Adaptive Gaussian process approximation for Bayesian inference with expensive likelihood functions

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Abstract

We consider Bayesian inference problems with computationally intensive likelihood functions. We propose a Gaussian process (GP) based method to approximate the joint distribution of the unknown parameters and the data, built upon a recent work [7]. In particular, we write the joint density approximately as a product of an approximate posterior density and an exponentiated GP surrogate. We then provide an adaptive algorithm to construct such an approximation, where an active learning method is used to choose the design points. With numerical examples, we illustrate that the proposed method has competitive performance against existing approaches for Bayesian computation.

1. Introduction

The Bayesian inference is a popular method to estimate unknown parameters from data, and a major advantage of the method is its ability to quantify uncertainty in the inference results [3]. In this work we consider Bayesian inference problems where the likelihood functions are highly expensive to evaluate. A typical example of this type of problems is the Bayesian inverse problems [22], where the parameters of interest can not be observed directly and need to be estimated from indirect data. Such problems arise from many real-world applications, ranging from carbon capture [10] to chemical kinetics [4]. In Bayesian
inverse problems, the mappings from the parameter of interest to the observable quantities, often known as the forward models, are often computationally intensive, e.g., involving simulating large scale computer models.

Due to the high computational cost, common numerical implementations of Bayesian inferences, such as the Markov chain Monte Carlo (MCMC) [1] methods can be prohibitively expensive. A simple idea to accelerate the computation of the posterior is to construct a computationally inexpensive surrogate or an approximation of the posterior distribution with a limited number of likelihood function evaluations. To this end, a particular convenient choice for surrogate function is the Gaussian Process (GP) model [23]. The idea of using the GP model to approximate the posterior or the likelihood function dates back to the the so-called Bayesian quadrature (or Bayesian Monte Carlo) approaches [16, 19, 8], which were designed to perform numerical integrations in a Bayesian fashion (for example, to compute the evidence in Bayesian inference problems [18]). Unlike the Bayesian quadrature methods, the goal of this work is to construct an approximation of the posterior distribution. To this end, a recent work [7] approximates the joint distribution of the unknown parameter and the data (which can also be viewed as the un-normalized posterior distribution) with an exponentiated GP model, where the design points, i.e., the points where the likelihood function is evaluated, are chosen with an active learning strategy. In particular, they determine the the design points by sequentially maximizing the variance in the posterior approximation. The method presented in this work also intends to approximate the joint distribution (or the un-normalized posterior, and in what follows the two terms with be used interchangeably). The new contributions of the proposed method are two-fold. First, we write the joint distribution as a product of an approximate posterior density and an exponentiated GP surrogate. The intuition behind this formulation is that, the GP model can be more effectively constructed if we can factor out a good approximation of the posterior (see Section 2.3 for a detailed explanation). As we may not know a good approximate posterior density in advance, we develop an algorithm to adaptively construct the product-form approximation of the joint distribution. Our second contribution is that we employ a different active learning strategy to choose the design points. Namely, we use the entropy rather than the variance as the selection criterion, which can better represent the uncertainty in the approximation of the joint distribution. Numerical examples illustrate that the proposed method can substantially improve the performance of the GP approximation.

The rest of the paper is organized as the following. In Section 2 we present the adaptive GP algorithm to construct the posterior approximation and the active leaning method to determine the design points. In section 3, we give two examples to illustrate the performance of the proposed method. Finally section 4 provides some concluding remarks.
2. The adaptive GP method

2.1. Problem Setup

A Bayesian inference problem aims to estimate an unknown parameter $x$ from data $d$, and specifically it computes the posterior distribution of $x$ using the Bayes’ formula:

$$\pi(x|d) \propto \pi(x,d) = l(x|d)\pi(x),$$

where $l(d|x)$ is the likelihood function and $\pi(x)$ is the prior distribution of $x$. When the Bayesian method is applied to inverse problems, the data and the forward model enter the formulation through the likelihood function. Namely, suppose that there is a function (termed as the forward function or the forward model) that maps the parameter of interest $x$ to the observable quantity $y$:

$$y = G(x) + \epsilon,$$

where $\epsilon$ is the observation error. Now we further assume that the distribution density of the observation noise $\epsilon$, $p_\epsilon(\epsilon)$, is available, and it follows directly that the likelihood function is given by

$$l(d|x) = p_\epsilon(d - G(x)).$$

In what follows we shall omit the argument $d$ in the likelihood function and denote it as $l(x)$ for simplicity. It is easy to see that each evaluation of the likelihood function $l(x)$ requires to evaluate the forward function $G(x)$. In practice, the forward function $G(x)$ often represents a large-scale computer model, and thus the evaluation of $l(x)$ can be highly computational demanding. Due to the high computational cost, the brute-force Monte Carlo simulation can not be used for such problems, and we resort to an alternative method to compute the posterior distributions, using the GP surrogate model. A brief description of the GP method is provided in next section.

2.2. The GP model

Given a real-valued function $g(x)$, the GP or the Kriging method constructs a surrogate model of $g(x)$ in a nonparameteric Bayesian regression framework [23, 15, 17]. Specifically the target function $g(x)$ is cast as a Gaussian random process whose mean is $\mu(x)$ and covariance is specified by a kernel function $k(x,x')$, namely,

$$\text{COV}[g(x),g(x')] = k(x,x').$$

The kernel $k(x,x')$ is positive semidefinite and bounded. Now let us assume that $n$ evaluations of the function $g(x)$ are performed at parameter values $X^* := [x^*_1, \ldots, x^*_m]$, yielding function evaluations $y^* := [y^*_1, \ldots, y^*_n]$, where

$$y^*_i = g(x^*_i) \quad \text{for} \quad i = 1, \ldots, m.$$Suppose that we want to predict the function values at points $D := [x_1, \ldots, x_{m'}]$, i.e., $y = [y_1, \ldots, y_{m'}]$ where $y_i = g(x_i)$. The sets $X^*$ and $D$ are often known as
the training and the test points respectively. The joint prior distribution of \((y^*, y)\) is,
\[
\begin{bmatrix}
    y^* \\
    y
\end{bmatrix} \sim \mathcal{N}
\left(
    \begin{bmatrix}
        \mu(X^*) \\
        \mu(D)
    \end{bmatrix},
    \begin{bmatrix}
        K(X^*,X^*) & K(X^*,D) \\
        K(D,X^*) & K(D,D)
    \end{bmatrix}
\right),
\]
(2)
where we use the notation \(K(A,B)\) to denote the matrix of the covariance evaluated at all pairs of points in set \(A\) and in set \(B\). The posterior distribution of \(y\) is also Gaussian:
\[
y \mid D, X^*, y^* \sim \mathcal{N}(u, \Sigma),
\]
(3a)
where the posterior mean is
\[
u = \mu(D) + K(D,X^*)K(X^*,X^*)^{-1}(y - \mu(D)),
\]
(3b)
and the posterior covariance matrix is
\[
\Sigma = K(D,D) - K(D,X^*)K(X^*,X^*)^{-1}K(X^*,D).
\]
(3c)
Here we only provide a brief introduction to the GP method tailored for our own purposes, and readers who are interested in further details may consult the aforementioned references.

2.3. The adaptive GP algorithm

Now we discuss how to use the GP method to compute the posterior distribution in our problem. A straightforward idea is to construct the surrogate model directly for the log-likelihood function \(\log l(x)\), and such a method has been used in the aforementioned works \([18, 7]\). A difficulty in this approach is that the target function \(\log l(x)\) can be highly nonlinear and fast varying, and thus are not well described by a GP model. We here present an adaptive scheme to alleviate the difficulty.

We first write the unnormalized posterior, i.e., the joint distribution \(\pi(x, d)\), as
\[
f(x) = l(x)\pi(x) = \exp(g(x))p(x),
\]
where \(p(x)\) is a probability distribution that we are free to choose and
\[
g(x) = \log(f(x)/p(x)).
\]
(4)
We work on the log posterior distribution since the log smoothes out a function and is more conducive for the GP modeling. Also, by doing this we ensure the non-negativity of the obtained approximate posterior. We then sample the function \(g(x)\) at certain locations and construct the GP surrogate of \(g(x)\). It should be noted that, the distribution \(p(x)\) plays an important role in the surrogate construction as a good choice of \(p(x)\) can significantly improve the accuracy of the GP surrogate models. In particular, if we take \(p(x)\) to be exactly the posterior \(p(x|d)\), it follows immediately that \(g(x)\) in Eq (4) is a constant. This then gives us the intuition that, if \(p(x)\) is a good approximation to the posterior
distribution $p(x|d)$, $g(x)$ is a mildly varying function which is easy to approximate. In other word, we can improve the performance of the GP surrogate by factoring out a good approximation of the posterior. Certainly, this can not be done in one step, as the posterior is not known in advance. We present here an adaptive framework to construct a sequence of pairs \( \{p_n(x), \exp(\hat{g_n}(x))\} \), the product of which evolves to a good approximation of the unnormalized posterior $f(x)$. Roughly speaking the algorithm performs the following iterations: in the $n$-th cycle, given the current guess of the posterior distribution $p_n(x)$, we construct a GP surrogate $\hat{g}_n(x)$ of $g_n(x)$ which is given by

$$g_n(x) = \log(f(x)/p_n(x)),$$

and we then compute a new (and possibly better) posterior approximation $p_{n+1}(x)$ using

$$p_{n+1}(x) \propto \exp(\hat{g}_n(x))p_n(x).$$

The complete scheme is described in Algorithm 1.

**Algorithm 1 The adaptive GP algorithm**

```plaintext
1: let $p_0(x) = \pi(x)$; let $n = 0$;
2: choose $m_0$ initial design points: $\{x_1, \ldots, x_{m_0}\}$, and compute $y_i = f(x_i)$ for $i = 1 \ldots m_0$;
3: let $S_0 = \{(x_1, y_1), \ldots, (x_{m_0}, y_{m_0})\}$;
4: for $n=0$ do $n_{\text{max}}$
5: let $g_n(x) = \log(f(x)/p_n(x))$;
6: construct a GP surrogate model $\hat{g}_n(x)$ for the function $g_n(x)$ with data set $S_n$;
7: draw a set of samples from the approximate posterior $\exp(\hat{g}_n(x))p_n(x)$ with MCMC, denoted as $X_n$;
8: obtain an estimated PDF from samples $X_n$, denoted as $p_{n+1}$;
9: if $n < n_{\text{max}}$ then
10: select $m$ design points: $\{x_1, \ldots, x_m\}$, evaluate $f(x_i)$ for $i = 1 \ldots m$, and let $S_{n+1} = S_n \cup \{(x_1, y_1), \ldots, (x_m, y_m)\}$;
11: end if
12: end for
```

Some remarks on the implementation of Algorithm 1 are listed in order:

- In Line 6, we construct the GP model for $g_n(x)$ using the procedure described in Section 2.2.
- In Line 7, we resort to the MCMC method to draw a rather large samples from the approximate posterior distribution; this procedure, however, does not require to evaluate the true likelihood function and is not computationally expensive.
- In Line 8, we need to compute the density function of a distribution $p_{n+1}$ from the samples $X_n$, and here we use the Gaussian mixture method [14] to estimate the density.
Finally in Line 10, we need to determine the design points, i.e., the locations where we evaluate the true function. The choice of design points is critical to the performance of the proposed adaptive GP algorithm, and we use an active learning method to determine the points, which is presented in Section 2.4.

2.4. Active learning for the design points

In the GP literature, the determination of the design points is often cast as an experimental design problem, i.e., the to find the experimental parameters that can provide us the most information. The problem has received considerable attention and a number of methods and criteria have been proposed to select the points, such as, the Mutual Information criterion [11], the Integrated Mean Square Error (IMSE) [20], the Integrated Posterior Variance (IVAR) [5], and the active learning MacKay (ALM) criterion [12], just to name a few. Here we choose to use an active learning strategy, that adds one design point a time, primarily for that it is easy to implement.

A common active learning strategy is to choose the point that has the largest uncertainty, and to this end we need a function that can measure or quantify the uncertainty in the approximation reconstructed. In the usual GP problems, the variance of the GP model \( \hat{g}(x) \) is a natural choice for such a measure of uncertainty (which yields the ALM method), because the distribution of \( \hat{g}(x) \) is Gaussian. In our problems, however, the function of interest is the posterior approximation \( \hat{f}(x) = \exp(\hat{g}(x))p(x) \) rather than the GP model \( \hat{g}(x) \) itself, and thus we should measure the uncertainty in \( \hat{f}(x) \). In [7], the variance of the posterior approximation \( \hat{f} \) is used as the measure function. However, since the distribution of \( \hat{f}(x) \) is not Gaussian, the variance may not provide a good estimate of the uncertainty. Here following [21], we choose to quantify the uncertainty in \( \hat{f}(x) \) using the entropy of it, and use it as the design criterion.

Specifically, suppose that, at point \( x \), the distribution of \( \hat{f}(x) \) is \( \pi_f(\hat{f}) \), and the entropy of \( \hat{f}(x) \) is defined as

\[
H(\hat{f}(x)) = - \int \log(\pi_f(\hat{f}))\pi_f(\hat{f})d\hat{f}.
\]

Thus we choose a new design point by

\[
\max_{x \in \Omega} H(\hat{f}(x)),
\]

where \( \Omega \) is the state space of \( x \). In the present problem, the distribution of \( \hat{g}(x) \) is Gaussian and let us assume its mean and variance are \( \mu \) and \( \sigma^2 \) respectively. It follows that the distribution of \( \hat{f}(x) \) is log-normal and the entropy of it can be computed analytically:

\[
H(\hat{f}) = \mu + \frac{1}{\ln(2\pi e \sigma^2)}.
\]

(5)

Now suppose that we have a set of existing data points, and we want to choose another \( m \) design points. We use the following scheme to sequentially choose the \( m \) new points:
1. Construct a GP model \( \hat{g}(x) \) for \( g(x) \) using the existing data points and set the iteration counter to be \( i = 0 \);
2. Compute \( x^* = \text{arg max}_{x \in \Omega} H(\hat{f}(x)) \);
3. Evaluate \( y^* = g(x^*) \) and let \( i = i + 1 \);
4. Update the GP model \( \hat{g} \) by adding the new data point \((x^*, y^*)\);
5. If \( i < m \), return to Step 2; otherwise, terminate the iteration.

Note that the key in the adaptive scheme is Step 2, where we seek the point \( x \) that maximizes the entropy \( H(\hat{f}(x)) \) in the state space \( \Omega \). This is a quite challenging problem from an optimization perspective, because the gradient of the objective function can not be easily obtained and the problem may have multiple local maxima. However, in the numerical tests, we have found that, our algorithm does not strictly require the optimality of the solution and it performs well as long as a good design point can be found in each step. Thus here we use a stochastic search method, the simulated annealing algorithm [9], to find the design point. We have also tested other meta-heuristic optimization algorithms, and the resulting performances are quite similar.

3. Numerical examples

3.1. The Rosenbrock function

We first test our method on a two-dimensional mathematical example. The likelihood function is

\[
l(x) = \exp \left( -\frac{1}{100} (x_1 - 1)^2 - (x_1^2 - x_2)^2 \right),
\]

which is the well-known Rosenbrock function, and the prior \( \pi(x) \) is a uniform distribution defined on \([-5, 5] \times [-5, 5]\). The resulting unnormalized posterior is shown in in Fig. 1. The function is challenging for many Bayesian computation methods such as the MCMC algorithms due to its “banana shape”, and thus it is often used as a test problem.

We now apply the proposed adaptive GP method to compute the posterior for this problem. First we note that, in this example and the other one, the GP hyperparameters are selected using the type II maximum likelihood method. Moreover, in this example, we let \( m_0 = m = 20 \) and the samples in \( S_0 \) were randomly drawn according to the prior distribution. In the algorithm, we need to sample from the approximate posterior distribution in each iteration, and here we draw 20,000 samples with the delayed rejection adaptive Metropolis algorithm (DRAM) [6]. We reinstate that the 20,000 MCMC samples are generated from the approximate posterior distribution and thus it does not require to evaluate the true likelihood function. We also set the number of iterations \( n_{\text{max}} = 10 \) and so totally we make 200 evaluations of the true likelihood function. To illustrate the performance of our method, we plot the maximum entropy of the approximation resulted in each iteration in Fig. 2 (left) and the Kullback-Leibler distance (KLD) between the approximate posterior and the true posterior distribution in Fig. 2 (right). Note that, ideally the
maximum entropy should decay with respect to the number of iterations, while the result shown in Fig. 2 fluctuates. This is because that the random search algorithm used may not identify the global optimal solution in all the iterations; nevertheless, as is shown in Fig. 2 (right), the KLD between the true posterior and the approximation decreases very well as the iteration proceeds, suggesting that the non-optimality in the random search algorithm does not significantly affect the performance of the proposed method. We then plot the approximate posterior obtained in the 1st, 4th, 7th and 10th iterations in Figs. 3, in which we can visualize how the quality of the approximation increases as the iterations proceed. In each of the plots, we also show the design points (red dots) that have been used up to the given iteration. Finally, as a comparison, we also compute the GP approximation of the posterior with two other methods. The first method is probably the most straightforward one: i.e. we randomly draw a number of design points from the prior distribution and use them to construct a GP approximation of the log-likelihood function. The second one is the method developed in [7]. We emphasize that, our method constructs the GP approximation by adaptively factoring out the approximate posterior distribution, which is another major difference from the two aforementioned alternative methods. We show the approximate posterior distributions computed with the two alternative methods in Figs 4, both with 200 design points that are marked as red dots in the figures. We can see from the figures that, the results of both methods differ evidently from the true posterior distribution, suggesting that the proposed adaptive scheme and active learning strategy do significantly improve the quality of the GP approximation constructed.

3.2. Genetic toggle switch

We now apply the proposed method to a real-world inference problem. Namely, we consider the kinetics of a genetic toggle switch, which was first
Figure 2: Left: the maximum entropy plotted against the number of iterations. Right: the KLD between from the true posterior to the GP approximation plotted against the number of iterations.

Figure 3: The approximate posterior distribution obtained at the 1st, 4th, 7th and 10th iterations respectively. The red dots are the design points that have been used.
studied in [2] and later numerically investigated in [13]. The toggle switch consists of two repressible promotors arranged in a mutually inhibitory network: promoter 1 an promoter 2. Either promoter transcribes a repressor for the other one, and moreover, either repressor may be induced by an external chemical or thermal signal. Genetic circuits of this form can be modeled by the following differential-algebraic equation system [2]:

\[
\begin{align*}
\frac{du}{dt} &= \frac{\alpha_1}{1 + \nu^\beta} - u, \\
\frac{dv}{dt} &= \frac{\alpha_2}{1 + w^\gamma} - v, \\
w &= \frac{u}{1 + ([\text{IPTG}]/K)^\eta}.
\end{align*}
\]

In the equations above, \(u\) and \(v\) are respectively the concentration of repressors 1 and 2; \(\alpha_1\) and \(\alpha_2\) are the effective rates of synthesis of the repressors; \(\gamma\) and \(\beta\) represent cooperativity of repression of the two promotors; and \([\text{IPTG}]\) is the concentration of IPTG, the chemical compound that induces the switch. Parameters \(K\) and \(\eta\) describe binding of IPTG with the first repressor. For more details of the model, we refer to [2].

|   | \(\alpha_1\) | \(\alpha_2\) | \(\gamma\) | \(\beta\) | \(\eta\) | \(K\) |
|---|---|---|---|---|---|---|
| \(n\) | [120, 200] | [15.8, 16.0] | [2.1, 2.9] | [0.85, 1.15] | [1.3, 2.7] | [2.3, 3.7] \(\times 10^{-5}\) |

Table 1: The prior domains of the parameters.

The experiments are performed with several selected values of \([\text{IPTG}]\): \(1 \times 10^{-5}, 5 \times 10^{-4}, 7 \times 10^{-4}, 1 \times 10^{-3}, 3 \times 10^{-3}, 5 \times 10^{-3}\) respectively, and for each
experiment, the measurement of $v$ is taken at $t = 10$. The goal is to infer the six parameters
\[
x = [\alpha_1, \alpha_2, \gamma, \beta, \eta, K],
\]
from the measurements of $v$. We use synthetic data in this problem, and specifically we assume that the true values of the parameters are
\[
x_{\text{true}} = [143, 15.95, 2.70, 0.96, 2.34, 2.70 \times 10^{-5}].
\]
The data is simulated using the model described by Eqs. (7) with the true parameter values and measurement noise is then added to the simulate data. The measurement noise here is assumed Gaussian and zero-mean, with a variance $\sigma^2 = 5 \times 10^{-4}$.

We assume that the priors of the six parameters are all uniform and independent of each other, where the domains of the uniform priors are given in Table 1. We apply our method to approximate the posterior distribution, where we use 10 iterations with 100 design points in each iteration, resulting totally 1000 evaluations of the true likelihood function. We note that each evaluation of the likelihood function involves a full simulation of the underlying model described by Eqs. (7). After obtaining the approximate posterior distribution, we draw $3 \times 10^5$ samples from it using a DRAM MCMC simulation. As a comparison, we also draw $3 \times 10^5$ samples from the true posterior distribution with a DRAM simulation. We show the mean and the standard deviations (SD) of the six parameters computed by both methods in Table 2. One can see from the results that, the GP method can accurately compute the posterior mean for all the parameters; on the other hand, the SD computed by the GP method are rather accurate for all parameters except that the SD of $\alpha_2$ is overestimated by the GP method. To further evaluate the performance of the GP method, we estimate the marginal posterior distribution of the six parameters from the samples and show the results in Fig. 5. Once again, we can see that the GP method can provide rather good approximation for all the marginals except that of the parameter $\alpha_2$ as the variance of it is overestimated. Given that the GP method only uses 1000 evaluations of the likelihood function, the numerical results indicate that the GP method is a very competitive alternative to the MCMC simulation, especially for problems with computationally intensive likelihood functions.

4. Conclusions

In summary, we have proposed an algorithm to construct GP based approximation for the un-normalized posterior distribution. The method expresses the un-normalize posterior as a product an approximate posterior density and an exponentiated GP model, and an adaptive scheme is presented to construct such an approximation. We also provide an active learning method that uses maximum entropy as the selection criterion to determine the sampling points. With numerical examples, we show that the method can obtain a rather good approximation of the posterior with a limited number of evaluations of the
Table 2: A comparison of the mean and the standard deviations of the six parameters computed by direct MCMC simulation and the proposed GP approximation method.

|       | $\alpha_1$ | $\alpha_2$ | $\gamma$ | $\beta$  | $\eta$  | $K$      |
|-------|------------|------------|----------|----------|----------|----------|
| Mean  | MCMC       | 158        | 15.95    | 2.54     | 0.97     | 2.14     | $2.97 \times 10^{-5}$ |
|       | GP         | 157        | 15.95    | 2.52     | 0.97     | 2.15     | $2.93 \times 10^{-5}$ |
| SD    | MCMC       | 21.8       | 0.011    | 0.225    | 0.044    | 0.358    | $4.03 \times 10^{-6}$ |
|       | GP         | 21.8       | 0.022    | 0.216    | 0.060    | 0.339    | $3.83 \times 10^{-6}$ |

Figure 5: The marginal distributions of the six parameters, computed with standard MCMC simulation (solid lines) and the proposed adaptive GP method (dashed lines).

likelihood functions. We believe the proposed method can be useful in a wide range of practical Bayesian inference problems where the likelihood function are expensive to evaluate.

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References

[1] Christophe Andrieu, Nando De Freitas, Arnaud Doucet, and Michael I Jordan. An introduction to MCMC for machine learning. *Machine learning*, 50(1-2):5–43, 2003.
[2] Timothy S Gardner, Charles R Cantor, and James J Collins. Construction of a genetic toggle switch in escherichia coli. *Nature*, 403(6767):339–342, 2000.

[3] Andrew Gelman, John B Carlin, Hal S Stern, and Donald B Rubin. *Bayesian data analysis*, volume 2. Chapman & Hall/CRC Boca Raton, FL, USA, 2014.

[4] Andrew Golightly and Darren J Wilkinson. Bayesian parameter inference for stochastic biochemical network models using particle Markov chain Monte Carlo. *Interface focus*, 1(6):807–820, 2011.

[5] Alex Gorodetsky and Youssef Marzouk. Mercer kernels and integrated variance experimental design: connections between gaussian process regression and polynomial approximation. *SIAM/ASA Journal on Uncertainty Quantification*, 4(1):796–828, 2016.

[6] Heikki Haario, Marko Laine, Antonietta Mira, and Eero Saksman. DRAM: efficient adaptive MCMC. *Statistics and Computing*, 16(4):339–354, 2006.

[7] Kirthevasan Kandasamy, Jeff Schneider, and Barnabás Póczos. Bayesian active learning for posterior estimation. In *Proceedings of the 24th International Conference on Artificial Intelligence*, pages 3605–3611. AAAI Press, 2015.

[8] Marc Kennedy. Bayesian quadrature with non-normal approximating functions. *Statistics and Computing*, 8(4):365–375, 1998.

[9] Scott Kirkpatrick, C Daniel Gelatt, Mario P Vecchi, et al. Optimization by simulated annealing. *Science*, 220(4598):671–680, 1983.

[10] Bledar A Konomi, Georgios Karagiannis, Kevin Lai, and Guang Lin. Bayesian treed calibration: an application to carbon capture with ax sorbent. *Journal of the American Statistical Association*, in press.

[11] Andreas Krause, Ajit Singh, and Carlos Guestrin. Near-optimal sensor placements in Gaussian processes: Theory, efficient algorithms and empirical studies. *Journal of Machine Learning Research*, 9(Feb):235–284, 2008.

[12] David JC MacKay. Information-based objective functions for active data selection. *Neural computation*, 4(4):590–604, 1992.

[13] Youssef Marzouk and Dongbin Xiu. A stochastic collocation approach to bayesian inference in inverse problems. *Communications in Computational Physics*, 6(4):826–847, 2009.

[14] Geoffrey McLachlan and David Peel. *Finite mixture models*. John Wiley & Sons, 2004.
[15] Jeremy Oakley and Anthony O’Hagan. Bayesian inference for the uncertainty distribution of computer model outputs. *Biometrika*, 89(4):769–784, 2002.

[16] Anthony O’Hagan. Bayes–Hermite quadrature. *Journal of statistical planning and inference*, 29(3):245–260, 1991.

[17] Anthony O’Hagan and JFC Kingman. Curve fitting and optimal design for prediction. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 1–42, 1978.

[18] Michael Osborne, Roman Garnett, Zoubin Ghahramani, David K Duvenaud, Stephen J Roberts, and Carl E Rasmussen. Active learning of model evidence using Bayesian quadrature. In *Advances in neural information processing systems*, pages 46–54, 2012.

[19] Carl Edward Rasmussen and Zoubin Ghahramani. Bayesian Monte Carlo. *Advances in neural information processing systems*, pages 505–512, 2003.

[20] Jerome Sacks, William J Welch, Toby J Mitchell, and Henry P Wynn. Design and analysis of computer experiments. *Statistical science*, pages 409–423, 1989.

[21] Paola Sebastiani and Henry P Wynn. Maximum entropy sampling and optimal Bayesian experimental design. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 62(1):145–157, 2000.

[22] Albert Tarantola. *Inverse problem theory and methods for model parameter estimation*. SIAM, 2005.

[23] Christopher KI Williams and Carl Edward Rasmussen. Gaussian processes for machine learning. *the MIT Press*, 2(3):4, 2006.