N^{-1} \) in (17) with \( C_N^{-1} t^T C_N^{-1} \).

Here we focus on the ARD squared exponential kernel (1); for other kernels such as polynomial kernels, we can derive their gradients in a similar way. For the ARD kernel, \( dK_{XB} \) and \( dK_{BB} \) in (17) can be computed as

\[
dK_{XB} = K_{XB} \circ dH \quad dK_{BB} = K_{BB} \circ dF
\]

where \( H \) and \( F \) are defined as

\[
H = 2X^T \text{diag}(\eta) B - (X^T \circ X^T) \eta 1^T - 1 \eta^T (B \circ B)
\]

\[
F = 2B^T \text{diag}(\eta) B - (B^T \circ B^T) \eta 1^T - 1 \eta^T (B \circ B)
\]

Utilizing the following identities, \( \text{tr}(P^T Q) = \text{vec}(P)^T \text{vec}(Q), \text{vec}(P \circ Q) = \text{diag}(\text{vec}(P)) \text{vec}(Q) \), where \( \text{vec}(\cdot) \) vectorizes a matrix into a column vector, we
can derive the gradients of the trace terms in (17):
\[
\frac{\text{tr}(C_N^{-1}K_{XB}K_{BB}^{-1}dK_{BX})}{dB} = 2R\Sigma^T\text{diag}(\eta) - 2(R11^T) \circ \left( B^T \text{diag}(\eta) \right)
\]
\[
\frac{\text{tr}(C_N^{-1}K_{XB}d(K_{BB}^{-1})K_{BX})}{dB} = -4SB\Sigma^T\text{diag}(\eta) + 4(S11^T) \circ \left( B^T \text{diag}(\eta) \right)
\]
where
\[
R = (K_{BB}^{-1}K_{BX}C_N^{-1}) \circ K_{BX}
\]
\[
S = (K_{BB}^{-1}K_{BX}C_N^{-1}K_{XB}K_{BB}^{-1}) \circ K_{BB}
\]
Substituting (18) and (19) into (17), we easily obtain the gradient over all the hyperparameters and use it to maximize the log marginal likelihood (12).

4.2 Joint optimization

4.2.1 Gradient over B

Define \( \tilde{K}_{BB} = U\Sigma^{-1}(w)U^T \) and recall that columns of \( U \) are eigenvectors of \( K_{BB} \). Then we have
\[
C_N = K_{XB}\tilde{K}_{BB}^{-1}K_{BX} + \sigma^2 I
\]
Now the gradient computation is similar to what we have for the sequential optimization but with a critical difference in \( dK_{BB} \) since the eigenvectors \( U \) depend on \( B \).

4.2.2 Gradient over \( \eta \)

Based on the eigen-decomposition, we have
\[
R(B) = (\tilde{K}_{BB}^{-1}CB) \circ CB
\]
\[
S(B) = (\tilde{K}_{BB}^{-1}CBC_{BB}^{-1}K_{XB}K_{BB}^{-1}) \circ \tilde{K}_{BB}^{-1}
\]
Using similar derivations, we can obtain
\[
\frac{\text{tr}(C_N^{-1}K_{XB}K_{BB}^{-1}dK_{BX})}{d\eta} = 21^T(B^T \circ (R\Sigma^T)) - (1^T R^T)(B \circ B) - (1^T (R^T)X \circ X^T)
\]
\[
\frac{\text{tr}(C_N^{-1}K_{XB}d(K_{BB}^{-1})K_{BX})}{d\eta} = -21^T(B^T \circ (SB\Sigma^T)) + 2(1^T (S^T)B \circ B)
\]
Again, we can obtain \( \frac{\text{tr}(C_N^{-1}tt^TC_{N}dC_{N})}{dB} \) by replacing \( C_N^{-1} \) in (20) and (21) by \( C_N^{-1}tt^TC_N^{-1} \). Then combining the above equations with (13) and (17), we have the gradients over \( \eta \).

4.3 Computational complexity

For either sequential or joint optimization, the overall computational complexity is \( O(\max(M^2, D)N) \) where \( D \) is the data dimension.
5 Related work

Our work is closely related to the seminal work by Williams and Seeger [2001]. But they differ in multiple aspects. First, we define a valid probabilistic model based on an eigen-decomposition of the GP prior. By contrast, the previous approach by Williams and Seeger [2001] aims at a low-rank approximation to the finite covariance/kernel matrix used in GP training—purely from a numerical approximation perspective—and its predictive distribution is not well-formed in a probabilistic framework (e.g., it may give a negative variance of the predictive distribution). Second, while the Nyström method simply uses the first few eigenvectors, we maximize the model marginal likelihood to adjust their weights in the covariance function. Third, exploring the clustering property of the eigenfunctions of the Gaussian kernel, our approach can conduct semi-supervised learning, while the previous one cannot. The semi-supervised learning capability of EigenGP is investigated in another paper of us. Forth, the Nyström method lacks a principled way to learn model hyperparameters including the kernel width and the basis points. By contrast, EigenGP learns all the hyperparameters from data in a principled empirical Bayesian framework. Forth, while the Nyström method can well approximate a stationary GP given a large number of basis points, the estimated basis points and weights in EigenGP’s covariance function make it suitable for nonstationary data.

Our model also bears similarity to relevance vector machine (RVM) [Tipping, 2000] and sparse spectrum Gaussian process (SSGP) by Lázaro-Gredilla et al. [2010]. However, based on the K-L expansion of a covariance function, the basis functions of ours is different those used in RVM or SSGP. Furthermore, with the additional term (11) in the model, EigenGP+ can give nonzero prediction variance when a test sample is far from the training samples.

6 Experimental results

In this section, we compare EigenGP and alternative methods on synthetic and real benchmark datasets. The alternative methods include the sparse GP methods—FITC, SSGP, and the Nyström method—as well as RVMs. We implemented the Nyström method ourselves and downloaded the software implementations for the other methods: FITC, http://www.gatsby.ucl.ac.uk/~asnelson/SPGP_dist.zip; SSGP, http://www.tsc.uc3m.es/~miguel/code/ssgpr_code.zip; and RVM, http://www.vectoranomaly.com/downloads/SB2_Release_200.zip. We used the ARD kernel for all the methods except RVMs (since they do not estimate the lengthscales in this kernel) and optimized all the hyperparameters via evidence maximization. For RVMs, we chose the squared exponential kernel with the same lengthscale for all the dimensions and applied a 10-fold cross-validation on the training data to select the lengthscale. On large real data, we used the values of $\eta$, $a_0$, and $\sigma^2$ learned from the full GP on a subset that was 1/10 of the training data to initialize all the methods except RVMs. For the rest configurations, we used the default setting of the downloaded software packages. For our own model, we denote the versions with sequential and joint optimization as EigenGP and EigenGP*, respectively.

To evaluate the test performance of each method, we measure the normalized mean square error (NMSE),

$$\text{NMSE} = \frac{\sum_{i=1}^{n}(t_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(t_i - \hat{y}_i)^2},$$

where $t_i$ and $y_i$ are the response value and the predictive mean for the $i$-th test point, and $m$ is the average response value of the training data.

6.1 Approximation quality on synthetic data

As in Section 3.1, we use the synthetic data from the FITC paper for the comparative study. To let all the methods have the same computational complexity, we set the number of basis functions (or points) $M = 5$. The results are summarized in Figure 2.

For the Nyström method, we used the kernel width learned from the full GP and applied K-means to choose the basis locations [Zhang et al., 2008]. Figure 2a shows that it does not fare well. Figure 2b demonstrates that the prediction of SSGP oscillates outside the range of the training samples, probably due to the fact that the sinusoidal components are global and span the whole data range (increasing the number of basis functions would improve SSGP’s predictive performance, but increase the computational cost.). As shown by Figure 2c, although FITC provides better predictive uncertainty in the region far from the training data, it fails to capture the turns of the data accurately for $x$ near 3. By contrast, EigenGP better models the data than the other methods around the training data.

Using the full GP predictive mean as the label for $x \in [-1, 7]$ (we do not have the true $y$ values in the test data), we compute the NMSE of all the methods to compare their approximation quality. The results are averaged over 10 runs, each with different random seeds, and reported in Table 1 (column 2). In this table, we have two versions of the Nyström method. For the first version, the kernel width is learned from the full GP and the basis locations are chosen by K-means as before; for the second version, its hyperparameters are learned by evidence maximization. Note that the evidence maximization algorithm for the Nyström approximation is novel too—developed by us for the comparative analysis. Table 1 shows that both EigenGP and EigenGP* approximate the mean of the full GP model more accurately than the other methods. We also compute the values of the KL divergence between the predictive distributions of the full GP and the sparse GPs and report them in the Appendix.

Furthermore, we add the difference term (11) into the
kernel function and denote this version of our algorithm as EigenGP*. It gives better predictive variance when far from the training data but its predictive mean is slightly worse than the version without this term (11); the NMSE of EigenGP* is 0.035±0.005. Thus, on the other datasets, we only use the versions without this term (EigenGP and EigenGP*) for their simplicity and effectiveness.

We also visualize the performance of all these methods with a higher computational complexity. Specifically, we set \( M = 10 \). Again, both versions of the Nyström method give poor predictive distributions. And SSGP still leads to extra wavy patterns outside the training data. Both FITC and the two versions of EigenGP (with and without the difference term in the kernel) give good predictions. The details are given in the Appendix.

![Figure 2](image_url)

**Figure 2:** Predictions of four sparse GP methods. Red dots represent training data, blue curves are predictive mean, red curves are two standard deviations above and below the mean curves, and the black crosses correspond to the inducing variables.

6.2 Prediction accuracy on nonstationary data

We then compare all the sparse GP methods on an one-dimensional nonstationary synthetic dataset with 200 training and 500 test samples. The underlying function is \( y = x \sin(x^2) \) where \( x \in (0, 3) \) and the standard deviation of the white noise is 0.5. This function is nonstationary in the sense that its frequency and amplitude increase when \( x \) increases from 0. We randomly generated the data 10 times and set the number of basis points (functions) to be 15 for all the competitive methods. Using the true function value as the label, we compute the average NMSE and the standard errors and report them in Table 1. For the Nyström method, the marginal likelihood optimization leads to much smaller error than the K-means based approach. However, both of them fare poorly when compared with the alternative methods. Table 1 also shows that EigenGP and EigenGP* achieve a striking 25,000 fold error reduction compared with Nyström*, and a 10-fold error reduction compared with the second best method, SSGP.

We further illustrate the predictive mean and standard deviation on a typical run in Figure 3. As shown in Figure 3a, the predictive mean of SSGP contains reasonable high frequency components for \( x \in (2, 3) \) but, as a stationary GP model, these high frequency components give extra wavy patterns in the left region of \( x \). In addition, the predictive mean on the right is smaller than the true one, probably affected by the small dynamic range of the data on the left. Figure 3b shows that the predictive mean of FITC at \( x \in (2, 3) \) has lower frequency and smaller amplitude than the true function—perhaps influenced by the low-frequency part on the left \( x \in (0, 2) \). Actually because of the low-frequency part, FITC learns a large kernel width \( \eta \); the average kernel width learned over the 10 runs is 207.75. This extremely large value affects the quality of learned basis points—for example, lacking of basis points for the high frequency region on the right. By contrast, using the same initial kernel width as FITC, EigenGP learns a suitable kernel width—on average, \( \eta = 0.07 \)—and provides good predictions as shown in Figure 3c.

### Table 1: NMSE on synthetic data

| Method     | dataset 1       | dataset 2       |
|------------|-----------------|-----------------|
| Nyström    | 537 ± 119       | 54013 ± 6957    |
| Nyström*   | 11 ± 3          | 1400 ± 288      |
| FITC       | 0.10 ± 0.03     | 0.48 ± 0.06     |
| SSGP       | 0.39 ± 0.05     | 0.44 ± 0.06     |
| EigenGP    | 0.02 ± 0.002    | 0.05 ± 0.008    |
| EigenGP*   | 0.03 ± 0.01     | 0.04 ± 0.003    |

6.3 Accuracy vs. time on real benchmark data

To evaluate the trade-off between prediction accuracy and computational cost, we use three large real datasets. The first dataset is California Housing from lib.stat.cmu.edu/. We randomly split the 8 dimensional data into 10,000 training and 10,640 test points. The second dataset is Physicochemical Properties of Protein Tertiary Structures (PPPTS) from http://archive.ics.uci.edu/ml/datasets/Physicochemical+Properties+of+Protein+Tertiary+Structure. We randomly split the 9 dimensional data into 20,000 training and 25,730 test points. The third dataset is Pole Telecomm available at www.cs.su.oz.au/~nitin. It contains 10,000
training and 5000 test samples, each of which has 26 features. On these datasets, we varied the rank or the number of basis functions (or points): $M = 20, 50, 100, 150$.

The test error and the training time of these methods are shown in Figure 4. We ran the Nyström method based on the marginal likelihood maximization, which is better than using K-means to set the basis points. Again, the Nyström method performed orders of magnitude worse than the other methods: with $M = 20, 50, 100, 150$, on California Housing, the Nyström method uses 181, 526, 1013, and 1631 seconds for training, respectively, and gives the NMSE $2.3 \times 10^7, 1.4 \times 10^4, 7.0 \times 10^3, \text{and } 5.4 \times 10^2$; on PPPTS, the training times are 391, 1078, 2232, and 3337 seconds and the NMSEs are $3.8 \times 10^8, 2.0 \times 10^6, 6.7 \times 10^5, \text{and } 8.1 \times 10^4$; and on Pole Telecomm, the training times are 292, 660, 1098, and 3818 seconds and the NMSEs are $7.8 \times 10^4, 2.4 \times 10^3, 1.2 \times 10^3, \text{and } 5.0 \times 10^3$.

For RVMs, we include the cross-validation time in its training time because choosing an appropriate kernel width is an important part of RVM training. Since RVM learns the number of basis functions automatically from the data, it gives a single result for each dataset, shown as in Figure 4.

As shown in Figure 4, EigenGP achieves the lowest prediction error given comparable computational time. Compared with EigenGP based on the sequential optimization, EigenGP∗ achieves similar prediction errors, but takes longer because the joint optimization has a higher computational complexity.

7 Conclusions

In this paper we have presented a simple yet effective sparse Gaussian process method, EigenGP, and applied it to regression. Despite its similarity to the Nyström method, EigenGP can improve its prediction quality by several orders of magnitude. EigenGP can also be applied to other learning tasks, including classification, semi-supervised learning and multi-task learning.

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APPENDIX

In the Appendix, we first report the KL divergence between the predictive posterior processes of the full GP and each of the sparse GP model on the first two synthetic datasets, for which we can run the full GP learning. The KL divergence shows us how well each sparse GP method approximates the full GP, but this divergence does not suggest exactly which method has better predictive performance.

Table A.1: KL Divergence

| Method     | dataset 1 | dataset 2 |
|------------|-----------|-----------|
| Nyström    | 16 ± 5    | 10 ± 0.6  |
| Nyström*   | 23 ± 15   | 25 ± 8    |
| FITC       | 0.18 ± 0.02 | 16 ± 15  |
| SSGP       | 1.35 ± 0.1 | 0.53 ± 0.05 |
| EigenGP    | 0.32 ± 0.01 | 0.11 ± 0.02 |
| EigenGP*   | 0.31 ± 0.01 | 0.05 ± 0.003 |

Then we visualize the predictions of the sparse GP methods with $M = 10$ on the first synthetic data in Figure A.1.

(a) Nyström (b) Nyström*

(c) SSGP (d) FITC

(e) EigenGP (f) EigenGP*+

For the Nyström method, we report its results in Figure A.1a when the kernel width are learned from the full GP and the basis locations are chosen by K-means. Figure A.1b shows the results of the Nyström method when the kernel width and the basis locations learned from evidence maximization. For both cases, the Nyström method gives poor predictions. SSGP, FITC and the two versions of EigenGP all give reasonable predictions.

Figure A.1: Predictions with $M = 10$. Red dots represent data, blue curves are predictive mean, red curves are ± two standard deviations around the mean curves, and the black crosses correspond to the inducing variables. EigenGP* denotes the version of EigenGP with the difference term in the covariance function. It better captures the uncertainty when far from the training data but gives a similar predictive mean as the version without the additional term.