**Function Optimization with Posterior Gaussian Derivative Process**

Sucharita Roy and Sourabh Bhattacharya*

**Abstract**

Function optimization is a research area that has wide applications in all scientific disciplines. Yet, for any sufficiently large class of optimization problems it is considerably difficult to single out any optimization methodology that can outperform the others in terms of theoretical foundation, accuracy, computational efficiency or robustness. Indeed, given any optimization problem, it is customary to search for methods that might be effective, and in most cases, some heuristic method is ultimately taken into consideration.

In this article, we propose and develop a novel Bayesian algorithm for optimization of functions whose first and second partial derivatives are known. The basic premise is the Gaussian process representation of the function which induces a first derivative process that is also Gaussian. The Bayesian posterior solutions of the derivative process set equal to zero, given data consisting of suitable choices of input points in the function domain and their function values, emulate the stationary points of the function, which can be fine-tuned by setting restrictions on the prior in terms of the first and second derivatives of the objective function. These observations motivate us to propose a general and effective algorithm for function optimization that attempts to get closer to the true optima adaptively with in-built iterative stages.

We provide theoretical foundation to this algorithm, proving almost sure convergence to the true optima as the number of iterative stages tends to infinity. The theoretical foundation hinges upon our proofs of almost sure uniform convergence of the posteriors associated with Gaussian and Gaussian derivative processes to the underlying function and its derivatives in appropriate fixed-domain infill asymptotics setups; rates of convergence are also available. We also provide Bayesian characterization of the number of optima using information inherent in our optimization algorithm.

We illustrate our Bayesian optimization algorithm with five different examples involving maxima, minima, saddle points and even inconclusiveness. Our examples range from simple, one-dimensional problems to challenging 50 and 100-dimensional problems. While we obtain encouraging and interesting results in each case, we shed light on various issues regarding computation and accuracy along the way. A general and important issue is that our algorithm is able to capture significantly more accurate solutions than the existing optimization algorithms thanks to the posterior simulation approach embedded in our method.

**Keywords:** Dirichlet process; Fixed-domain infill asymptotics; Function optimization; Gaussian derivative process; Importance resampling; Parallel processing; Transformation based Markov Chain Monte Carlo (TMCMC).

1 **Introduction**

There is no scientific discipline that does not require function optimization. Hence, it is needless to mention that there exists an enormous literature on the topic, with a plethora of optimization techniques and algorithms. Most of the existing algorithms are deterministic and heuristic in nature, focussing on quick computations via popular software usage. The solutions provided by most such algorithms are often found to be reasonable in practical applications, even though there need not be any guarantee of convergence to the true optima. Indeed, optimization algorithms are generally designed depending upon the problem at hand, and it seems to be almost impossible to pinpoint towards any optimization method that works for a even a relatively large class of problems. Among stochastic optimization methods, we consider the simulated annealing methodology to be a general purpose procedure, but it is crucially important to very carefully choose the sequence of “temperatures” to converge to the optima in practice,

*Sucharita Roy is an Assistant Professor and Head of the Department of Mathematics in St. Xavier’s College, Kolkata, pursuing PhD in Interdisciplinary Statistical Research Unit, Indian Statistical Institute, 203, B. T. Road, Kolkata 700108. Sourabh Bhattacharya is an Associate Professor in Interdisciplinary Statistical Research Unit, Indian Statistical Institute, 203, B. T. Road, Kolkata 700108. Corresponding e-mail: sourabh@isical.ac.in.
and even in moderately high dimensions this often turns out to be an extremely difficult exercise. Effective choice of proposal distributions also plays a major role in practical convergence, which is again a difficult issue in high dimensions.

In this article, we propose and develop a novel Bayesian algorithm for optimization of functions whose first and second partial derivatives are available. Our approach is to embed the underlying function, along with its derivatives, in a random function scenario, driven by Gaussian processes and the induced derivative Gaussian processes, the latter forming the crux of our methodology. In a nutshell, with data consisting of suitable choices of input points in the function domain and their function values, we first obtain the posterior derivative process corresponding to the original Gaussian process. Then we construct the posterior distribution of the solutions corresponding to setting random partial derivative functions to the null vector. This posterior is expected to emulate the stationary points of the objective function. Now consider a uniform prior on the function domain having the constraints that the first partial derivatives are reasonably close to the null vector and that the matrix of second order partial derivatives is positive definite (for minimization problem, and negative definite for maximization problem). Due to the prior constraints, the resultant posterior solutions may be expected to approximately emulate the true optima even if the dataset is not large enough.

However, for small datasets, the prior constraints will be usually too restrictive to let any posterior simulation method progress. Hence, we shall begin with posterior solution simulations associated with less restrictions, such as that the Euclidean norm of the partial derivative vector is bounded above by some reasonably large constant. Once adequate posterior solution simulations are obtained, we shall consider iterative stages, where we shall progressively simulate from the posterior with finer prior restrictions, and at each stage augmenting realizations (and their function values) that meet the finer restrictions, to the original dataset. Thus, as the iterations tend to infinity, the resulting posteriors are expected to converge to the true optima. These key concepts lead to an effective, general-purpose optimization algorithm.

As can be anticipated from the above intuitions, convergence of the algorithm depends crucially on convergence of the posterior derivative process to the true function derivatives. And such convergence depends upon appropriate design of the input points of the function domain. As such, under appropriate fixed-domain infill asymptotics setups, we prove almost sure uniform convergence of the posteriors corresponding to Gaussian and Gaussian derivative processes to the objective function and its derivatives. Interestingly, we are also able to obtain rates of convergence under a particular infill asymptotics setup. To our knowledge, these results are new and are of independent interest. Utilizing these results, we prove almost sure convergence of our optimization algorithm to the true optima as the number of iterations tends to infinity. As an aside, we also provide Bayesian characterization of the number of optima, borrowing information from our optimization algorithm.

To illustrate our ideas, we consider five different optimization problems involving maxima, minima, saddle points and even inconclusiveness. The problems vary from simple, one-dimensional to challenging 50 and 100-dimensional situations. On application of our Bayesian optimization algorithm with increased sophistication demanded by the increasingly challenging examples, we obtain encouraging and insightful results in each case. We elucidate various issues on accuracy and computation as we proceed with the applications.

A general and important feature of our Bayesian optimization algorithm is that it is able to recognize significantly more accurate solutions than the existing optimization algorithms. This interesting ability can be attributed to the posterior simulation approach ingrained in our Bayesian optimization concept. Indeed, the posterior simulation approach ensures that our algorithm can explore regions of the input space around any given solution obtained by any other approach, and neighborhoods of such solution must contain at least one new solution which is at least as close to the true optimum compared to the given solution.

It must be mentioned that function optimization methods using traditional Gaussian process posteriors do exist in the literature (see, for example, Frazier (2018) and the references therein), but these methods consider the objective function to be a “black box” and assume that the derivatives are unavail-
able. These methods would naturally be far less accurate compared to ours when the derivatives are available. We are also not aware of any convergence result for such “derivative-free” Gaussian process methods which make use of so-called “acquisition functions” to progress. Since there are many choices of acquisition functions, each with its own merits and demerits, it seems doubtful if such methods can have solid foundation, letting alone reliability in practical implementations. In this article, we shall not concern ourselves with the existing Bayesian optimization methods.

The rest of this article is structured as follows. In Section 2 we provide details on derivation of the posterior associated with Gaussian derivative process and in Section 3 we derive the form of the posterior for the random optima associated with the solutions of the Gaussian derivative process set equal to zero, along with other desirable restrictions using objective function derivatives. Almost sure uniform convergence results for posteriors associated with Gaussian process and Gaussian process derivatives are presented in Section 4, along with the proofs. In Section 5 we introduce our general-purpose Bayesian optimization algorithm, and in Section 6 we establish Bayesian characterization of the number of optima of the objective function. Illustration of our Bayesian optimization algorithm with various optimization problems is taken up in Section 7. Summarization of our contribution, along with concluding remarks, are provided in Section 8.

2 Posterior Gaussian derivative process

2.1 Details of the objective function

Consider any function \( f : \mathbb{R}^d \rightarrow \mathbb{R} \), where \( \mathbb{R} \) is the real line and \( d \geq 1 \) is the dimension of the input space, assumed to be finite. We further assume that the second order partial derivatives of \( f \), namely, \( \partial^2 f / \partial x_i \partial x_j \) exist and are continuous for all \( x \in \mathcal{X} \subseteq \mathbb{R}^d \) for \( i, j = 1, \ldots, d \). The objective is to optimize the function \( f(x) \) with respect to \( x \in \mathcal{X} \). In this article, we assume that \( \mathcal{X} \) is compact.

2.2 Data from the objective function

Assume that corresponding to arbitrary inputs \( \{x_1, \ldots, x_n\} \in \mathcal{X} \), where \( n > 1 \), the output vector \( f_n = (f(x_1), \ldots, f(x_n))^T \) is available. Here \( T \) denotes transpose. Let \( D_n = \{ (x_i, f(x_i)) : i = 1, \ldots, n \} \).

2.3 Gaussian process representation of the objective function

Let \( g : \mathbb{R}^d \rightarrow \mathbb{R} \) denote a random function such that given \( D_n, g(x_i) = f(x_i) \) for \( i = 1, \ldots, n \).

Since Gaussian processes have the above interpolation property, we model \( g(\cdot) \) by a Gaussian process with mean function \( \mu(\cdot) \) and covariance function \( \sigma^2 c(\cdot, \cdot) \), where \( \sigma^2 \) is the process variance. In other words, \( E[g(x)] = \mu(x) \) for any \( x \in \mathcal{X} \) and \( \text{Cov}(g(x), g(y)) = \sigma^2 c(x, y) \) for all \( x, y \in \mathcal{X} \). Let \( \mu(\cdot) \) be continuous in \( \mathcal{X} \) and \( c(\cdot, \cdot) \) be Lipschitz continuous on \( \mathcal{X} \times \mathcal{X} \). Then \( g(\cdot) \) is actually a continuous-path Gaussian process with mean function \( \mu(\cdot) \) and covariance function \( \sigma^2 c(\cdot, \cdot) \).

We shall use the notation \( g_n \) to denote \( (g(x_1), \ldots, g(x_n))^T \) when distribution of this vector will be considered and \( f_n \) when this vector is conditioned upon.

2.4 Gaussian derivative process

For \( x = (x_1, \ldots, x_d) \) and \( y = (y_1, \ldots, y_d) \), let us assume that the second order mixed partial derivatives

\[
\frac{\partial^2 c(x^*, y^*)}{\partial x_i \partial y_i} = \frac{\partial^2 c(x, y)}{\partial x_i \partial y_i} \bigg|_{x=x^*,y=y^*}
\]

are Lipschitz continuous on \( \mathcal{X} \times \mathcal{X} \) for \( i = 1, \ldots, d \).

With the above assumption on the covariance function and with the further assumption that \( \mu(\cdot) \) is twice continuously differentiable with continuous mixed second order partial derivatives, for \( x =
corresponding to the original continuous-path Gaussian process \( g(\cdot) \) exists for \( i = 1, \ldots, d \), for all \( x^* \in \mathcal{X} \). Specifically, for \( i = 1, \ldots, d \), \( g_i'(\cdot) = \partial g(\cdot)/\partial x_i \) is a continuous-path Gaussian process with mean function \( \mu_i'(\cdot) = \partial \mu(\cdot)/\partial x_i \) and covariance function \( \sigma^2 \partial^2 g(\cdot)/\partial x_i \partial y_j \).

For general details on Gaussian and Gaussian derivative processes, see, for example, Adler (1981), Adler and Taylor (2007).

### 2.5 Joint distribution of Gaussian variables and Gaussian derivative variables

Note that, given \( x^*, y^* \in \mathcal{X} \),

\[
g_i'(x^*) = \frac{\partial g(x^*)}{\partial x_i} = \frac{\partial g(x)}{\partial x_i} \bigg|_{x=x^*},
\]

the covariance term is given by (2.1),

\[
\text{Cov} \left( g_i'(x^*), g_j'(x^*) \right) = \sigma^2 \frac{\partial^2 c(x, y)}{\partial x_i \partial y_j} \bigg|_{x=x^*, y=x^*};
\]

(2.1)

\[
\text{Cov} \left( g_i'(x^*), y_j(x^*) \right) = \sigma^2 \frac{\partial c(x, y)}{\partial x_i} \bigg|_{x=x^*, y=y^*}.
\]

(2.2)

With the above covariance forms, for given \( x^* \in \mathcal{X} \), we have

\[
\left( g_1'(x^*), \ldots, g_d'(x^*), g(x_1), \ldots, g(x_n) \right)^T \sim N_{d+n} \left( \mu_{d+n}, \sigma^2 \Sigma_{d+n \times d+n} \right),
\]

(2.3)

that is, the vector on the left hand side of (2.3) has the \( (d + n) \)-variate normal distribution with mean vector \( \mu_{d+n} \) and covariance matrix \( \sigma^2 \Sigma_{d+n \times d+n} \). Here

\[
\nu_{d+n}(x^*) = \left( \mu_d'(x^*)^T, \mu_n^T \right)^T,
\]

(2.4)

where \( \mu_d'(x^*) = (\partial \mu(x^*)/\partial x_1, \ldots, \partial \mu(x^*)/\partial x_d)^T \) with \( \partial \mu(x^*)/\partial x_i = \partial \mu(x)/\partial x_i \bigg|_{x=x^*} \) for \( i = 1, \ldots, d \), and \( \mu_n = (\mu(x_1), \ldots, \mu(x_n))^T \). Also,

\[
\Sigma_{d+n \times d+n}(x^*) = \begin{pmatrix} \Sigma_{11}^{d \times d}(x^*) & \Sigma_{12}^{d \times n}(x^*) \\ \Sigma_{21}^{n \times d}(x^*) & \Sigma_{22}^{n \times n}(x^*) \end{pmatrix},
\]

(2.5)

where \( \Sigma_{11}^{d \times d} \) is the \( d \)-th order correlation matrix with \( (i, j) \)-th element \( \sigma^{-2} \text{Cov} \left( g_i'(x^*), g_j'(x^*) \right) \) where the covariance term is given by (2.1), \( \Sigma_{12}^{d \times n}(x^*) \) is the \( d \times n \) matrix with \( (i, j) \)-th element \( \sigma^{-2} \text{Cov} \left( g_i'(x^*), g(x_j) \right) \), where the covariance term is of the same form as (2.2) with \( y^* \) replaced with \( x_j \), \( \Sigma_{21}^{n \times d}(x^*) \) is the transpose of \( \Sigma_{12}^{d \times n}(x^*) \), and \( \Sigma_{22}^{n \times n}(x^*) \) is the \( n \times n \) matrix with \( (i, j) \)-th element \( c(x_i, x_j) \), the correlation between \( g(x_i) \) and \( g(x_j) \). In our examples, we shall consider the squared exponential correlation function having the form

\[
c(x, y) = \exp \left( -\frac{1}{2} (x - y)^T \Lambda^{-1} (x - y) \right),
\]

(2.6)

for \( x, y \in \mathcal{X} \), where \( \Lambda \) is a \( d \times d \) diagonal matrix with positive diagonal elements \( \lambda_i; i = 1, \ldots, d \). It follows that \( \Sigma_{11} = \Lambda^{-1} \) and for \( j = 1, \ldots, n \), the \( j \)-th column of \( \Sigma_{12}(x^*) \) is \(-\Lambda^{-1}(x^* - x_j)c(x^*, x_j)\).
2.6 Posterior distribution of the Gaussian derivatives given the data and parameters

From (2.3) it follows that the joint posterior distribution of \( g'(x^*) = (g'_1(x^*), \ldots, g'_d(x^*))^T \) given \( x^* \), \( D_n \), and other parameters \( \theta \), is the following \( d \)-variate normal distribution:

\[
\pi \left( g'(x^*) | \sigma^2, \theta, D_n \right) \equiv N_d \left( \bar{\mu}(x^*), \sigma^2 \bar{\Sigma}(x^*) \right),
\]

(2.7)

where

\[
\bar{\mu}(x^*) = \mu'(x^*) + \Sigma_{12}(x^*) \Sigma_{22}^{-1} (f_n - \mu_n);
\]

(2.8)

\[
\bar{\Sigma}(x^*) = \Sigma_{11}(x^*) - \Sigma_{12}(x^*) \Sigma_{22}^{-1} \Sigma_{21}(x^*).
\]

(2.9)

2.7 Prior and posterior distributions of the parameters

In our examples we assume that \( \mu(x) = h(x)^T \beta \), where \( h(x)^T = (1, x_1, \ldots, x_d) \) and \( \beta = (\beta_0, \beta_1, \ldots, \beta_d)^T \in \mathbb{R}^d \). Let \( H_{d \times d + 1} = (h(x_1), \ldots, h(x_n))^T \).

2.7.1 Priors for the parameters

We assume that a priori

\[
\pi(\beta | \sigma^2) \equiv N_{d+1} \left( \beta_0, \sigma^2 \Sigma_0 \right),
\]

(2.10)

where \( \beta_0 \) is the mean vector and \( \Sigma_0 \) is the positive definite covariance matrix, and

\[
\pi \left( \sigma^{-2} \right) \equiv \mathcal{G}(a, b),
\]

(2.11)

the gamma distribution with mean \( a/b \) and variance \( a/b^2 \), where \( a, b > 0 \).

2.7.2 Posteriors for the parameters

Let us first obtain the posterior distribution of \( \sigma^{-2} \) given \( D_n \). Note that

\[
\pi(\sigma^{-2} | D_n) \propto \pi(\sigma^{-2}) \pi(g_n | \sigma^{-2}) = \pi(\sigma^{-2}) \int \pi(g_n | \sigma^{-2}, \beta) \pi(\beta | \sigma^2) \, d\beta.
\]

(2.12)

To obtain \( \pi(g_n | \sigma^{-2}, \beta) = \int \pi(g_n | \sigma^{-2}, \beta) \pi(\beta | \sigma^2) \, d\beta \) note that

\[
\pi(g_n | \sigma^{-2}, \beta) \equiv N_n \left( H\beta, \sigma^2 \Sigma_{22} \right)
\]

(2.13)

and since \( \pi(\beta | \sigma^2) \) has the normal distribution (2.10), it follows that

\[
\pi(g_n | \sigma^{-2}) \equiv N_n \left( H\beta_0, \sigma^2 \left( H\Sigma_0 H^T + \Sigma_{22} \right) \right).
\]

(2.14)

Combining (2.14) with (2.12) and (2.11) it follows that

\[
\pi(\sigma^{-2} | D_n) \equiv \mathcal{G} \left( a + \frac{d}{2}, b + \frac{1}{2} \left( f_n - H\beta_0 \right)^T \left( H\Sigma_0 H^T + \Sigma_{22} \right)^{-1} \left( f_n - H\beta_0 \right) \right).
\]

(2.15)

Also, combining (2.13) and (2.10) it is easy to see that

\[
\pi(\beta | D_n, \sigma^2) \equiv N_{d+1} \left( \left( H^T \Sigma_{22}^{-1} H + \Sigma_0^{-1} \right)^{-1} \left( H^T \Sigma_{22}^{-1} f_n + \Sigma_0^{-1} \beta_0 \right), \sigma^2 \left( H^T \Sigma_{22}^{-1} H + \Sigma_0^{-1} \right)^{-1} \right).
\]

(2.16)
2.8 Marginal posterior distribution of the derivative process

Now, from (2.7) it follows that

\[
\pi \left( g'(x^*) | \sigma^2, \beta, D_n \right) \equiv N_d \left( A\beta + \Sigma_{12}(x^*) \Sigma_{22}^{-1} (f_n - H\beta), \sigma^2 \bar{\Sigma}(x^*) \right),
\]

where \( A^{d \times d+1} = (0^{d \times 1} \, \mathbb{I}_d) \). Here \( 0^{d \times 1} \) is the \( d \)-dimensional null vector and \( \mathbb{I}_d \) is the identity matrix of order \( d \). Integrating (2.17) with respect to (2.16) we obtain

\[
\pi \left( g'(x^*) | \sigma^2, D_n \right) \equiv N_d \left( \hat{\mu}'(x^*), \sigma^2 \bar{\Sigma}(x^*) \right),
\]

where \( \hat{\mu}'(x^*) \) and \( \bar{\Sigma}(x^*) \) are given by

\[
\hat{\mu}'(x^*) = A\beta + \Sigma_{12}(x^*) \Sigma_{22}^{-1} (f_n - H\beta);
\]

\[
\bar{\Sigma}(x^*) = \bar{\Sigma}(x^*) + (A - \Sigma_{12}(x^*) \Sigma_{22}^{-1} H) (H^T \Sigma_{22}^{-1} H + \Sigma_0^{-1})^{-1} (A - \Sigma_{12}(x^*) \Sigma_{22}^{-1} H)^T,
\]

with

\[
\hat{\beta} = (H^T \Sigma_{22}^{-1} H + \Sigma_0^{-1})^{-1} (H^T \Sigma_{22}^{-1} f_n + \Sigma_0^{-1} \beta_0).
\]

Integrating (2.18) with respect to (2.15) we obtain

\[
\pi \left( g'(x^*) | D_n \right) \equiv t_d \left( \hat{\mu}'(x^*), \frac{a + \frac{d}{2}}{b + \frac{1}{2} (f_n - H\beta_0)^T (H \Sigma_0 H^T + \Sigma_{22})^{-1} (f_n - H\beta_0)} \right),
\]

where for any \( d \)-dimensional vector \( \mu, d \)-th order covariance matrix \( \Sigma \), and \( \alpha > 0 \), \( t_d (\mu, \Sigma^{-1}, \alpha) \) is a \( d \)-variate Student’s \( t \) distribution with density at \( x \in \mathbb{R}^d \) given by

\[
t_d (x : \mu, \Sigma^{-1}, \alpha) = C \left[ 1 + \alpha^{-1} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]^{-(\alpha + d) / 2},
\]

where

\[
C = \frac{\Gamma \left( \frac{\alpha + d}{2} \right)}{\Gamma \left( \frac{\alpha}{2} \right)} (\alpha \pi)^{\frac{d}{2}},
\]

with \( \Gamma(\cdot) \) denoting the gamma function.

3 Posterior distribution of random optima corresponding to the posterior derivative process

From (2.22) we obtain the following posterior density at \( g'(x^*) = 0 \):

\[
\pi \left( g'(x^*) = 0 | D_n \right) \propto \left[ 1 + \frac{\hat{\mu}'(x^*)^T \bar{\Sigma}(x^*)^{-1} \hat{\mu}'(x^*)}{2b + (f_n - H\beta_0)^T (H \Sigma_0 H^T + \Sigma_{22})^{-1} (f_n - H\beta_0)} \right]^{-(\alpha + d)}.
\]

Now, with prior \( \pi(x^*) \) on \( x^* \), the posterior of \( x^* \), given \( g'(x^*) \) and \( D_n \) can be obtained as follows:

\[
\pi(x^* | g'(x^*), D_n) \propto \pi(x^*) \pi(g'(x^*), g_n | x^*)
\]

\[
= \pi(x^*) \pi(g'(x^*) | D_n, x^*) \pi(g_n | x^*)
\]

\[
= \pi(x^*) \pi(g'(x^*) | D_n, x^*) \pi(g_n)
\]

\[
\propto \pi(x^*) \pi(g'(x^*) | D_n, x^*).
\]

(3.2)
In the second step of (3.2), \( \pi(g_n | x^*) \) is the marginal distribution of \( g_n \), integrated over the parameters. Since this does not depend upon \( x^* \), we denoted this as \( \pi(g) \) in the third step of (3.2). From (3.2) it then follows that

\[
\pi(x^*|g'(x^*) = 0, D_n) \propto \pi(x^*) \pi(g'(x^*) = 0 | D_n, x^*). \quad (3.3)
\]

Now, \( \pi(g'(x^*) = 0 | D_n, x^*) \) will also depend upon parameters of the covariance function, which will be unknown generally. It is legitimate to estimate them using the maximum likelihood estimation method (see, for example, Santner et al. (2003)) and treat them as fixed.

The formula (3.3) holds for any prior \( \pi(x^*) \) for \( x^* \). However, we shall consider a uniform prior on \( \mathcal{X} \) constrained by the first and second derivatives of \( f(\cdot) \). The details are presented below.

### 3.1 Prior for \( x^* \)

Without loss of generality, let us assume that our objective is to obtain the minima of the function \( f(\cdot) \) on \( \mathcal{X} \). For \( i, j = 1, \ldots, d \), let \( f''_{ij}(x^*) = \left. \frac{\partial^2 f(x)}{\partial x_i \partial x_j} \right|_{x=x^*} \) denote the second order partial derivatives of the objective function \( f(\cdot) \) at any \( x^* \in \mathcal{X} \). Let \( \Sigma''(x^*) \) stand for the \( d \times d \) matrix of such second order partial derivatives at \( x^* \) with \( (i,j) \)-th element \( f''_{ij}(x^*) \). Let \( \Sigma''(x^*) > 0 \) denote that \( \Sigma''(x^*) \) is positive definite. Then we consider the following prior for \( x^* \):

\[
\pi(x^*) \propto I_B(\epsilon)(x^*), \quad (3.4)
\]

where, for any set \( A \) and vector \( x \), \( I_A(x) = 1 \) if \( x \in A \) and zero otherwise. Also, for any \( x \) and \( \epsilon > 0 \),

\[
B(\epsilon) = \mathcal{X} \cap \left\{ x : \| f'(x) \|_d < \epsilon \right\} \cap \left\{ x : \Sigma''(x) > 0 \right\}, \quad (3.5)
\]

where \( \| \cdot \|_d \) denotes the Euclidean norm in the \( d \)-dimensional Euclidean space.

### 4 Almost sure uniform convergence of posterior Gaussian and Gaussian derivative processes

Consider the joint posterior distribution of

\[
\pi(g(\cdot), g'(\cdot)|D_n) = \pi(g(\cdot)|D_n) \pi(g'(\cdot)|g(\cdot), D_n). \quad (4.1)
\]

Then the marginal posterior \( \pi(g'(\cdot)|D_n) \) is of the same form as (2.22), and the marginal posterior distribution \( \pi(g(\cdot)|D_n) \) in (4.1) corresponds to the \( t_1 \) process, the form of which is not relevant for our purpose.

For \( n \geq 1 \), let \( X_n \) denote the \( n \) input points in \( D_n \). Note that even after marginalizing out the parameters of the Gaussian process with respect to their posteriors (here \( \beta \) and \( \sigma^2 \)), the interpolation property of \( g(\cdot) \) given \( D_n \) is preserved. That is, the marginal posterior \( \pi(g(x^*)|D_n) \) gives full posterior mass to \( f(x^*) \) if \( x^* \in X_n \).

Let \( g_n(\cdot) \) denote any random function associated with any non-null set of the marginalized posterior measure of \( g(\cdot) \) given \( D_n \) (here, the \( t_1 \) posterior measure). Also, let \( g'_n(\cdot) \) denote any \( d \)-dimensional random function associated with any non-null set of the marginalized posterior measure of \( g'(\cdot) \) given \( D_n \), the form of which is provided explicitly by (2.22). Theorems 2, 3, 4 and 5 prove almost sure uniform convergence of \( g_n(\cdot) \) and \( g'_n(\cdot) \) to \( f(\cdot) \) and \( f'(\cdot) \) respectively, as \( n \to \infty \). In particular, Theorems 4 and 5 also provide rates of such convergences. Before introducing the theorems, we first state and prove a lemma that will aid in proving the theorems.

**Lemma 1** Consider a sequence of real-valued continuous functions \( \{ f_n \}_{n=1}^{\infty} \) on any compact set \( \mathcal{X} \)
such that \( f_n(x) \to f(x) \) for all \( x \in \mathcal{X} \), where \( f \) is some real-valued continuous function on \( \mathcal{X} \). Then

\[
\lim_{n \to \infty} \sup_{x \in \mathcal{X}} |f_n(x)| < \infty.
\]

**Proof.** Note that \( f_n \), for \( n \geq 1 \), and \( f \) are actually uniformly continuous since \( \mathcal{X} \) is compact. Now let us first consider an arbitrary \( x_1 \in \mathcal{X} \). Then due to pointwise convergence of \( f_n \) to \( f \), for any \( \epsilon > 0 \), there exists \( n_1 \geq 1 \) such that for \( n \geq n_1 \), \( |f_n(x_1) - f(x_1)| < \epsilon \). Moreover, due to uniform continuity of \( f_n \) and \( f \), there exists an open neighborhood \( \mathcal{N}(x_1) \) of \( x_1 \) such that \( |f_n(x) - f(x)| < \epsilon_1 \) for all \( x \in \mathcal{N}(x_1) \), where \( \epsilon_1 \) is some positive finite constant. Since \( f \) is continuous on the compact set \( \mathcal{X} \), it is uniformly bounded. Hence, \( \sup_{x \in \mathcal{N}(x_1)} |f_n(x)| < M_1 \) for all \( n \geq n_1 \), where \( M_1 \) is some positive finite constant.

Now consider another point \( x_2 \in \mathcal{X} \setminus \mathcal{N}(x_1) \). Then similar argument shows that \( \sup_{x \in \mathcal{N}(x_2)} |f_n(x)| < M_2 \) for all \( n \geq n_2 \geq n_1 \), where \( \mathcal{N}(x_2) \) is some appropriate open neighborhood of \( x_2 \) and \( M_2 \) is some positive finite constant.

Thus, starting with \( \mathcal{N}(x_1) \) and the associated bound \( \sup_{x \in \mathcal{N}(x_1)} |f_n(x)| < M_1 \), continuing the procedure for \( i \geq 2 \), we can construct neighborhoods \( \mathcal{N}(x_i) \) with \( x_i \in \mathcal{X} \setminus \bigcup_{j=1}^{i-1} \mathcal{N}(x_j) \) and bounds \( M_i \) such that for all \( n \geq n_i \geq n_{i-1} \geq \cdots \geq n_2 \geq n_1 \), \( \sup_{x \in \mathcal{N}(x_i)} |f_n(x)| < M_i \). Note that \( \mathcal{X} \subseteq \bigcup_{i=1}^{\infty} \mathcal{N}(x_i) \). That is, the set of neighborhoods \( \{ \mathcal{N}(x_i) : i = 1, 2, \ldots \} \) constitutes an open cover for \( \mathcal{X} \). Since \( \mathcal{X} \) is compact, there exists a finite sub-cover for \( \mathcal{X} \), say, \( \{ \mathcal{N}(x_i) : j = 1, 2, \ldots, K \} \), where \( K \) is finite. Now, by our construction, for \( n \geq n_j \), \( \sup_{x \in \mathcal{N}(x_j)} |f_n(x)| < M_j \), for \( j = 1, \ldots, K \). Let \( n_0 = \max\{n_{ij} : j = 1, \ldots, K\} \) and \( M = \max\{M_j : j = 1, \ldots, K\} \). Then for all \( n \geq n_0 \), \( \sup_{x \in \mathcal{X}} |f_n(x)| < M < \infty \). ■

**Theorem 2** Consider a fixed-domain infill asymptotics framework such that for any \( x \in \mathcal{X} \), there exists \( x_n \in \mathcal{X}_n \) for \( n \geq 1 \) satisfying

\[
\lim_{n \to \infty} \|x_n - x\|_d = 0.
\]

Also assume that points of the form \( x_n + h_n \in \mathcal{X}_n \), where \( h_n \to 0 \), as \( n \to \infty \).

For \( x = (x_1, \ldots, x_d) \) and \( y = (y_1, \ldots, y_d) \), let the correlation function be such that

\[
\frac{\partial^2 c(x^*, y^*)}{\partial x_i \partial y_i} = \frac{\partial^2 c(x, y)}{\partial x_i \partial y_i} \bigg|_{x=x^*, y=y^*}
\]

exists for all \( x^*, y^* \in \mathcal{X} \) and is Lipschitz continuous on \( \mathcal{X} \times \mathcal{X} \) for \( i = 1, \ldots, d \). Then, for almost all sequences \( \{g_n(\cdot)\}_{n=1}^{\infty} \)

\[
\sup_{x \in \mathcal{X}} |g_n(x) - f(x)| \to 0, \text{ as } n \to \infty.
\]

**Proof.** Consider any \( x \in \mathcal{X} \). Then there exists \( x_n \in \mathcal{X}_n \) for \( n \geq 1 \) satisfying (4.2). Now by Taylor’s series expansion up to the first order,

\[
g_n(x_n) = g_n(x) + (x_n - x)^T g_n'(c_n),
\]

where \( c_n \) lies on the line joining \( x \) and \( x_n - x \).

Now, for \( i = 1, \ldots, d \), consider the \( i \)-th partial derivative \( g_{in}(\cdot) \) of \( g_n(\cdot) \). With any sequence \( h_{in} \to 0 \) as \( n \to \infty \), we have

\[
\frac{g_n(x_{i1}, \ldots, x_{i-1,n}, x_{in} + h_{in}, x_{i+1,n}, \ldots, x_{dn}) - g_n(x_n)}{h_{in}} = g_{in}'(x_{in}^*),
\]

(4.5)
where \( x^*_n = (x_{1n}, \ldots, x_{i-1,n}, x^*_n, x_{i+1,n}, \ldots, x_{dn}) \); here \( x^*_n \) lies between \( x_{in} \) and \( x_{in} + h_{in} \). Since \((x_{1n}, \ldots, x_{i-1,n}, x_{in} + h_{in}, x_{i+1,n}, \ldots, x_{dn})^T \in X_n \) and \( x_n \in X_n \), \( g_n(x_{1n}, \ldots, x_{i-1,n}, x_{in} + h_{in}, x_{i+1,n}, \ldots, x_{dn}) = f(x_{1n}, \ldots, x_{i-1,n}, x_{in} + h_{in}, x_{i+1,n}, \ldots, x_{dn}) \) and \( g_n(x_n) = f(x_n) \), almost surely. Hence, from (4.5) it follows that

\[
g'_{in}(x^*_n) = f'_i(z_n), \text{ almost surely,} \tag{4.6}
\]

with \( z_n = (x_{1n}, \ldots, x_{i-1,n}, x_{in}, x_{i+1,n}, \ldots, x_{dn}) \), where \( z_{in} \) lies between \( x_{in} \) and \( x_{in} + h_{in} \). Clearly, \( z_n \to x \), as \( n \to \infty \). Hence, taking limits of both sides of (4.6) as \( n \to \infty \), and using continuity of \( f'_i(\cdot) \), yields

\[
\lim_{n \to \infty} g'_{in}(x^*_n) = f'_i(x), \text{ almost surely.} \tag{4.7}
\]

Now, by the hypothesis of Lipschitz continuity of the second order mixed partial derivatives of the correlation function ensures existence and sample path continuity of the partial derivatives \( g'_{in}(\cdot) \), for \( i = 1, \ldots, d \), for any \( n \geq 1 \). Since \( X \) is compact, \( g'_{in}(\cdot) \) are uniformly continuous on \( X \), for \( i = 1, \ldots, d \), for any \( n \geq 1 \). Uniform continuity of \( g'_{in}(\cdot) \) for all \( n \geq 1 \) implies that for any \( \epsilon > 0 \),

\[
|g'_{in}(x^*_n) - g'_{in}(x)| < \epsilon, \quad \text{whenever } \|x^*_n - x\|_d < \delta, \quad \text{where } \delta (> 0) \text{ depends upon } \epsilon \text{ only.}
\]

Now, since \( x^*_n \to x \) as \( n \to \infty \), there exists \( n_0 (\geq 1) \) depending upon \( \delta \) such that \( \|x^*_n - x\|_d < \delta \) for \( n \geq n_0 \). Further, using (4.7) we obtain for any \( x \in X \), the following:

\[
\lim_{n \to \infty} g'_{in}(x) = \lim_{n \to \infty} g'_{in}(x^*_n) + \lim_{n \to \infty} (g'_{in}(x) - g'_{in}(x^*_n)) = f'_i(x), \text{ almost surely.} \tag{4.8}
\]

That is, \( g'_{in}(\cdot) \) converges pointwise to \( f'_i(\cdot) \) almost surely, as \( n \to \infty \). Moreover, \( g'_{in}(\cdot) \) is almost surely continuous on \( X \) for all \( n \geq 1 \) and \( f'_i(\cdot) \) is continuous on \( X \). Since \( X \) is compact, we invoke Lemma 1 to conclude that there exists a positive, finite constant \( M \) depending upon \( f'_i(\cdot); i = 1, \ldots, d \) such that

\[
\lim_{n \to \infty} \sup_{x \in X} |g'_{in}(x)| < M, \text{ almost surely, for } i = 1, \ldots, d. \tag{4.9}
\]

Hence, using the Cauchy-Schwartz inequality in (4.4), boundedness of the partial derivatives \( g'_{in}(\cdot) \) for \( i = 1, \ldots, d \) for large enough \( n \) and (4.2), we obtain

\[
|g_n(x_n) - g_n(x)| = |(x_n - x)^T g'_n(c_n)| \leq \|x_n - x\|_d \times \|g'_n(c_n)\|_d \to 0, \text{ as } n \to \infty. \tag{4.10}
\]

Hence, using (4.10) and continuity of \( f(\cdot) \) we obtain, for any \( x \in X \),

\[
\lim_{n \to \infty} g_n(x) = \lim_{n \to \infty} g_n(x_n) = \lim_{n \to \infty} f(x_n) = f(\lim_{n \to \infty} x_n) = f(x), \tag{4.11}
\]

proving pointwise convergence of \( g_n(\cdot) \) to \( f(\cdot) \).

Thus, we have shown that \( g_n(\cdot) \) converges pointwise to \( f(\cdot) \) on \( X \) almost surely, as \( n \to \infty \) (equation (4.11)), and also that the partial derivatives of \( g_n(\cdot) \) are uniformly bounded in the limit almost surely (equation (4.9)). The latter also implies that \( g_n(\cdot) \) is almost surely Lipschitz continuous on \( X \). Since \( X \) is compact, by the stochastic Ascoli lemma (see, for example, Billingsley (2013)), it follows that (4.3) holds.

**Theorem 3** Consider a fixed-domain infill asymptotics framework such that for any \( x \in X \), there exists \( x_n \in X_n \) for \( n \geq 1 \) satisfying (4.2) and that points of the form \( x_n + h_n \in X_n \), where \( h_n \to 0 \), as \( n \to \infty \).

For \( x = (x_1, \ldots, x_d) \) and \( y = (y_1, \ldots, y_d) \), let the correlation function be such that

\[
\frac{\partial^4 c(x^*, y^*)}{\partial x_i \partial y_i \partial x_j \partial y_j} = \frac{\partial^4 c(x, y)}{\partial x_i \partial y_i \partial x_j \partial y_j} \bigg|_{x \to x^*, y \to y^*},
\]

exists for all \( x^*, y^* \in X \) and is Lipschitz continuous on \( X \times X \) for \( i, j = 1, \ldots, d \).
Then, for almost all sequences \( \{ g_n'() \}_{n=1}^{\infty} \),

\[
\sup_{x \in \mathcal{X}} \| g_n'(x) - f'(x) \|_d \to 0, \text{ as } n \to \infty. \tag{4.12}
\]

**Proof.** Note that for \( i = 1, \ldots, d \), pointwise convergence of \( g_n'(\cdot) \) to \( f'(\cdot) \) as \( n \to \infty \), is already shown by (4.8), in the proof of Theorem 2. Hence, if we can show that for \( i, j = 1, \ldots, d \), the second order partial derivatives \( g_n''(\cdot) \) are uniformly bounded on \( \mathcal{X} \) as \( n \to \infty \), then this would imply that \( g_n''(\cdot) \) are almost surely Lipschitz continuous on \( \mathcal{X} \) for large enough \( n \). Since \( \mathcal{X} \) is compact, this would then imply by the stochastic Ascoli result that \( \sup_{x \in \mathcal{X}} | g_n''(x) - f''(x) | \to 0 \), almost surely, as \( n \to \infty \), for \( i = 1, \ldots, d \), which is equivalent to (4.12). Hence, in the rest of the proof, we show that \( \lim_{n \to \infty} \sup_{x \in \mathcal{X}} | g_n''(x) | < \infty \).

As before, let us fix any \( x \in \mathcal{X} \). Hence, by hypothesis, there exists \( x_n \in X_n \) for \( n \geq 1 \), such that \( x_n \to x \) as \( n \to \infty \). Also let \( h_n \to 0 \), as \( n \to \infty \). Using Taylor’s series expansion of \( g_n(x_n + h_n) \) up to the second order we obtain

\[
g_n(x_n + h_n) = g_n(x_n) + h_n g_n'(x_n) + \frac{h_n^2}{2} g_n''(x_n^*) h_n, \tag{4.13}
\]

where \( x_n^* \) lies on the line joining \( x_n \) and \( x_n + h_n \). Existence and sample path continuity of the second order partial derivatives \( g_n''(\cdot) \) for \( i, j = 1, \ldots, d \), which constitute the elements of the matrix \( g_n''(\cdot) \), are guaranteed by the hypothesis of existence and Lipschitz continuity of \( \frac{\partial^2 \phi(x, y)}{\partial x \partial y} \).

Now, given \( i \in \{1, \ldots, d\} \), let \( h_{in} \) denote the vector with \( h_n \) at the \( i \)-th co-ordinate and 0 at the remaining co-ordinates. Then (4.13) reduces to

\[
g_n(x_n + h_{in}) = g_n(x_n) + h_n g_n'(x_n) + \frac{h_n^2}{2} g_n''(x_{i1n}^*), \tag{4.14}
\]

where \( x_{i1n}^* \) lies on the line joining \( x_n \) and \( x_n + h_{in} \). Similar arguments also yield

\[
g_n(x_n - h_{in}) = g_n(x_n) - h_n g_n'(x_n) + \frac{h_n^2}{2} g_n''(x_{i2n}^*), \tag{4.15}
\]

where \( x_{i2n}^* \) lies on the line joining \( x_n - h_{in} \) and \( x_n \). From (4.15) we obtain

\[
h_n g_n'(x_n) = g_n(x_n) - g_n(x_n - h_{in}) + \frac{h_n^2}{2} g_n''(x_{i2n}^*), \tag{4.16}
\]

which we substitute in (4.14) to obtain \( g_n(x_n + h_{in}) = 2g_n(x_n) - g_n(x_n - h_{in}) + \frac{h_n^2}{2} (g_n''(x_{i1n}^*) + g_n''(x_{i2n}^*)) \). Thus, denoting the first and second order partial derivatives of \( f(\cdot) \) by \( f_1(\cdot) \) and \( f_2(\cdot) \), we obtain, almost surely,

\[
\frac{1}{2} \left( g_n''(x_{i1n}^*) + g_n''(x_{i2n}^*) \right) = \frac{g_n(x_n + h_{in}) - 2g_n(x_n) + g_n(x_n - h_{in})}{h_n^2}
\]

\[
= \frac{f(x_n + h_{in}) - 2f(x_n) + f(x_n - h_{in})}{h_n^2}
\]

\[
= \frac{1}{2} \left( f_1''(x_{i3n}^*) + f_2''(x_{i4n}^*) \right), \tag{4.16}
\]

where \( x_{i3n}^* \) lies on the line joining \( x_n \) and \( x_n + h_{in} \) and \( x_{i4n}^* \) lies on the line joining \( x_n - h_{in} \) and \( x_n \). Now, since for \( k = 1, 2, 3, 4 \), \( x_{ikn} \to x \) as \( n \to \infty \), and since \( g_n''(\cdot) \) is continuous for all \( n \geq 1 \) and \( f_1''(\cdot) \) is also continuous, it is easy to see that for \( k = 1, 2, g_n''(x_{ikn}) \sim g_n''(x) \) and \( f_1''(x_{ikn}) \sim f_1''(x) \) for \( k = 3, 4 \), as \( n \to \infty \), where for any two sequences \( a_n \) and \( b_n \), \( a_n \sim b_n \) stands for \( a_n/b_n \to 1 \) as \( n \to \infty \). An implicit assumption in the above arguments on asymptotic equivalence is that \( f_1''(x) \neq 0 \) and \( g_n''(x) \to 0 \) almost surely, as \( n \to \infty \). Hence, taking limits of both sides of (4.16) yields, for each \( x \in \mathcal{X} \),

\[
\lim_{n \to \infty} g_n''(x) = f_1''(x) \text{ almost surely}, \tag{4.17}
\]
proving pointwise convergence of \( g''_{ij} (\cdot) \) to \( f''_{ij} (\cdot) \) almost surely as \( n \to \infty \), for each \( i = 1, \ldots, d \) when \( f''_{ii}(x) \neq 0 \) and \( g''_{ii}(x) \to 0 \) almost surely, as \( n \to \infty \). Note that if \( f''_{ii}(x) = 0 \) and \( g''_{ii}(x) \to 0 \) almost surely as \( n \to \infty \), then (4.17) holds trivially. In other words, (4.17) holds for all \( x \in \mathcal{X} \).

Now, in (4.13), let \( h_{ijn} \) be the vector with \( h_n \) at the \( i \)-th and \( j \)-th co-ordinates and zero elsewhere. Then (4.13) boils down to

\[
g_n(x_n + h_{ij}) = g_n(x_n) + h_n(g''_{in}(x_n) + g'_{jn}(x_n)) + \frac{h_n^2}{2} \left( g''_{in}(x_{ij}^*) + g''_{jn}(x_{ij}^*) + 2g''_{in}(x_{ij}^*) \right),
\]

where \( x_{ij}^* \) lies on the line joining \( x_n \) and \( x_n + h_{ij} \). Substituting \( h_n g''_{in}(x_n) = g_n(x_n) - g_n(x_n - h_{in}) + \frac{h_n^2}{2} g''_{in}(x_{in}) \) and \( h_n g''_{jn}(x_n) = g_n(x_n) - g_n(x_n - h_{jn}) + \frac{h_n^2}{2} g''_{jn}(x_{jn}) \) in (4.18), where \( x^*_i \) lies on the line joining \( x_n - h_{in} \) and \( x_n \), and \( x^*_j \) lies on the line joining \( x_n - h_{jn} \) and \( x_n \), we obtain

\[
g_n(x_n + h_{ij}) = 3g_n(x_n) - g_n(x_n - h_{in}) - g_n(x_n - h_{jn}) + \frac{h_n^2}{2} \left( g''_{in}(x_{in}) + g''_{jn}(x_{jn}) + g''_{in}(x_{in}) + g''_{jn}(x_{jn}) \right) + h_n^2 g''_{ij}(x_{ij}).
\]

Now, continuity of \( g''_{ij}(\cdot) \) for \( n \geq 1 \), continuity of \( f''_{ij}(\cdot) \), and (4.17) imply that as \( n \to \infty \), \( g''_{in}(x_{in}) \sim g''_{in}(x) \sim f''_{in}(x) \sim f''_{ij}(x) \), almost surely. Similarly, \( g''_{in}(x_{in}^*) \sim f''_{in}(x_{in}) \sim g''_{in}(x_{in}^*) \sim f''_{ij}(x_{in}) \), almost surely, as \( n \to \infty \). These, applied to (4.19), yield

\[
g''_{ij}(x_{ij}^*) = \frac{g_n(x_n + h_{ij}) - 3g_n(x_n) + g_n(x_n - h_{in}) + g_n(x_n - h_{jn})}{h_n^2} - \frac{1}{2} \left( \left[ g''_{in}(x_{in}^*) + g''_{in}(x_{ij}) \right] + \left( g''_{jn}(x_{in}^*) + g''_{jn}(x_{ij}) \right) \right)
\]

\[
\quad = \frac{f(x_n + h_{ij}) - 3f(x_n) + f(x_n - h_{in}) + f(x_n - h_{jn})}{h_n^2} - \frac{1}{2} \left( \left[ g''_{in}(x_{in}^*) + g''_{in}(x_{ij}) \right] + \left( g''_{jn}(x_{in}^*) + g''_{jn}(x_{ij}) \right) \right)
\]

\[
\quad \sim \frac{f(x_n + h_{ij}) - 3f(x_n) + f(x_n - h_{in}) + f(x_n - h_{jn})}{h_n^2} - \left( f''_{ii}(x_n) + f''_{ij}(x_n) \right),
\]

almost surely, as \( n \to \infty \). Again, implicit in (4.21) is the assumption that \( f''_{ii}(x) \neq 0 \), \( f''_{ij}(x) \neq 0 \), \( g''_{in}(x) \to 0 \) and \( g''_{jn}(x) \to 0 \) almost surely, as \( n \to \infty \). However, if either or both of \( f''_{ii}(x) = 0 \) and \( g''_{in}(x) \to 0 \) and \( f''_{ij}(x) = 0 \) and \( g''_{jn}(x) \to 0 \), then the relevant expressions in (4.20) and (4.21) converge to zero almost surely, as \( n \to \infty \). Hence, the above asymptotic equivalence for \( g''_{ij}(x_{ij}) \) remains valid for all \( x \in \mathcal{X} \).

Taylor’s series expansion of \( f(x_n + h_{ij}) \) in the same way as (4.18), where \( x_{ij}^* \) must be replaced with some \( x_{ij}^{**} \) lying on the line joining \( x_n \) and \( x_n + h_{ij} \), yields the same asymptotic expression (4.21) for \( f''_{ij}(x_{ij}^{**}) \). In other words, we have

\[
g''_{ij}(x_{ij}^{**}) \sim f''_{ij}(x_{ij}^{**}), \quad \text{almost surely, as } n \to \infty.
\]

Hence, taking limit of both sides of (4.22), using continuity of \( g''_{ij}(\cdot) \) for \( n \geq 1 \) and continuity of \( f''_{ij}(\cdot) \) gives

\[
\lim_{n \to \infty} g''_{ij}(x) = f''_{ij}(x), \quad \text{almost surely, for all } x \in \mathcal{X},
\]

(4.23)

Since \( g''_{ij}(\cdot) \) is almost surely continuous for all \( n \geq 1 \) and \( f''_{ij}(\cdot) \) is continuous, with \( \mathcal{X} \) being compact, the pointwise convergence result (4.23) lets us conclude, using Lemma 1, that \( \lim_{n \to \infty} \sup_{x \in \mathcal{X}} |g''_{ij}(x) - f''_{ij}(x)| < \infty \).

Theorems 2 and 3 prove almost sure uniform convergence of \( g_n(\cdot) \) and \( g'_n(\cdot) \) to \( f(\cdot) \) and \( f'(\cdot) \), respectively.
respectively. However, the rates of convergence are not provided by these theorems. Further fine-tuning the structure of the set of input points $X_n$ helps achieve desired rates of convergence, as we show next in Theorems 4 and 5.

**Theorem 4** Let $X = \prod_{i=1}^{d} X_i$, where, for $i = 1, \ldots, d$, $X_i$ are compact subsets of $\mathbb{R}$. For each $i \in \{1, \ldots, d\}$, let $x_{i,j} < x_{2i} < \cdots < x_{n_i}$ be an ordered set of points partitioning $X_i$, with $h_i = \max_{1 \leq j \leq n_i - 1} (x_{j+1} - x_{ji})$. For $i = 1, \ldots, d$, and for $j = 1, \ldots, n_i$, let input points of the form $(x_1^*, \ldots, x_{i-1}^*, x_{i,j}^*, x_{i+1}^*, \ldots, x_d^*) \in \prod_{j \neq i} X_j$ may be arbitrary.

For $x = (x_1, \ldots, x_d)$ and $y = (y_1, \ldots, y_d)$, let the correlation function be such that

$$\frac{\partial^4 c(x^*, y^*)}{\partial x_i \partial y_i \partial x_j \partial y_j} \bigg|_{x = x^*, y = y^*}$$

exists for all $x^*, y^* \in X$ and is Lipschitz continuous on $X \times X$ for $i, j = 1, \ldots, d$.

Then, letting $h = \max_{1 \leq i \leq d} h_i$, the following holds for almost all sequences $\{g_n'(\cdot)\}_{n=1}^{\infty}$ with the above forms of the input points:

$$\sup_{x \in X} \|g_n'(x) - f'(x)\|_d = O \left(\sqrt{h}\right), \text{ as } n \to \infty. \quad (4.24)$$

The constant associated with $O \left(\sqrt{h}\right)$ depends only upon $d$ and $f(\cdot)$.

**Proof.** For any $i \in \{1, \ldots, d\}$, and for arbitrary $X^*_{-i} = (x_1^*, \ldots, x_{i-1}^*, x_{i+1}^*, \ldots, x_d^*) \in \prod_{j \neq i} X_j$, for any $x \in X_i$, let

$$g_{in}(x|X^*_{-i}) = g_{n}(x_1^*, \ldots, x_{i-1}^*, x, x_{i+1}^*, \ldots, x_d^*); \quad (4.25)$$

$$f_{i}(x|X^*_{-i}) = f(x_1^*, \ldots, x_{i-1}^*, x, x_{i+1}^*, \ldots, x_d^*). \quad (4.26)$$

Since $x \in X_i$, it must belong to some interval of the form $[x_{ji}, x_{j+1}^*]$, for some $j \in \{1, 2, \ldots, n_i - 1\}$. Let us fix that $j$. For $y = x_{ji}$ and $y = x_{j+1}$, $g_{in}(y|X^*_{-i}) = f_{i}(y|X^*_{-i})$ by interpolation property of the posterior Gaussian process, assuming that $(x_1^*, \ldots, x_{i-1}^*, y, x_{i+1}^*, \ldots, x_d^*) \in X_n$ for $y = x_{ji}$ and $y = x_{j+1}$. That is, $g_{i}(y|X^*_{-i}) - f_{i}(y|X^*_{-i}) = 0$ for $y = x_{ji}$ and $y = x_{j+1}$. Hence, by Rolle’s theorem, $g_{in}'(y|X^*_{-i}) - f_{i}'(y|X^*_{-i}) = 0$, for some $u \in (x_{ji}, x_{j+1})$. This permits the following representation:

$$g_{in}'(y|X^*_{-i}) - f_{i}'(y|X^*_{-i}) = \int_u (g_{in}'(v|X^*_{-i}) - f_{i}'(v|X^*_{-i})) \, dv, \quad (4.27)$$

The hypothesis of Lipschitz continuity of the 4-th order mixed partial derivatives of the correlation function ensures existence and sample path continuity of $g_{in}'(v|X^*_{-i})$. Hence, by the Cauchy-Schwartz inequality we obtain from (4.27), the following:

$$|g_{in}'(y|X^*_{-i}) - f_{i}'(y|X^*_{-i})|$$

$$\leq \left[ \int_u (g_{in}''(v|X^*_{-i}) - f_{i}''(v|X^*_{-i}))^2 \, dv \right]^{1/2} \times |x - u|^{1/2}$$

$$\leq \left[ \int_{X_i} (g_{in}''(v|X^*_{-i}) - f_{i}''(v|X^*_{-i}))^2 \, dv \right]^{1/2} \times h_i^{1/2}$$

$$\leq \sup_{X^*_{-i} \in \prod_{j \neq i} X_j} \int_{X_i} (g_{in}'(v|X^*_{-i}) - f_{i}'(v|X^*_{-i})) \, dv \right]^{1/2} \times h^{1/2}. \quad (4.28)$$

Now, since the hypotheses of this theorem constitute a special case of Theorem 3, the result of almost sure uniform boundedness of $|g_{in}'(\cdot)|$ as $n \to \infty$, is valid here. Specifically, from the proof of Theorem
3 in this case it holds that \( \lim_{n \to \infty} \sup_{(u, X^*_i) \in \mathcal{X}} |g''_n(u|X^*_i)| < \infty \). This, along with continuity of \( f''_i(v|X^*_i) \) and compactness of \( \mathcal{X} \), shows that (4.28) is \( O(\sqrt{h}) \). Hence, switching to our usual notation, it follows that

\[
\sup_{x \in \mathcal{X}} (g'_n(x) - f'_i(x))^2 = O(h), \quad \text{almost surely, as } n \to \infty. 
\] (4.29)

Since \( \sup_{x \in \mathcal{X}} \sum_{i=1}^d (g'_n(x) - f'_i(x))^2 \leq \sum_{i=1}^d \sup_{x \in \mathcal{X}} (g'_n(x) - f'_i(x))^2 \), it follows from (4.29) that

\[
\sup_{x \in \mathcal{X}} \|g'_n(x) - f'(x)\|_d = O(\sqrt{h}), \quad \text{almost surely, as } n \to \infty,
\]

proving (4.24). Note that the constant associated with \( O(\sqrt{h}) \) above depends only upon \( d \) and \( f \).

The following result holds as a consequence of Theorem 4.

**Theorem 5** Under the conditions of Theorem 4, the following holds with the forms of the input points as specified in Theorem 4: for almost all sequences \( \{g_n(\cdot)\}_{n=1}^\infty \),

\[
\sup_{x \in \mathcal{X}} |g_n(x) - f(x)| = O(h^{3/2}), \quad \text{as } n \to \infty. 
\] (4.30)

The constant associated with \( O(h^{3/2}) \) depends only upon \( d \) and \( f \).

**Proof.** As in the proof of Theorem 4, for any \( x \in \mathcal{X}_i \), it must belong to some interval of the form \([x_{ji}, x_{j+1}]\), for some \( j \in \{1, 2, \ldots, \tilde{n}_i - 1\} \). Let us fix that \( j \). Now, \( g_n(x_{ji}|X^*_i) = f_i(x_{ji}|X^*_i) \) almost surely, by interpolation property of the posterior process \( g_n(\cdot) \), assuming that \((x^*_1, \ldots, x^*_j, x_{ji}, x^*_{j+1}, \ldots, x^*_d) \in X_n \). Hence,

\[
g_n(x|X^*_i) - f_i(x|X^*_i) = \int_{x_{ji}}^x \left( g'_n(v|X^*_i) - f'_i(v|X^*_i) \right) dv. 
\] (4.31)

The Cauchy-Schwartz inequality applied to (4.31) gives

\[
|g_n(x|X^*_i) - f_i(x|X^*_i)| \leq \left( \int_{x_{ji}}^x \left( g'_n(v|X^*_i) - f'_i(v|X^*_i) \right)^2 dv \right)^{1/2} \times |x-x_{ji}|^{1/2}. 
\] (4.32)

From (4.28) it follows that the integral on the right hand side of (4.32) is \( O(h) \times |x-x_{ji}| \), almost surely, as \( n \to \infty \). Recall that the constant associated with \( O(h) \times |x-x_{ji}| \) depends only upon \( d \) and \( f \). Since \( |x-x_{ji}| \) is bounded above by \( h \), it follows that the right hand side of (4.32) is \( O(h^{3/2}) \), almost surely, as \( n \to \infty \). Switching to the usual notation, it is seen that (4.30) holds.

**Remark 6** As \( h \to 0 \), \( g'(\cdot) \) uniformly converges to \( f'(\cdot) \) at the rate \( h^{1/2} \) and \( g(\cdot) \) uniformly converges to \( f(\cdot) \) at the rate \( h^{3/2} \), almost surely with respect to their posteriors.

**Remark 7** In Theorems 2, 3, 4 and 5 we have referred to the posterior (2.22), which corresponds to a linear mean structure of the Gaussian process prior and conjugate priors for \( \beta \) and \( \sigma^2 \). However, as can be seen from the proofs, both the theorems continue to hold for any mean function that has continuous second order mixed partial derivatives and any prior on the parameters, including the parameters of the correlation function such that the posteriors of the parameters are proper.

**Remark 8** The hypotheses of Theorems 4 and 5 require input points of the form \((x^*_1, \ldots, x^*_i, x_{ji}, x^*_{i+1}, \ldots, x^*_d) \) to belong to \( D_n \) for \( i = 1, \ldots, d \), and for \( j = 1, \ldots, \tilde{n}_i \), where \((x^*_1, \ldots, x^*_i, x^*_{i+1}, \ldots, x^*_{d}) \subseteq \bigcup_{j \neq i} X_j \) may be chosen arbitrarily. Now observe that if \( X_i = [a, b] \), for \( i = 1, \ldots, d \), for some \( a < b \), then we can set \( \tilde{n}_i = n \) and \( h_i = h \), for \( i = 1, \ldots, d \). In such cases, inclusion of the set of \( n^d \) points \( \{(x_{j1}, \ldots, x_{jd}) : j_1, \ldots, j_d \in \{1, \ldots, n\} \} \) in \( D_n \) is sufficient for Theorems 4 and 5 to hold. However,
when $d$ and $n$ are even moderately large, $n^d$ is an extremely large number, which would prohibit computation of $\Sigma_{22}^{-1}$, and hence computation of the posterior of $g'(\cdot)$. Hence, for practical purposes it makes sense to refer to the general setup of Theorems 2 and 3.

5 Algorithm for optimization with the Gaussian process derivative method

We now propose a general methodology for function optimization, which judiciously exploits the posterior form (3.3). Without loss of generality, we consider the minimization problem for notational convenience. In a nutshell, the initial stage (say, the 0-th stage) of the methodology involves simulations from $\pi(x^\ast|g'(x^\ast) = 0, D_n)$ satisfying $\|f'(\cdot)\|_d < \epsilon$ for some $\epsilon > 0$ and $\Sigma''(\cdot) > 0$. In the subsequent stages $k = 1, 2, \ldots$, previous stage realizations satisfying $\|f'(\cdot)\|_d < \eta_k$, where $\eta_k \to 0$ as $k \to \infty$, are successively augmented with $D_n$ and realizations from the posterior associated with the augmented data are generated at each stage $k$ by a judicious importance resampling strategy. As $k \to \infty$, the posteriors given the successively augmented data converge to the true optima.

The importance of the 0-th stage simulation algorithm for generating realizations from $\pi(x^\ast|g'(x^\ast) = 0, D_n)$ satisfying the restrictions $\|f'(\cdot)\|_d < \epsilon$ for some $\epsilon > 0$ and $\Sigma''(\cdot) > 0$, is enormous, particularly because the entire $d$-dimensional random variable $x^\ast$ must be updated in a single block to meet the restrictions. Traditional MCMC algorithms are not known to be efficient in such problems as even for moderately large dimensions good proposal distributions are difficult to devise, and the acceptance rates can be poor, along with poor mixing properties. In this regard, the transformation based Markov Chain Monte Carlo (TMCMC) proposed by Dutta and Bhattacharya (2014) is an effective methodology. Indeed, TMCMC is designed to update all (or most of) the components of the high-dimensional random variable in a single block using appropriate deterministic transformations of some single (or low-dimensional) random variable. As such, this strategy drastically reduces effective dimensionality, which is responsible for maintaining good acceptance rates in spite of high dimensions. Good mixing properties can also be ensured by judiciously choosing the relevant “move-types”, and judicious mixtures of additive and multiplicative transformations usually lead to desired mixing properties. For details on TMCMC and its properties, see Dutta and Bhattacharya (2014), Dey and Bhattacharya (2016), Dey and Bhattacharya (2017), Dey and Bhattacharya (2019). As such, we recommend TMCMC for our optimization methodology.

We provide the detailed Bayesian optimization methodology below as Algorithm 1.
Algorithm 1 Optimization with Gaussian process derivatives

(1) First simulate $N$ realizations $\{x^*_1, \ldots, x^*_N\}$ from $\pi(x^*|g'(x^*) = 0, D_n)$ given by (3.3) using TMCMC, where the prior for $x^*$ is given by (3.4) for some pre-fixed $\epsilon > 0$. This includes simulations from posteriors associated with most plausible functions $g(\cdot)$ satisfying $g'(x^*) = 0$ for $x^* \in X$, given $D_n$. That is, $\{x^*_i; \; i = 1, \ldots, N\}$, represents the set of solutions for $g'(x^*) = 0$ for functions $g(\cdot)$ that satisfy $g(x_i) = f(x_i); \; i = 1, \ldots, n$. Thanks to the prior (3.4), these solutions further satisfy $\|f'(x^*_i)\|_d < \epsilon$ and $\Sigma''(x^*_i) > 0$, for $i = 1, \ldots, N$. Note that $\Sigma''(x^*) > 0$ can be checked by computing the eigenvalues and checking if all the eigenvalues are positive. But a more efficient alternative is to check if Cholesky decomposition of $\Sigma''(x^*)$ is possible, the information of which is provided by the subroutines of the BLAS and LAPACK libraries. We exploit the latter for our implementation.

(2) For stages $k = 1, 2, 3, \ldots,$

   (i) For $i = 1, \ldots, N$, compute importance weights proportional to

   \[
   w_k(x^*_i) = \begin{cases} 
   1 & \text{if } k = 1; \\
   w_{k-1}(x^*_i) \times \frac{\pi(g'(x^*_i) = 0 | D_{n+\sum_{j=1}^{k-1} n_j} x^*_i)}{\pi(g'(x^*_i) = 0 | D_{n+\sum_{j=1}^{k-2} n_j} x^*_i)} & \text{if } k \geq 2,
   \end{cases}
   \tag{5.1}
   \]

   where $n_0 = 0$.

   (ii) Select a subsample $\{x^*_1, \ldots, x^*_M\}$ from $\{x^*_1, \ldots, x^*_N\}$ with probabilities proportional to $w_k(x^*_i); \; i = 1, \ldots, N$. Note that, as $M \to \infty$ and $N \to \infty$ such that $M/N \to 0$, $x^*_i$; $j = 1, \ldots, M$, follow the distribution $\pi(x^*|g'(x^*) = 0, D_{n+\sum_{j=1}^{k-1} n_j})$. The recursively computed importance weights $w_k(x^*_i); \; i = 1, \ldots, N$, are expected to be stable, since for $\pi(g'(x^*_i) = 0 | D_{n+\sum_{j=1}^{k-1} n_j} x^*_i)$ each stage $k$, for $i = 1, \ldots, N$, the factors $\pi(g'(x^*_i) = 0 | D_{n+\sum_{j=1}^{k-2} n_j} x^*_i)$ in (5.1) are not expected to be very different from 1 if $n_{k-1}$ is not significantly greater than zero. Note that the importance weights $w_k(x^*_i)$, for $i = 1, \ldots, N$, can be computed simultaneously on parallel processors. This, along with stability of the recursive formulation (5.1), is expected to make for an efficient computational strategy.

   (iii) For $j = 1, \ldots, M$, check if $\|f'(x^*_j)\|_d < \eta_k$, where $\eta_k \to 0$ as $k \to \infty$. If $x^*_j$ satisfies this condition, then $x^*_j$ is a realization from $\pi(x^*|g'(x^*) = 0, D_{n+\sum_{j=1}^{k-1} n_j})$, where the prior for $x^*$ is uniform on $B(\eta_k)$, the form of which is given by (3.5).

   (iv) Let $n_k \geq 0$ realizations among the $M$ realizations satisfy the condition $\|f'(x^*_j)\|_d < \eta_k$. Without loss of generality, assume that $x^*_j; \; j = 1, \ldots, n_k$ are such realizations. Compute $f(x^*_j); \; j = 1, \ldots, n_k$, and augment $(x^*_j, f(x^*_j)); \; j = 1, \ldots, n_k$, with $D_{n+\sum_{j=0}^{k-1} n_j}$ to form $D_{n+\sum_{j=0}^{k} n_j}$.

   (v) Store the realizations $\{x^*_j; \; j = 1, \ldots, n_k\}$.
5.1 Further discussion of Algorithm 1

Algorithm 1 begins by simulating from the posterior of $x^*$ satisfying $\|f'(x^*)\|_d < \epsilon$ and $\Sigma''(x^*) > 0$. In the subsequent steps $k \geq 1$, the set of realizations $\{x^*_{ij} : j = 1, \ldots, n_k\}$ generated by importance resampling further satisfy $\|f'(x^*_{ij})\|_d < \eta_k$ along with $\Sigma''(x^*_{ij}) > 0$, for $j = 1, \ldots, n_k$. The implication is that, $\epsilon$ may be chosen somewhat larger to achieve reasonably good TMCMC mixing acceptance rates. Indeed, if $n$ is not large enough, then $g'$ is not expected to be sufficiently close to $f'$, and hence for too small $\epsilon$, $\{x^* : \|f'(x^*)\|_d < \epsilon\}$ would be too small a region to contain the solutions $\{x^* : \|g'(x^*)\|_d = 0\}$, given $D_n$. This would result in poor TMCMC mixing.

Once adequate mixing with reasonable acceptance rates are achieved with relatively small $n$ and relatively large $\epsilon$, the subsequent steps increase the data size by augmenting the data with those values that satisfy $\|f'(x^*_{ij})\|_d < \eta_k$. Thus, in the subsequent steps, these data points help better approximate the region around the stationary points of $f$ by the posterior, and enables more simulations from the region $\|f'(x^*_{ij})\|_d < \eta_k$, finally leading to convergence of the solutions $\{x^* : g_k'(x^*) = 0, \Sigma''(x^*) > 0\}$ to $\{x^* : f'(x^*) = 0, \Sigma''(x^*) > 0\}$, almost surely, as $k \to \infty$, where $g_k'(\cdot)$ denotes any realization from the posterior of $g'(\cdot)$ given $D_{n+\sum_{j=0}^{k-1} n_j}$. This intuition is formalized below as Theorem 9.

**Theorem 9** Consider the setup of Theorem 3 (or more specifically, that of Theorem 4). Then, as $k \to \infty$, the set $\{x^*_{ij} : j = 1, \ldots, n_k\}$ of Algorithm 1 almost surely contains all the local minima of the objective function $f(\cdot)$, as $M \to \infty$ and $N \to \infty$ such that $M/N \to 0$.

**Proof.** Note that at stage $k$, as $M \to \infty$ and $N \to \infty$ such that $M/N \to 0$, $x^*_{ij} : j = 1, \ldots, n_k$, arise from $\pi(x^* g'(x^*) = 0, D_{n+\sum_{j=0}^{k-1} n_j})$, subject to $\|f'(x^*_{ij})\|_d < \eta_k$ and $\Sigma''(x^*_{ij}) > 0$ for $j = 1, \ldots, n_k$. These realizations are solutions of $g_k'(x^*) = 0$ and $\Sigma''(x^*) > 0$ when the data observed is $D_{n+\sum_{j=0}^{k-1} n_j}$. By Theorem 3 (or more specifically by Theorem 4), as $k \to \infty$ (equivalently, as $h \to 0$ in Theorem 4), $g_k'(\cdot)$ uniformly converges to $f'(\cdot)$ almost surely. Hence, as $k \to \infty$,

$$\{x^* : g_k'(x^*) = 0, \|f'(x^*)\|_d < \eta_k, \Sigma''(x^*) > 0\} \to \{x^* : f'(x^*) = 0, \Sigma''(x^*) > 0\},$$

(5.2)

almost surely.

Due to (5.2), as $k \to \infty$, the set $\{x^*_{ij} : j = 1, \ldots, n_k\}$ contains all the local minima of the objective function $f(\cdot)$, as $M \to \infty$ and $N \to \infty$ such that $M/N \to 0$. $\blacksquare$

**Remark 10** In step (2) (iv) of Algorithm 1 we have suggested augmentation of all realizations $(x^*_{ij}, f(x^*_{ij}))$ satisfying $\|f'(x^*_{ij})\|_d < \eta_k$ to the existing data $D_{n+\sum_{j=0}^{k-1} n_j}$. In practice, augmentation of all such realizations may enlarge the dataset to such an extent that invertibility of the resultant $\Sigma_{22}$ may be infeasible or numerically unstable, so that computation of the corresponding posterior densities of $g'(x^*_{ij}) = 0$, and hence the importance weights (5.1), may not yield reliable results. Hence in practice, as a rule of thumb, we recommend augmenting at most $5$ realizations satisfying $\|f'(x^*_{ij})\|_d < \eta_k$, which we consider in all our applications.

**Remark 11** As the stage number $k$ in step (2) of Algorithm 1 increases, $n_k$ decreases. Hence, in practice, $n_k$ will be zero after some large enough $k$. When $d$ is large, due to the curse of dimensionality, only the first few stages are expect to yield positive $n_k$.

**Remark 12** In step (1) of Algorithm 1, that is, in the TMCMC step, as well as in any stage $k$ of step (2) of the algorithm provided that $n_k$ is sufficiently large, desired credible regions of the respective posterior distributions of $x^*$ can be obtained. These quantify the uncertainty in a posteriori learning about the optima, given $\|f'(\cdot)\|_d < \epsilon$ or $\|f'(\cdot)\|_d < \eta_k$. As $k \to \infty$, the uncertainty decreases, and the credibility regions shrink to the points representing the true optima. However, as mentioned in Remark 6, in practice, particularly for large $d$, $n_k$ would be zero for most stages $k$, which would preclude computation of credible regions for most stages.
Remark 13 Note that if it is known beforehand that there is a single global minimum of \( f(\cdot) \) on \( X \), then step (2) of Algorithm 1 is not required. It is then sufficient to report \( x^*_i \), as the (approximate) minimizer of \( f(\cdot) \), where \( i^* = \min\{f(x^*_i) : i = 1, \ldots, N\} \).

6 Bayesian characterization of the number of local minima of the objective function with recursive posteriors

Steps (2) (iii) and (2) (iv) can be combined to obtain a Bayesian characterization of the number of local minima of the objective function. In this regard, for stage \( j \), let us define \( Y_j = \sum_{r=1}^{M} I_{B(\eta_j)}(x^*_r) \), where \( B(\eta_j) \) is given by (3.5). Thus, \( \{Y_j = m\} \) with probability \( p_{mj} \), for \( m = 0, 1, 2, \ldots, M \). Since \( M \to \infty \), we allow \( Y_j \) to take values on the entire set of non-negative integers. That is, we set

\[
P(Y_j = m) = p_{mj}; \quad m = 0, 1, 2, \ldots, \quad (6.1)
\]

the infinite-dimensional multinomial distribution, where \( 0 \leq p_{mj} \leq 1 \) for \( m = 0, 1, 2, \ldots \) and \( j \geq 1 \). Further, \( \sum_{m=0}^{\infty} p_{mj} = 1 \) for all \( j \geq 1 \). We assume that the true probabilities \( p_{m0} \in [0, 1]; \quad m = 0, 1, 2, \ldots, \) such that \( \sum_{m=0}^{\infty} p_{m0} = 1 \), are unknown. Indeed, if \( f(\cdot) \) has finite number of local minima, then there must exist \( \tilde{m} \geq 0 \) such that \( p_{\tilde{m}0} = 1 \) and \( p_{m0} = 0 \) for \( m \neq \tilde{m} \). For infinite number of local minima, we must have \( p_{m0} = 0 \) for any finite integer \( m \geq 0 \).

We adopt the approach of Roy and Bhattacharya (2020) based on Dirichlet process (Ferguson (1973)) to obtain the posterior distribution of the infinite set of parameters \( \{p_{mk}; \quad m = 0, 1, 2, \ldots\} \). Roy and Bhattacharya (2020) came up with the following strategy for characterizing possibly infinite number of limit points of infinite series, which we usefully employ for our current purpose, albeit with a definition of \( Y_j \) that is different from that of Roy and Bhattacharya (2020).

Let \( \mathcal{Y} = \{1, 2, \ldots\} \) and let \( B(\mathcal{Y}) \) denote the Borel \( \sigma \)-field on \( \mathcal{Y} \) (assuming every singleton of \( \mathcal{Y} \) is an open set). Let \( \mathcal{P} \) denote the set of probability measures on \( \mathcal{Y} \). Then, at the first stage,

\[
\pi(Y_1 | P_1) \equiv P_1, \quad \text{ (6.2)}
\]

where \( P_1 \in \mathcal{P} \). We assume that \( P_1 \) is the following Dirichlet process:

\[
\pi(P_1) \equiv \text{DP}(G), \quad \text{ (6.3)}
\]

where, the probability measure \( G \) is such that, for every \( j \geq 1 \),

\[
G(Y_j = m) = \frac{1}{2^m}. \quad \text{ (6.4)}
\]

Then

\[
\pi(P_1 | y_1) \equiv \text{DP}(G + \delta_{y_1}),
\]

where, for any \( x, \delta_x \) denotes point mass at \( x \).

At the second stage, we set the prior for \( P_2 \) to be the posterior of \( y_1 \) corresponding to \( \text{DP} \left( (1 + \frac{1}{2^2}) G \right) \) prior for \( P_1 \). That is, \( \pi(P_2) \equiv \text{DP} \left( (1 + \frac{1}{2^2}) G + \delta_{y_1} \right) \). Then, with respect to this prior for \( P_2 \), the posterior of \( P_2 \) is given by

\[
\pi(P_2 | y_2) \equiv \text{DP} \left( (1 + \frac{1}{2^2}) G + \delta_{y_1} + \delta_{y_2} \right).
\]

Continuing this recursive process as obtain that, at the \( k \)-th stage, the posterior of \( P_k \) is a Dirichlet process, given by

\[
\pi(P_k | y_k) \sim \text{DP} \left( \sum_{j=1}^{k} \frac{1}{2^j} G + \sum_{j=1}^{k} \delta_{y_j} \right). \quad \text{ (6.5)}
\]
It follows from (6.5) that

$$E(p_{mk}|y_k) = \frac{\frac{1}{m} \sum_{j=1}^{k} \frac{1}{j^2} + \sum_{j=1}^{k} I(y_j = m)}{\sum_{j=1}^{k} \frac{1}{j^2} + k},$$

(6.6)

$$Var(p_{mk}|y_k) = \frac{\left(\sum_{j=1}^{k} \frac{1}{j^2} + \sum_{j=1}^{k} I(y_j = m)\right) \left((1 - \frac{1}{2m}) \sum_{j=1}^{k} \frac{1}{j^2} + k - \sum_{j=1}^{k} I(y_j = m)\right)}{\left(\sum_{j=1}^{k} \frac{1}{j^2} + k + 1\right)^2} \left(\sum_{j=1}^{k} \frac{1}{j^2} + k + 1\right).$$

(6.7)

The theorem below characterizes the number of local minima of the objective function $f(\cdot)$ in terms of the limit of the marginal posterior probabilities of $p_{mk}$, denoted by $\pi_m(\cdot|y_k)$, as $k \to \infty$.

**Theorem 14** Assume the conditions of Theorem 4, and in Algorithm 1, assume that $M \to \infty$ and $N \to \infty$ such that $M/N \to 0$. Then $f(\cdot)$ has $\bar{m} \geq 0$ local minima if and only if

$$\pi_{\bar{m}}(\mathcal{N}_1|y_k) \to 1, \text{ almost surely with respect to the posterior (3.3)},$$

(6.8)

as $k \to \infty$. In the above, $\mathcal{N}_1$ is any neighborhood of 1 (one).

**Proof.** First, let us assume that $f(\cdot)$ has $\bar{m} \geq 0$ local minima. Then, by Theorem 9, Algorithm 1 converges to the $\bar{m}$ local minima almost surely, as $k \to \infty$, provided that $M \to \infty$ and $N \to \infty$ such that $M/N \to 0$. Hence, there exists $j_0 \geq 1$, such that for $j \geq j_0$, $y_j = \bar{m}_0$. Thus, almost surely, $I(y_j = \bar{m}) = 1$, for $j \geq j_0$. Consequently, it easily follows from (6.6) and (6.7) that almost surely, as $k \to \infty$,

$$E(p_{mk}|y_k) \to 1, \text{ and}$$

(6.9)

$$Var(p_{mk}|y_k) = O\left(\frac{1}{k}\right) \to 0.$$  

(6.10)

Now let $\mathcal{N}_1$ denote any neighborhood of 1, and let $\epsilon \ (> 0)$ be sufficiently small such that $\mathcal{N}_1 \supseteq \{1 - p_{mk} < \epsilon\}$. Then using Markov’s inequality we obtain

$$\pi_{\bar{m}}(\mathcal{N}_1|y_k) \geq \pi_{\bar{m}}(1 - p_{mk} < \epsilon|y_k)$$

$$= 1 - \pi_{\bar{m}}(1 - p_{mk} \geq \epsilon|y_k)$$

$$\geq 1 - \frac{E(1 - p_{mk}|y_k)^2}{\epsilon^2}$$

$$= 1 - \frac{1 - 2E(p_{mk}|y_k) + E(p_{mk}^2|y_k)}{\epsilon^2}.$$  

(6.11)

Now, as $k \to \infty$, $E(p_{mk}|y_k) \to 1$ by (6.9), and $E(p_{mk}^2|y_k) = Var(p_{mk}|y_k) + [E(p_{mk}|y_k)]^2 \to 1$ by (6.9) and (6.10). Hence, the right hand side of (6.11) converges to 1 almost surely, as $k \to \infty$. This proves (6.8).

Now assume that (6.8) holds for any neighborhood $\mathcal{N}_1$ of 1. Let us fix $\eta \in (0, 1)$. Then given any $\epsilon \in (0, 1 - \eta)$,

$$\pi_{\bar{m}}(1 - p_{mk} < \epsilon|y_k) \to 1,$$  

(6.12)

almost surely as $k \to \infty$. The left hand side of (6.12) admits the following Markov’s inequality:

$$\pi_{\bar{m}}(1 - p_{mk} < \epsilon|y_k) = \pi_{\bar{m}}(p_{mk} > 1 - \epsilon|y_k) < \frac{E(p_{mk}|y_k)}{1 - \epsilon}.$$  

(6.13)

Due to (6.12), validity of (6.13) for all $\epsilon \in (0, 1 - \eta)$, and almost sure upper boundedness of $p_{mk}$ by 1,
it follows that
\[ E(p_{m,k}|y_k) \to 1, \text{ almost surely, as } k \to \infty. \tag{6.14} \]

Now, if \( f(\cdot) \) is assumed to have \( m^* \) local minima where \( m^* \neq \tilde{m} \), then due to (6.9) we must have
\[ E(p_{m^*,k}|y_k) \to 1, \text{ almost surely, as } k \to \infty. \tag{6.15} \]

Also note that since \( 0 \leq p_{m,k} \leq 1 \) for all \( m \) and \( k \), the dominated convergence theorem ensures the following, almost surely:
\[ 1 = \lim_{k \to \infty} \sum_{m=1}^{\infty} E(p_{m,k}|y_k) = \sum_{m=1}^{\infty} \lim_{k \to \infty} E(p_{m,k}|y_k). \tag{6.16} \]

Hence, (6.15) implies that \( E(p_{\tilde{m},k}|y_k) \to 0, \) almost surely, as \( k \to \infty. \) But this would contradict (6.14). Hence, \( f(\cdot) \) must have \( \tilde{m} \) local minima. ¥

7 Experiments

We consider application of Algorithm 1 to 5 different optimization problems, ranging from simple to challenging, several of which are problems of finding both maxima and minima, and one is concerned with saddle points and inconclusiveness in addition to maximum. Encouragingly, all our experiments bring forth the versatility of Algorithm 1 in capturing all the optima, saddlepoints, as well as inconclusiveness of the problems.

As regards TMCMC, in our examples, we expectedly find that in the less challenging, low-dimensional problems, additive TMCMC is sufficient, while in the more challenging cases, we consider appropriate mixtures of additive and multiplicative moves, followed by a further move of a specialized mixture of additive and multiplicative transformations to improve mixing.

In most of our experiments, we discard the first \( 10^5 \) TMCMC iterations as burn-in and store every 10-th TMCMC realization in the next \( 5 \times 10^5 \) iterations, to obtain 50000 realizations before proceeding to step (2) of Algorithm 1. However, in the 4-th example, due to inadequate mixing, we discard the first \( 10^6 \) iterations and store every 10-th realization in the next \( 5 \times 10^6 \) iterations to obtain \( 5 \times 10^5 \) TMCMC realizations. For the resample size in step (2), we set \( M = 1000. \)

For the posterior of \( g(\cdot) = 0 \) given by (3.1), we set \( a = b = 0.1, \beta_0 = 0 \) and \( \Sigma_0 = I_d, \) for all the examples, where \( d \) is the dimension relevant to the problem. In all the examples, we also set \( \mathcal{X} = [-10, 10]^d \) and the initial input size \( n = 10. \) With \( x_i = (x_{i1}, \ldots, x_{id}) \) for \( i = 1, \ldots, n, \) we choose the inputs points as \( x_{ik} = -10 + 2(i - 1), \) for \( i = 1, \ldots, n \) and for \( k = 1, \ldots, d. \) We then evaluate \( f(\cdot) \) at each \( x_i; \) \( i = 1, \ldots, n, \) to form \( D_n \) with \( n = 10. \) As we shall demonstrate, this strategy, in conjunction with the rest of the methodology, leads to adequate estimation of the optima in our examples.

7.1 Example 1

We begin with a simple example, where the goal is to obtain the maxima and minima of the function
\[ f(x) = 2x^3 - 3x^2 - 12x + 6. \tag{7.1} \]

Here \( f'(x) = 6(x - 2)(x + 1) \) and \( f''(x) = 6(2x - 1). \) Hence, this function has a maximum at \( x = -1 \) and minimum at \( x = 2. \)

We apply step (1) of Algorithm 1 with \( \epsilon = 1, \) implementing additive TMCMC with equal move-type probabilities for forward and backward transformations. Specifically, at iteration \( t = 1, 2, \ldots, \) letting \( x^{(t-1)} \) denote the TMCMC realization at iteration \( t - 1, \) we draw \( \epsilon \sim N(0, 1) \) and consider the transformation \( y = x^{(t-1)} + b|\epsilon|, \) where \( b \) takes the values 1 and \( -1 \) with equal probabilities. We set
Figure 7.1: TMCMC trace plots for Example 1.

\[ x^{(t)} = y \text{ with probability} \]
\[ \alpha = \min \left\{ 1, \frac{\pi(y)\pi(g'(y) = 0|D_n, y)}{\pi(x^{(t-1)})\pi(g'(x^{(t-1)} = 0|D_n, x^{(t-1)})} \right\}, \]

and set \( x^{(t)} = x^{(t-1)} \) with the remaining probability. This is of course same as the ordinary random walk Metropolis algorithm since the dimension here is \( d = 1 \); see Dutta and Bhattacharya (2014) for ramifications and detailed discussions. Figure 7.1 shows the trace plots of \( x^* \) for maximum and minimum, where to reduce the figure file size, we thinned the original TMCMC sample of size \( N = 50000 \) to 10000 by displaying every 5-th realization. The trace plots indicate adequate mixing properties of TMCMC. We run step (2) of Algorithm 1 for \( k = 1, \ldots, S \) stages with \( S = 40 \), setting \( \eta_k = 1/(10 + k - 1)^2 \), computing the importance weights for the \( N \) TMCMC realizations at each stage on 100 64-bit cores in a VMWare parallel computing environment. The cores have 2.80 GHz speed, and have access to 1 TB memory. All our codes are written in C, using the Message Passing Interface (MPI) protocol for parallel processing. As such, our entire exercise is completed in about 2 minutes. We obtain \( \hat{x}_{\max} = -0.999995 \) and \( \hat{x}_{\min} = 2.000023 \), as our estimates of the maximum and the minimum, respectively, which are quite accurate.

7.2 Example 2

We now consider maximization and minimization of the function \( f(x) = \sin(x) \) for \( x \in [-10, 10] \). Here, the true maxima are \( x_{\max} = \{ \frac{\pi}{2} - 2\pi = -4.712389, \frac{\pi}{2} = 1.570796, \frac{\pi}{2} + 2\pi = 7.853982 \} \), and the minima are \( x_{\min} = \{-7.853982, -1.570796, 4.713289 \} \).

We implement Algorithm 1 in the same way as in Example 1. Figure 7.2 displays the TMCMC trace plots, thinned to 10000 realizations to reduce figure file sizes. Clear tri-modality can be visualized from both the trace plots. After implementing step (2) of Algorithm 1 for \( S = 40 \) stages on VMWare parallel computing architecture, we obtain \( \hat{x}_{\max} = \{-4.712551, 1.570655, 7.860879 \} \) and \( \hat{x}_{\min} = \{-7.854051, -1.570423, 4.713222 \} \), which turn out to be adequate approximations to the truths. Again, the entire exercise takes about 2 minutes.

7.3 Example 3

Let us now consider a two-dimensional example, given by \( f(x_1, x_2) = x_1x_2(x_1 + x_2)(1 + x_2) \).
The first derivatives are given by \( f'_1(x_1, x_2) = 2x_2(x_1 + x_2)(x_2 + 1) \) and \( f'_2(x_1, x_2) = x_1(3x_2^2 + 2x_2(x_1 + 1) + x_1) \).

The second derivatives are \( f''_{11}(x_1, x_2) = 2x_2(x_2 + 1), \) \( f''_{12}(x_1, x_2) = f''_{21}(x_1, x_2) = 4x_1x_2 + 3x_2^2 + 2(x_1 + x_2) \) and \( f''_{22}(x_1, x_2) = 2x_1(3x_2 + x_1 + 1) \).

Consider the determinant \( D(x_1, x_2) = f''_{11}(x_1, x_2)f''_{22}(x_1, x_2) - [f''_{12}(x_1, x_2)]^2. \) Now, if \((a, b)\) is any critical point of \( f(\cdot) \) satisfying \( f'_1(a, b) = 0 \) and \( f'_2(a, b) = 0\), then \( (a, b) \) is a local maximum if \( D(a, b) > 0 \) and \( f''_{11}(a, b) < 0; \) \( (a, b) \) is a local minimum if \( D(a, b) > 0 \) and \( f''_{11}(a, b) > 0; \) \( (a, b) \) is a saddle point if \( D(a, b) < 0. \) Furthermore, if \( D(a, b) = 0, \) then \( (a, b) \) may be either maximum, minimum or even a saddle point, that is, the derivative test remains inconclusive in such cases.

In this example, it is easy to verify that there are four critical points \((0, 0), (0, -1), (1, -1)\) and \((\frac{3}{5}, -\frac{3}{4})\). The last point is a local maximum; \((0, -1)\) and \((1, -1)\) are saddle points, and the derivative test remains inconclusive about \((0, 0)\).

We implement Algorithm 1 using the above conditions on \( D(x^*) \) and \( f''_{11}(x^*) > 0 \), along with the condition \( \|f'(x^*)\|_2 < \epsilon \), with \( \epsilon = 1 \), in the prior for \( x^* = (x^*_1, x^*_2) \), for detection of maxima, minima, saddle points and inconclusiveness.

We implement additive TMCMC with equal move-type probabilities for forward and backward transformations. In these cases, at iteration \( t = 1, 2, \ldots \), letting \( x^{(t-1)} \) denote the TMCMC realization at iteration \( t - 1 \), we draw \( \varepsilon \sim N(0, 1) \) and consider the transformation \( y = x^{(t-1)} + b|\varepsilon| \), where, \( b = (b_1, b_2)^T \) and each of \( b_1 \) and \( b_2 \) independently takes the values 1 and \(-1\) with equal probabilities. We set \( x^{(t)} = y \) with probability

\[
\alpha = \min \left\{ 1, \frac{\pi(y) \pi(g'(y) = 0 | D_n, y)}{\pi(x^{(t-1)}) \pi(g'(x^{(t-1)}) = 0 | D_n, x^{(t-1)})} \right\},
\]

and set \( x^{(t)} = x^{(t-1)} \) with the remaining probability. Note that unlike the one-dimensional setup, this additive TMCMC is no longer equivalent to random walk Metropolis (see Dutta and Bhattacharya (2014) for details).

Implementation of Algorithm 1 for obtaining the maximum and the saddle points took about 7 minutes to complete on our VMWare, implemented on 100 cores.
7.3.1 Maximum

Figure 7.3 displaying the TMCMC trace plots for maxima finding, indicates quite adequate mixing. Running step (2) of Algorithm 1 for \( S = 40 \) steps yields \( \hat{x}_{\text{max}} = (0.376858, -0.752406) \), which is reasonably close to the true maximum.

7.3.2 Saddle points

Our initial TMCMC investigations revealed two modal regions roughly around \((0.1, -1.1)\) and \((1.1, -1.1)\). For better exploration of the two modal regions, we implemented two separate TMCMC runs beginning at the above two points, and continue Algorithm 1 to ultimately obtain two separate results after \( S = 40 \) stages at step (2), associated with the two different starting points. Figures 7.4 and 7.5 display the TMCMC trace plots associated with the two different starting points.

Running step (2) of Algorithm 1 for \( S = 40 \) steps yields \( \hat{x}_{\text{saddle}}^{(1)} = (-0.000309, -0.999580) \) and \( \hat{x}_{\text{saddle}}^{(2)} = (0.999433, -0.999915) \) as estimates of two saddle points, which are both reasonably close to the true saddle points.

7.3.3 Inconclusiveness

Investigation of situations where \( D(a, b) = 0 \) for any critical point \((a, b)\) yielded the TMCMC trace plots displayed as Figure 7.6. On completion of step (2) of Algorithm 1, we obtain \( \hat{x}_{\text{incon}} = (-0.000087, -0.000265) \) as the estimate of the stationary point regarding which conclusion can not be drawn using the second derivatives. Observe that \( \hat{x}_{\text{incon}} \) quite adequately estimates the actual point \((0, 0)\) where conclusion fails.

7.3.4 Minimum

Our attempt to implement TMCMC with the restrictions \( D(x^*) > 0 \) and \( f_{11}''(x^*) > 0 \) with \( \|f'(x^*)\|_2 < \epsilon \) did not yield any acceptance, even for arbitrary initial values. In other words, we could not obtain any solution that satisfies all the above restrictions, and hence conclude that there is no critical point on \( \mathcal{X} \) that satisfy the above restrictions.
Figure 7.4: TMCMC trace plots for Example 3 for finding the first saddle point.

(a) TMCMC for first saddle point: first co-ordinate.

(b) TMCMC for first saddle point: second co-ordinate.

Figure 7.5: TMCMC trace plots for Example 3 for finding the second saddle point.

(a) TMCMC for second saddle point: first co-ordinate.

(b) TMCMC for second saddle point: second co-ordinate.
(a) TMCMC for inconclusiveness: first co-ordinate.  
(b) TMCMC for inconclusiveness: second co-ordinate.  

Figure 7.6: TMCMC trace plots for Example 3 for investigating inconclusiveness.

7.4 Example 4

Table 14.2 of Lange (2010) reports quarterly data on AIDS deaths in Australia during 1983–1986, which is considered for illustration of fitting Poisson regression model. Specifically, for $i = 1, \ldots, 14$, Lange (2010) considers the model $Y_i \sim \text{Poisson}(\lambda_i)$, with $\lambda_i = \exp(\beta_0 + \beta_1)$. Lange (2010) computed the maximum likelihood estimate (MLE) of $\beta = (\beta_0, \beta_1)$ using Fisher’s scoring method, which is equivalent to Newton’s method in this case. The final estimate obtained is $\hat{\beta}_{\text{MLE}} = (0.3396, 0.2565)$.

In our notation, the function to maximize is $f(x_1, x_2) = -\sum_{i=1}^{14} \exp(x_1 + ix_2) + \sum_{i=1}^{14} y_i(x_1 + ix_2)$, with respect to $x = (x_1, x_2)$. Note that this is a concave maximization problem and hence the second derivative is irrelevant. We thus consider the only constraint $\|f'(x^*)\|_2 < \epsilon$ for our implementation, with $\epsilon = 1$. However, additive TMCMC did not exhibit adequate mixing properties in this example, and hence we consider a mixture of additive and multiplicative TMCMC that is expected to improve mixing by using a mixture of localised moves of additive TMCMC and non-local (“random dive”) moves of multiplicative TMCMC (see Dutta (2012), Dey and Bhattacharya (2016) for details). We strengthen the mixture TMCMC strategy with a further step of a mixture of specialized additive and multiplicative moves, which has parallels with Liu and Sabati (2000). The detailed TMCMC algorithm, for general dimension $d$, is provided below as Algorithm 2.

In our case, $d = 2$, and we choose $a_j^{(1)} = a_j^{(2)} = 0.05$, for $j = 1, 2$; we also set $p = q = 1/2$. However, in spite of such a sophisticated TMCMC algorithm, we failed to achieve excellent mixing in this example, even with long TMCMC runs, discarding the first $10^6$ iterations and storing every 10-th realization in the next $5 \times 10^5$ iterations. The trace plots of all stored $5 \times 10^5$ realizations shown in Figure 7.7 indeed demonstrate that the TMCMC chain does not have excellent mixing properties. In fact, the trace plots correspond to a reasonable initial value, chosen to be the 4-th iterate of the Fisher scoring method (see Table 14.3 of Lange (2010)). The subsequent Fisher scoring iterates as initial values led to increasingly improved performance. But here our goal is to demonstrate that even when the mixing is less adequate, the estimates of the optima obtained by our method can still significantly outperform the existing techniques.

As it is known that this example is a concave maximization problem, step (2) of Algorithm 1 is unnecessary. Following Remark 13, we set $i^* = \min\{f(x_i^*) : i = 1, \ldots, N\}$ and report $x_i^*$, as the (approximate) maximizer of $f(\cdot)$. Thus, with the $N = 5 \times 10^5$ TMCMC realizations shown in Figure 7.7, we obtain the estimate $\hat{x}_{\text{MLE}} = (0.364422, 0.254428)$. For this value, $\|f'(\hat{x}_{\text{MLE}})\|_2 = 0.395978$. On the other hand, the MLE obtained by Lange (2010) yields $\|f'(\hat{\beta}_{\text{MLE}})\|_2 = 0.755344$, which is much away from zero compared to our method. In other words, $\hat{x}_{\text{MLE}}$ is much more reliable compared
Algorithm 2 Mixture TMCMC

(1) Fix $p, q \in (0, 1)$. Set an initial value $x^{(0)}$.

(2) For $t = 1, \ldots, N$, do the following:

1. Generate $U \sim U(0, 1)$.
   (a) If $U < p$, then do the following:
      (i) Generate $\varepsilon \sim N(0, 1)$, $b_j \sim \text{iid} U([-1, 1])$ for $j = 1, \ldots, d$, and set $y_j = x_j^{(t-1)} + b_j a_j^{(1)} \varepsilon$, for $j = 1, \ldots, d$. Here $a_j^{(1)}$ are positive scaling constants.
      (ii) Evaluate
      $$\alpha_1 = \min \left\{ 1, \frac{\pi(y)\pi'(g'(y) = 0|D_n, y)}{\pi(x^{(t-1)})\pi'(g'(x^{(t-1)})) = 0|D_n, x^{(t-1)}} \right\}.$$ 
      (iii) Set $\tilde{x}^{(t)} = y$ with probability $\alpha_1$, else set $\tilde{x}^{(t)} = x^{(t-1)}$.
   (b) If $U \geq p$, then
      (i) Generate $\varepsilon \sim U(-1, 1)$, $b_j \sim \text{iid} U([-1, 0, 1])$ for $j = 1, \ldots, d$, and set $y_j = x_j^{(t-1)} \varepsilon$ if $b_j = 1$, $y_j = x_j^{(t-1)}/\varepsilon$ if $b_j = -1$ and $y_j = x_j^{(t-1)}$ if $b_j = 0$, for $j = 1, \ldots, d$.
      Calculate $|J| = \varepsilon \sum_{j=1}^d b_j$.
      (ii) Evaluate
      $$\alpha_2 = \min \left\{ 1, \frac{\pi(y)\pi'(g'(y) = 0|D_n, y)}{\pi(x^{(t-1)})\pi'(g'(x^{(t-1)})) = 0|D_n, x^{(t-1)}} \times |J| \right\}.$$ 
      (iii) Set $\tilde{x}^{(t)} = y$ with probability $\alpha_2$, else set $\tilde{x}^{(t)} = x^{(t-1)}$.

2. Generate $U \sim U(0, 1)$.
   (a) If $U < q$, then do the following
      (i) Generate $\tilde{U} \sim U(0, 1)$ and $\varepsilon \sim N(0, 1)$. If $\tilde{U} < 1/2$, set $y_j = x_j^{(t)} + a_j^{(2)} |\varepsilon|$, for $j = 1, \ldots, d$; else, set $y_j = x_j^{(t)} - a_j^{(2)} |\varepsilon|$, for $j = 1, \ldots, d$. Here $a_j^{(2)}$ are positive scaling constants.
      (ii) Evaluate
      $$\alpha_3 = \min \left\{ 1, \frac{\pi(y)\pi'(g'(y) = 0|D_n, y)}{\pi(x^{(t)})\pi'(g'(x^{(t)})) = 0|D_n, x^{(t)}} \right\}.$$ 
      (iii) Set $x^{(t)} = y$ with probability $\alpha_3$, else set $x^{(t)} = \tilde{x}^{(t)}$.
   (b) If $U \geq q$, then
      (i) Generate $\varepsilon \sim U(-1, 1)$ and $\tilde{U} \sim U(0, 1)$. If $\tilde{U} < 1/2$, set $y_j = x_j^{(t)} \varepsilon$ for $j = 1, \ldots, d$ and $|J| = |\varepsilon|^d$, else set $y_j = x_j^{(t)} /\varepsilon$ for $j = 1, \ldots, d$ and $|J| = |\varepsilon|^{-d}$.
      (ii) Evaluate
      $$\alpha_4 = \min \left\{ 1, \frac{\pi(y)\pi'(g'(y) = 0|D_n, y)}{\pi(x^{(t)})\pi'(g'(x^{(t)})) = 0|D_n, x^{(t)}} \times |J| \right\}.$$ 
      (iii) Set $x^{(t)} = y$ with probability $\alpha_4$, else set $x^{(t)} = \tilde{x}^{(t)}$.

(3) Store the realizations $\{x^{(t)}; t = 0, 1, \ldots, N\}$ for Bayesian inference.
to $\hat{\beta}_{MLE}$, indicating that our method significantly outperforms the existing popular methods of MLE computation. This is indeed a general statement, since with good choices of initial values for TMCMC, which may typically be optima obtained by existing, popular optimization methods, we can explore regions in $\mathcal{X}$ which almost surely contain values that yield smaller $\|f\|_d$ compared to the optima obtained by other numerical methods. It is also encouraging to note that for this example TMCMC takes much less than a minute to yield $6 \times 10^6$ iterations on our VMWare, implemented on a single processor.

7.5 Example 5

Hunter and Lange (2000) refer to a nonlinear optimization problem of the form $Y_i \sim N(\mu_i, \sigma^2)$ for $i = 1, \ldots, m$, where

$$\mu_i = \sum_{j=1}^{d} \left[ \exp \left( -z_{ij}^2 \right) + z_{ij} \theta_{d-j+1} \right];$$

$z_{ij}$ being the $i$-th observation of the $j$-th covariate, for $i = 1, \ldots, m$ and $j = 1, \ldots, d$. The goal is to compute the MLE of $\theta = (\theta_1, \ldots, \theta_d)$, assuming that $\sigma$ is known. In our notation, the objective is to minimize

$$f(x) = \sum_{i=1}^{m} \left( y_i - \sum_{j=1}^{d} \left[ \exp \left( -z_{ij}^2 \right) + z_{ij} x_{d-j+1} \right] \right)^2,$$

with respect to $x$.

We consider 5 simulation experiments in this regard for $d = 2, 5, 10, 50, 100$. In each case we generate $\theta_{0j} \sim U(-1, 1)$ independently for $j = 1, \ldots, d$, $z_{ij} \sim N(0, 1)$ independently, for $i = 1, \ldots, m$ and $j = 1, \ldots, d$, and set, for $i = 1, \ldots, m$, $\mu_{0i} = \sum_{j=1}^{d} \left[ \exp \left( -z_{ij}^2 \right) + z_{ij} \theta_{0, d-j+1} \right]$. We finally generate the response data by simulating $Y_i \sim N(\mu_{0i}, \sigma^2_0)$ independently for $i = 1, \ldots, m$, where we set $\sigma^2_0 = 0.1$. For $d = 2, 5, 10, 50, 100$, we generate datasets of sizes $m = 10, 10, 20, 75, 200$.

Note that this is not a convex minimization problem and the matrix of second derivatives $\Sigma''(\cdot)$ plays an important role, along with $\|f'(\cdot)\|_d$. Thus it is important to check positive definiteness of $\Sigma''(\cdot)$ for any dimension $d$. We use the LAPACK library function “dpotrf” for Cholesky decomposition of $\Sigma''(\cdot)$, which contains a parameter “info”. Given any $x$, $info = 0$ indicates positive definiteness of $\Sigma''(x)$, while other values of $info$ rules out positive definiteness. Note that since this is not a convex minimization problem, step (2) of Algorithm 1 is necessary, unlike in Example 4.
We implement the mixture TMCMC algorithm 2 for all values of \( d \), with \( p = q = 1/2 \) and set \( a_j^{(1)} = a_j^{(2)} = 0.05 \) for \( j = 1, \ldots, d \).

### 7.5.1 Case 1: \( d = 2 \)

In the TMCMC step, we set \( \epsilon = 1 \) in the restriction \( \| f'(\cdot) \|_2 < \epsilon \). The trace plots, shown in Figure 7.8, exhibit adequate mixing. Running step (2) of Algorithm 1 till \( S = 40 \) stages with \( \eta_k = 1/(10 + k - 1) \) for \( k = 1, \ldots, S \), yielded the estimate of the MLE to be \( \hat{x}_{MLE} = (0.678854, 0.293575) \), for which \( \| f'(\hat{x}_{MLE}) \|_2 = 0.012514 \). The exercise 3 minutes on our VMWare, implemented in parallel on 100 cores.

However, examination of the samples obtained by importance resampling at the different stages of step (2) of Algorithm 1 did not reveal any evidence of multimodality, and hence it is pertinent to consider that estimate which corresponds to the minimum of \( \{ \| f'(x^*_i) \|_2 : i = 1, \ldots, N \} \), where \( x^*_i \) are the original TMCMC samples, with \( N = 50000 \). As such, we modify the previous estimate to \( \hat{x}_{MLE} = (0.678912, 0.293809) \), which yields \( \| f'(\hat{x}_{MLE}) \|_2 = 0.007221 \), which is somewhat closer to zero compared to that for the previous estimate. Note however, that the two estimates of MLE are quite close to each other.

### 7.5.2 Case 2: \( d = 5 \)

Here, for the 5-dimensional TMCMC, we set \( \epsilon = 3 \) in the restriction \( \| f'(\cdot) \|_5 < \epsilon \), as smaller values of \( \epsilon \) led to poor convergence. Note that the Euclidean norm increases with dimension (see, for example, Giraud (2015)), and so it is a natural requirement to increase \( \epsilon \) as dimension increases. Similarly, we had to increase \( \eta_k \) to \( \eta_k = 1.5/\log(10 + k) \) for implementing step (2) of Algorithm 1. The rest of the parameters of Algorithm 2 remain the same as for \( d = 2 \).

The trace plots exhibited reasonable mixing; those for the first and the last (5-th) co-ordinate of \( x^* \) are depicted in Figure 7.9. Running step (2) of Algorithm 1 till \( S = 40 \) stages we obtain \( \hat{x}_{MLE} = (0.663327, 0.431669, 0.045598, 0.239091, 0.301665) \), which corresponds to \( \min \{ \| f'(x^*_i) \|_5 : i = 1, \ldots, N \} = 0.254217 \), with \( N = 50000 \). Note the increase in \( \| f'(\cdot) \|_5 \) compared to those of the smaller dimensions. Again, this is clearly to be expected because of the curse of dimensionality. The exercise takes 4 minutes to complete on our VMWare.
7.5.3 Case 3: $d = 10$

Here, for $d = 10$, we had to set $\epsilon = 6$ for the restriction $\|f'(\cdot)\|_{10} < \epsilon$ in TMCMC for adequate convergence. We also set $\eta_k = 7/\log(10 + k - 1)$ for implementing step (2) of Algorithm 1.

Our investigation shows that the mixing of TMCMC is not inadequate. The trace plots of the first and the last co-ordinate of $x^*$ shown in Figure 7.10 also bear evidence to this. After implementing step (2) of Algorithm 1 till $S = 40$ stages, we obtain $\hat{x}_{MLE} = (0.472309, 0.10124, 0.079194, 0.108072, 0.096287, -0.511566, 0.517567, -0.887624, 0.637796, -0.317721)$ with $\|f'(\hat{x}_{MLE})\|_{10} = 1.917746$. On the other hand, $\min\{\|f'(x^*_i)\|_{10} : i = 1, \ldots, 50000\} = 1.902788$, which corresponds to $\hat{x}_{MLE} = (0.471200, 0.100131, 0.078085, 0.101934, 0.095178, -0.504813, 0.516459, -0.888733, 0.631659, -0.323859)$. Thus, both the estimates as well as the corresponding gradients are quite close to each other. Again note the increase in $\|f'(\cdot)\|_{10}$ compared to those of the smaller dimensions. The entire exercise takes 17 minutes on our VMWare to complete.
7.5.4 Case 4: \(d = 50\)

For this somewhat large dimension, we had to set \(\epsilon = 100\) and \(\eta_k = 200/\log(10 + k - 1)\). Figure 7.11, which displays all stored 50000 TMCMC realizations for \(x^*_1\) and \(x^*_50\) do not indicate excellent mixing, in spite of the sophistication of Algorithm 2. However, due to the high-dimension and complexity of the posterior this is not unexpected. As demonstrated by Example 4, we can still expect to get closer to the MLE compared to other optimization methods. In this case, we obtain \(\min\{\|f'(x^*_i)\|_{50} : i = 1, \ldots, 50000\}\) = 73.05261 while step (2) of Algorithm 1 implemented for till \(S = 100\) stages, of which only the first four stages consisted of positive \(n_k\), yielded \(\|f'(\hat{x}_{MLE})\|_{50} = 76.28244\). Thus, the norms of the gradients have increased considerably in this high dimension, compared to the previous \(d = 2, 5, 10\). Given the high dimension in this problem, the above gradient values 73.05261 and 76.28244 are quite close.

The TMCMC implementation took about 12 hours on a single core in our VMWare and step (2) of Algorithm 1 took additional 2 hours on 100 cores.

7.5.5 Case 5: \(d = 100\)

The curse of dimensionality now forced us to set \(\epsilon = 400\) for TMCMC convergence and \(\eta_k = 850/\log(10 + k - 1)\). It took around 15 hours to complete the TMCMC run; the trace plots shown in Figure 7.12 do not bear evidence of non-convergence, even though mixing is expectedly inadequate in such high dimension. Here we obtain \(\min\{\|f'(x^*_i)\|_{50} : i = 1, \ldots, 50000\}\) = 330.4483, while step (2) of Algorithm 1 implemented for till \(S = 100\) stages, of which only the first three stages yielded positive \(n_k\), produced \(\hat{x}_{MLE}\) such that \(\|f'(\hat{x}_{MLE})\|_{100} = 341.2009\). Given the high dimension, this value is quite close to the above minimum gradient. Implementation of step (2) of Algorithm 1 took 2 hours 36 minutes on 100 cores on our VMWare.

8 Summary and conclusion

In this article, we have proposed and developed a novel Bayesian algorithm for general function optimization, judiciously exploiting its derivatives in conjunction with posterior Gaussian derivative process given data consisting of input points from the function domain and their function evaluations. The posterior simulation approach inherent in our method ensures improved accuracy of our results compared to existing optimization algorithms. Another important feature of our algorithm is that for any desired de-
gree of accuracy, Bayesian credible regions of the optima of any desired level, become readily available after implementation of the algorithm.

Under appropriate fixed-domain infill asymptotics setup, we prove almost sure convergence of the algorithm to the true optima. Along the way, we establish almost sure uniform convergence of the posteriors corresponding to Gaussian and Gaussian derivative processes to the objection function and its derivatives, under the fixed-domain infill asymptotics setup, providing rates of convergence under a specific setup. We also establish Bayesian characterization of the number of optima of the objective function by exploiting the information existing in our algorithm.

Applications of our Bayesian optimization algorithm to various examples ranging from simple to challenging, led to encouraging and insightful results. Choice of initial values for starting TMCMC of our algorithm is seen to affect mixing, but as we argued, optima yielded by good existing optimization algorithms can act as good initial values for TMCMC. Moreover, we have also demonstrated that even with less adequate mixing, our Bayesian algorithm can still significantly outperform popular optimization methods. Thus, the TMCMC mixing issue is perhaps not too important, at least for low dimensional problem.

Dimensionality of the problem seems to be a far more serious issue. Indeed, our experimental results demonstrate that as dimension increases, accuracy of our algorithm deteriorates. High dimensionality also seriously affects TMCMC mixing by excessively restricting the input space through the prior constraints. These are only natural, but need to be dealt with seriously. Our future endeavors will address these issues.

Figure 7.12: TMCMC trace plots for Example 5 for finding MLE for dimension $d = 100$. 
References

Adler, R. J. (1981). *The Geometry of Random Fields*. John Wiley & Sons Ltd., New York.

Adler, R. J. and Taylor, J. E. (2007). *Random Fields and Geometry*. Springer, New York.

Billingsley, P. (2013). *Convergence of Probability Measures*. John Wiley & Sons Ltd., New York.

Dey, K. K. and Bhattacharya, S. (2016). On Geometric Ergodicity of Additive and Multiplicative Transformation Based Markov Chain Monte Carlo in High Dimensions. *Brazilian Journal of Probability and Statistics*, 30, 570–613. Also available at arXiv.

Dey, K. K. and Bhattacharya, S. (2017). A Brief Tutorial on Transformation Based Markov Chain Monte Carlo and Optimal Scaling of the Additive Transformation. *Brazilian Journal of Probability and Statistics*, 31, 569–617. Also available at arXiv.

Dey, K. K. and Bhattacharya, S. (2019). A Brief Review of Optimal Scaling of the Main MCMC Approaches and Optimal Scaling of Additive TMCMC Under Non-Regular Cases. *Brazilian Journal of Probability and Statistics*, 33, 222–266. Also available at arXiv.

Dutta, S. (2012). Multiplicative Random Walk Metropolis-Hastings on the Real Line. *Sankhya. Series B*, 74, 315–342. Also available at arXiv.

Dutta, S. and Bhattacharya, S. (2014). Markov Chain Monte Carlo Based on Deterministic Transformations. *Statistical Methodology*, 16, 100–116. Also available at http://arxiv.org/abs/1106.5850. Supplement available at http://arxiv.org/abs/1306.6684.

Ferguson, T. S. (1973). A Bayesian Analysis of Some Nonparametric Problems. *The Annals of Statistics*, 1, 209–230.

Frazier, P. I. (2018). A Tutorial on Bayesian Optimization. arXiv preprint.

Giraud, C. (2015). *Introduction to High-Dimensional Statistics*. CRC Press, New York.

Hunter, D. R. and Lange, K. (2000). Quantile Regression via an MM Algorithm. *Journal of Computational and Graphical Statistics*, 9(1), 60–77.

Lange, K. (2010). *Numerical Analysis for Statisticians*. Springer-Verlag, New York.

Liu, J. S. and Sabatti, S. (2000). Generalized Gibbs Sampler and Multigrid Monte Carlo for Bayesian Computation. *Biometrika*, 87, 353–369.

Roy, S. and Bhattacharya, S. (2020). Bayes Meets Riemann – Bayesian Characterization of Infinite Series With Application to Riemann Hypothesis. *International Journal of Applied Mathematics and Statistics*, 59, 81–128. Also available at https://arxiv.org/abs/1601.01452.

Santner, T. J., Williams, B. J., and I. Notz, W. (2003). *The Design and Analysis of Computer Experiments*. Springer-Verlag, New York.