On the construction of probabilistic Newton-type algorithms

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Abstract

It has recently been shown that many of the existing quasi-Newton algorithms can be formulated as learning algorithms, capable of learning local models of the cost functions. Importantly, this understanding allows us to safely start assembling probabilistic Newton-type algorithms, applicable in situations where we only have access to noisy observations of the cost function and its derivatives. This is where our interest lies. We make contributions to the use of the non-parametric and probabilistic Gaussian process models in solving these stochastic optimisation problems. Specifically, we present a new algorithm that unites these approximations together with recent probabilistic line search routines to deliver a probabilistic quasi-Newton approach. We also show that the probabilistic optimisation algorithms deliver promising results on challenging nonlinear system identification problems where the very nature of the problem is such that we can only access the cost function and its derivative via noisy observations, since there are no closed-form expressions available.

1 Introduction

We are in this paper concerned with the unconstrained nonlinear optimisation problem

\[
\hat{x} = \arg \min_x f(x),
\]

(1)
in situations when we only have access to noisy evaluations of the cost function \( f(x) \) and its derivatives. In the noise-free case, solving this problem has attracted enormous research attention for many decades and this has resulted in many variants of optimisation algorithms. Among these are the much celebrated class of quasi-Newton methods that are still—almost half a century after their inception—the state of the art methods when it comes to numerical solution of the unconstrained optimisation problem (1). This is true across most—if not all—branches of science where optimisation problems of the type (1) needs to be solved.

When \( f(x) \) and its derivatives are noisy, then these existing methods suffer from a fundamental problem. Specifically, the algorithms may fail to converge since they rely on knowledge of descent directions and line-search (or related) methods that are not geared towards noisy cost functions and gradient evaluations. Such stochastic optimisation problems are commonly occurring for example in the following situations; 1) If the dataset is very large it is not possible to evaluate the cost function on the entire dataset and instead it is divided into so-called mini-batches. This situation arises quite often in Machine Learning and in particular in deep learning applications. 2) When we employ numerical algorithms to compute the cost function and its derivatives. This occurs for example in nonlinear system identification using the maximum likelihood method when various particle filters are used to compute the intractable cost function and its gradients. We use nonlinear system identification as a case study in this paper.

There has recently been some very relevant and encouraging developments for dealing with these stochastic optimisation problems. More specifically it has been shown \cite{1, 2} that standard quasi-Newton methods like the BFGS method \cite{3, 4, 5, 6}, Broyden’s method \cite{7} and the DFP formula \cite{8, 9} all can be interpreted as particular instances of Bayesian linear regression or as Gaussian process regression. This line of research has shown that we can reinterpret the quasi-Newton algorithms as learning algorithms that estimate a local quadratic model to the cost function \cite{1, 10}.
Most of this recent development has taken place within the relatively new and vibrant direction of research commonly referred to as \textit{probabilistic numerics}, see probabilistic-numerics.org and [11].

Perhaps most importantly this line of research has opened up for genuinely new probabilistic optimisation algorithms, which is necessary in order to solve the problems we are facing when we only have noisy observations of the cost function and its derivatives. We will in this work explore these ideas and present a new algorithm that combines a new approach to modelling the Hessian matrix together with recent results for probabilistic line search routines. Importantly, we are able to ensure that the model of the Hessian is symmetric by making use of the half-vector operator [12]. Another technical contribution is that we propagate the uncertainty in the Hessian approximation between iterations of the algorithm. As a final contribution we have the application of these new algorithms to the challenging nonlinear system identification problem.

The key construction is provided by the Bayesian non-parametric Gaussian process (GP) [13, 14], which is very briefly introduced in Section 2. In that section we also outline the two main directions of development that exist when it comes to modelling optimisation problems using the GP. These two directions are then described and developed further in Sections 3 and 4. The algorithms are then profiled on the nontrivial nonlinear system identification application in Section 5. Finally, we state our conclusions and ideas for future direction of this research in Section 6.

2 Modeling optimisation problems using GPs

2.1 Background on the Gaussian process

The Gaussian process [13, 14] is by now an established model for nonlinear functions. The representation that is used by the GP in modeling a nonlinear function is non-parametric (meaning that it does not rely on any parametric functional form) and probabilistic (meaning that uncertainty is taken into account throughout the model).

The Gaussian process is formally defined as a (potentially infinite) collection of random variables such that any finite subset of it has a joint Gaussian distribution. Let us assume that we want to model some nonlinear function \( f(x) \) as a realisation from a Gaussian process. We then assign a prior distribution over the function \( f(x) \) given be the GP, which we denote by

\[
  f(x) \sim \mathcal{GP}(\mu(x), k(x, x')) ,
\]

(2)

where \( \mu(x) \) is some suitable mean function (for example, a strictly convex function centred on prior knowledge of the parameter values). The covariance function (also referred to as the kernel) \( k(x, x') \) represents the correlation between function values based on the two evaluation points \( x \) and \( x' \).

This prior can then be updated using observations of the function via the standard results on partitioned Gaussian distributions, see e.g. [14] for details.

2.2 Two existing directions

The idea of using the GP for optimisation is rather natural, especially in situations where we only have access to noisy observations of the cost function and its derivatives. The approaches available so far can very broadly be divided into two directions.

The first direction starts by assuming that the Hessian is distributed according to a GP. This Hessian is then updated via (potentially noisy) observations of the Hessian, the gradient and the cost function. The observations of the gradients and the cost function take the form of line integral observations of the GP, which can readily be incorporated. Henning recently outlined some promising and highly interesting developments along these lines [10, 1]. We follow this direction in Section 3.

The second direction instead tries to build a global model of the cost function and possibly also of its derivatives. Here the crucial observation is that the derivative of a GP is another GP [14]. This straightforwardly opens up for the possibility of modelling the cost function and possibly also its derivatives as a joint GP. This global GP model is then
updated using the (possibly noisy) observations of the cost function and its gradients. Developments along this line started in the global optimisation literature [15] under names such as Gaussian Process Optimisation (GPO) [16] and Bayesian optimisation [17]. This direction is following and developed in Section 4.

Interestingly the algorithms resulting from these two directions are highly suitable for standard nonlinear deterministic problems. We see great potential in new optimisation algorithms being created not only for the stochastic situation, but also for the classic deterministic problem.

3 Non-parametric quasi-Newton methods

3.1 A non-standard take on the quasi-Newton methods

The idea underlying the Newton and quasi-Newton methods is that they learn a local quadratic model $q(x_k, \delta)$ of the cost function $f(x)$ around the current iterate $x_k$

$$q(x_k, \delta) \triangleq f(x_k) + g(x_k)^T \delta + \frac{1}{2} \delta^T H(x_k) \delta,$$

(3)

where $\delta = x - x_k$, $g(x_k) = \nabla f(x)|_{x=x_k}$ denotes the gradient and $H(x_k) = \nabla^2 f(x)|_{x=x_k}$ denotes the Hessian. Note that (3) is a second order Taylor expansion of $f(x)$, i.e. $f(x) \approx q(x_k, \delta)$ in a close vicinity around $x_k$. The quasi-Newton methods compute an estimate of the Hessian based on zero and first order information (function values and their gradients). More specifically these methods are designed to represent the cost function according to the following model

$$f_q(x_k + \delta) = f(x_k) + g(x_k)^T \delta + \frac{1}{2} \delta^T B_k \delta,$$

(4)

for some positive definite matrix $B_k$. Note that

$$\nabla_\delta f_q(x_k + \delta) = g(x_k) + B_k \delta.$$ (5)

Quasi-Newton methods make a standing assumption that

$$\nabla_\delta f_q(x_k + \delta)|_{\delta=x_{k-1}-x_k} = \nabla_x f(x_{k-1}) = g(x_{k-1}).$$ (6)

Equations (5) and (6) combined result in $g(x_{k-1}) = g(x_k) + B_k (x_{k-1} - x_k)$, so that if we define

$$y_k \triangleq g(x_k) - g(x_{k-1}), \quad s_k \triangleq x_k - x_{k-1},$$ (7)

then we obtain the secant condition (quasi-Newton equation).

$$B_k s_k = y_k.$$ (8)

This equation is not enough to define the elements of the Hessian approximation $B_k$, we also know that by construction it has to be symmetric. From a learning point of view this is very helpful since it halves the number of unknown parameters to be estimated, but some extra care will have to be taken to ensure this. That said, the existing quasi-Newton algorithms can all be interpreted as employing some particular form of regularisation on $B_k$, for example, one that minimises changes from a previous Hessian approximation $B_{k-1}$. As such, we can solve the following optimisation problem to find a suitable $B_k$ as the solution to

$$\min_B \|B - B_{k-1}\|_W^2,$$

s.t. $B = B^T$, $B s_k = y_k$, (9)

where $W$ is a positive definite weighting matrix. It was Henning [1, 2] who recently showed this enlightening unifying interpretation of the quasi-Newton algorithms. In Appendix A we also provide an alternative derivation of the solution to (9) to complement the developments in [2]. As pointed out in [2] this opens up for some flexibility in finding new algorithms which we will continue exploring below.
3.2 Integral formulation of the quasi-Newton equation

In the previous section we formulated the key quasi-Newton equation (8) using derivatives. We can represent the same information using a line integral, which comes about by noting that if we define the line segment \( r_k(\tau) \) between the current iterate \( x_k \) and the previous iterate \( x_{k-1} \) as

\[
r_k(\tau) \triangleq x_{k-1} + \tau(x_k - x_{k-1}), \quad \tau \in [0, 1],
\]

then

\[
\int_0^1 \frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) d\tau = \nabla f(r_k(1)) - \nabla f(r_k(0)) = \nabla f(x_k) - \nabla f(x_{k-1}) \triangleq y_k.
\]

Now also note that by the chain rule

\[
\frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) = \nabla^2 f(r_k(\tau)) \frac{\partial r_k(\tau)}{\partial \tau} = \nabla^2 f(r_k(\tau))(x_k - x_{k-1}).
\]

Therefore,

\[
\int_0^1 \frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) d\tau = \int_0^1 \nabla^2 f(r_k(\tau))(x_k - x_{k-1}) d\tau.
\]

That is

\[
y_k = \int_0^1 \nabla^2 f(r_k(\tau))(x_k - x_{k-1}) d\tau.
\]

This means that the difference between gradients (i.e. \( y_k \)) can be considered a line integral observation of the Hessian matrix. Therefore, in theory we could update an estimate of the Hessian based on this and other such observations. However, since the Hessian is unknown we do not have any functional form for it. Hennig [10] introduced the idea of using a Gaussian process to represent the true Hessian. This is the approach we will take here as well. There are two key problems in building a Bayesian non-parametric model of the Hessian using a GP. Firstly, we have to be able to make use of the line integral observations (13) when learning the GP. This has been solved and used in other settings before, see e.g. [1, 18]. Secondly, how do we ensure that the resulting GP represents a Hessian, i.e. that its realisations are at least symmetric matrices? We will in the subsequent section develop a solution based on the so-called half-vector operator [12] to ensure that the GP employed in representing the Hessian is symmetric. Importantly, the fact that the gradient observations are potentially noisy does in fact not cause any problems at all, since this fits within the standard Gaussian process regression formulation.

3.3 Modelling the Hessian as a GP

The equivalent integral version of the quasi-Newton equation (8) was in the previous section shown to be

\[
y_k = \int_0^1 B(r_k(\tau)) s_k d\tau,
\]

where \( B(\cdot) \) denotes the model of the Hessian and \( s_k = x_k - x_{k-1} \). Note that since \( B(r_k(\tau)) s_k \) is a column vector we can straightforwardly apply the vectorisation operator inside the integral in (47) without changing the result,

\[
y_k = \int_0^1 \text{vec}(B(r_k(\tau)) s_k) d\tau = \int_0^1 (s_k^T \otimes I) \text{vec}(B(r_k(\tau))) d\tau = (s_k^T \otimes I) \int_0^1 \text{vec}(B(r_k(\tau))) d\tau,
\]

where \( \otimes \) denotes the Kronecker product. The whole point of this exercise is that we have now isolated the vectorised Hessian estimate \( \text{vec}(B(r_k(\tau))) \) inside the integral. One option would now be to place a GP prior on \( \text{vec}(B(r_k(\tau))) \), but that would not enforce the symmetry requirement we have on the Hessian estimate. We can solve this problem...
using the half-vectorisation operator\(^1\) vec\(\left(\cdot\right)\) \[12\]. Hence, we now assume that we have a GP prior on the unique elements in the Hessian estimate

\[ \tilde{B}(\tau) = \text{vech} \left( B(r_k(\tau)) \right), \]  

that is given by

\[ p \left( \tilde{B}(\tau) \right) = \mathcal{GP}(\mu_k(\tau), \kappa_k(\tau, t)). \]  

We can then retrieve the full Hessian estimate using the so-called duplication matrix \(D\), which is a matrix such that

\[ \text{vec} \left( B(r_k(\tau)) \right) = D \tilde{B}(\tau). \]  

More details and some useful results on the duplication matrix, the associated elimination matrix (vec\(\left(A\right) = L \text{vec} \left( A \right)\)) and their use are provided by \[12\]. It is now straightforward to also generalise the measurement (15) by adding some noise

\[ y_k = (s_k^T \otimes I) \int_0^1 D \tilde{B}(\tau) \, d\tau + e_k, \quad e_k \sim \mathcal{N}(0, R). \]  

It can now be shown that the joint GP for \(\tilde{B}(\tau)\) and \(y_k\) is given by

\[ p(\tilde{B}(\tau), y_k) = \mathcal{GP}(m_j, K_j), \]  

where \(\gamma_k(\tau, t)\) and \(\pi_k(\tau, t)\) are given by

\[ \gamma_k(\tau, t) = \left( \int_0^1 \kappa_k(\tau, t) \, d\tau \right) D^T (s_k \otimes I), \]  

and

\[ \pi_k(\tau, t) = (s_k^T \otimes I) D \left( \int_0^1 \int_0^1 \kappa_k(\tau, t) \, d\tau \, dt \right) D^T (s_k \otimes I) + R. \]  

Employing the standard results for conditioning of partitioned Gaussians we obtain the posterior distribution \(p(\tilde{B}(\tau) \mid y_k)\) from which we can then assemble back the full Hessian estimate.

\[ p(\tilde{B}(\tau) \mid y_k) = \mathcal{GP}(m, K), \]  

where

\[ m = \mu_k(\tau) + \gamma_k(\tau, t) \pi^{-1}(\tau, t) (y_k - (s_k \otimes I) \int_0^1 \mu_k(\tau) \, d\tau), \]  

\[ K = \kappa_k(\tau, t) - \gamma_k(\tau, t) \pi^{-1}(\tau, t) \gamma_k^T(\tau, t). \]  

Finally, the Hessian estimate is according to (50) given by

\[ p(\text{vec} \left( B(r_k(\tau)) \right) \mid y_k) = \mathcal{GP}(Dm, DKD^T). \]  

\(^1\)For a symmetric \(n \times n\) matrix \(A\) the vector vec\(\left( A \right)\) contains redundant information. More specifically, we do not need to keep the \(n(n-1)/2\) entries above the main diagonal. The half-vectorisation vec\(\left( A \right)\) of a symmetric matrix \(A\) is obtained by vectorising only the lower triangular part of \(A\).
3.4 Resulting optimisation algorithm

The above ideas are collected here in the form of an algorithm statement where the main theme is akin to quite standard gradient-based search algorithms. In particular, we compute a search direction based on gradient information and the Hessian approximation, and perform a line search along this direction using the cost function \( f(x) \) to regulate a potential decrease in the cost. Importantly, care must be taken when performing a line search in this setting since \( f(x) \) is stochastic. Here we employ the recent work in [19] that delivers a line search algorithm that handles noisy function and gradient evaluations and also satisfies Wolfe-like conditions on the calculated step length.

It is important to be specific about the covariance function employed below. Here we have opted to use a multi-variate version of the squared exponential covariance given by

\[
k_k(\tau, t) = \sigma^2 C_k e^{-\frac{1}{2} \tau^T (\tau) V r_k(t)}
\]

(25)

where the matrix \( C_k \) describes the covariance effect on each element of \( \widetilde{B}(\cdot) \), the matrix \( V \) acts as an inverse length scale, and \( \sigma^2 \) scales the entire covariance.

Algorithm 1 GP Hessian Approximation optimisation

Require: An initial estimate \( x_1 \) and a mean estimate of the Hessian matrix \( \mu_1(\cdot) = \text{vech} \left( B_1 \right) \), and a covariance matrix \( C_1 \), and a positive integer \( k_{\text{max}} > 0 \) that determines the maximum number of iterations.

1: Set \( k = 1 \) and perform the following.
2: \textbf{while} \( k < k_{\text{max}} \) \textbf{do}
3: \hspace{1em} Calculate a descent direction \( p_k \) based on the current Hessian approximation \( B_k \) and gradient \( g(x_k) \) (care should be taken to ensure this is a descent direction since \( B_k \) is not guaranteed to be positive definite).
4: \hspace{1em} Calculate a suitable step length \( \alpha_k \) along the direction \( p_k \) according to [19] and set \( x_{k+1} = x_k + \alpha_k p \).
5: \hspace{1em} Set \( k \rightarrow k + 1 \).
6: \hspace{1em} Update the Hessian approximation mean \( \widetilde{B}_k = m \) and set the covariance matrix \( C_k = K \) according to (23).
7: \textbf{end while}

4 Global GP representation

The approach adopted here is to optimise a surrogate function, rather than the cost function itself. It is important that the surrogate function maintain the global “shape” of the underlying cost function and at the same time remain amenable to classical optimisation methods for smooth functions.

As a potential surrogate function, here we employ the non-parametric class of GPs to model the cost function, its gradient and Hessian, similar to the development in [16]. In particular, we model the cost function \( f(x) \) via

\[
f(x) \sim \mathcal{GP}(\mu(x), h(x, x') ) ,
\]

(26)

where \( \mu(x) \) is some suitable mean function (for example, a strictly convex function centred on prior knowledge of the parameter values). Let us now introduce the notation

\[
g(x) = \nabla_x f(x), \quad h(x) = \text{vech} \left( \nabla_x^2 f(x) \right) ,
\]

(27)

for the gradient and the Hessian, respectively. Here we have again explicitly exploit the fact that the Hessian is symmetric and employ the half-vectorisation operator to this end. Recall that the derivative of a Gaussian process is another Gaussian process [14]. Hence, if the covariance function \( k(x, x') \) is twice differentiable, the stacked object \( (f(x), g^T(x), h^T(x))^T \) is guaranteed to be a Gaussian process with induced mean and covariance functions according to

\[
\begin{bmatrix}
  f(x) \\
g(x) \\
h(x)
\end{bmatrix} \sim \mathcal{GP} \begin{bmatrix}
  \frac{1}{\nabla_x} \\
  \frac{1}{\nabla_x^2} \\
end{bmatrix} \mu(x), \begin{bmatrix}
  \frac{1}{\nabla_x} \\
  \frac{1}{\nabla_x^2} \\
end{bmatrix} k(x, x') \begin{bmatrix}
  \frac{1}{\nabla_x} \\
  \frac{1}{\nabla_x^2}
\end{bmatrix}^T
\]

(28)
In the above, \( \nabla_x \) is used to present the vector of partial derivatives with respect to \( x \) and \( \nabla^2_x = \text{vech} \left( \nabla_x^2 \right) \) is used to represent the vector of operators that is formed by applying the half-vectorization operator to the following matrix of second order derivative operators

\[
\nabla^2_x \triangleq \begin{bmatrix}
\frac{\partial^2}{\partial x_1 \partial x_1} & \frac{\partial^2}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2}{\partial x_1 \partial x_n} \\
\frac{\partial^2}{\partial x_2 \partial x_1} & \frac{\partial^2}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2}{\partial x_2 \partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2}{\partial x_n \partial x_1} & \frac{\partial^2}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2}{\partial x_n \partial x_n}
\end{bmatrix}
\] (29)

Therefore, \( \nabla^2_x \in \mathbb{R}^{n \times n} \) and \( \nabla^2_x \in \mathbb{R}^{(n+1)/2 \times 1} \).

For a given value of the parameters \( x \), we obtain the following noisy measurements of the cost function \( f(x) \), its gradient \( g(x) \) and its Hessian \( h(x) \),

\[
\begin{align*}
\hat{f}(x) &= f(x) + v_c, & v_c &\sim \mathcal{N}(0, \sigma_c^2), \\
\hat{g}(x) &= g(x) + v_g, & v_g &\sim \mathcal{N}(0, \Sigma_g), \\
\hat{h}(x) &= h(x) + v_h, & v_h &\sim \mathcal{N}(0, \Sigma_h),
\end{align*}
\] (30)

where \( \sigma_c, \Sigma_g \) and \( \Sigma_h \) carries information about the nature of the noise. In a situation where we do not have access to one or more of the observations in (30) we simply just remove the corresponding line(s) and our development still holds.

Based on the above it is now possible to construct a joint GP consisting of both the true objects \( \ell(x) \) and the (possibly noisy) observations of them \( \hat{\ell}(x) \)

\[
\ell(x) = \begin{bmatrix} f(x) \\ g(x) \\ h(x) \end{bmatrix}, \quad \hat{\ell}(x) = \begin{bmatrix} \hat{f}(x) \\ \hat{g}(x) \\ \hat{h}(x) \end{bmatrix},
\] (31)

according to

\[
\begin{bmatrix} \ell(x) \\ \hat{\ell}(x) \end{bmatrix} \sim \mathcal{GP} \left( \begin{bmatrix} \mu_\ell(x) \\ \mu_{\hat{\ell}}(x) \end{bmatrix}, \begin{bmatrix} k_\ell,\ell(x,x') & k_\ell,\hat{\ell}(x,x') \\ k_{\hat{\ell}},\ell(x,x') & k_{\hat{\ell}},\hat{\ell}(x,x') \end{bmatrix} \right)
\] (32)

where

\[
\begin{align*}
\mu_\ell(x) &= \begin{bmatrix} \mu(x) \\ \nabla_x \mu(x) \\ \nabla^2_x \mu(x) \end{bmatrix}, & \mu_{\hat{\ell}}(x) &= \begin{bmatrix} \hat{\mu}(x) \\ \nabla_x \hat{\mu}(x) \\ \nabla^2_x \hat{\mu}(x) \end{bmatrix}
\end{align*}
\] (33)

and finally,

\[
k_\ell,\ell(x,x') = k_\ell,\ell(x,x') = \begin{bmatrix} k(x,x') & k(x,x')(\nabla^2_{\hat{\ell}})^T \\ \nabla_x k(x,x') & \nabla_x k(x,x')(\nabla^2_{\hat{\ell}})^T \\ \nabla^2_x k(x,x') & \nabla^2_x k(x,x')(\nabla^2_{\hat{\ell}})^T \end{bmatrix}
\] (34)

and

\[
k_{\hat{\ell}},\ell(x,x') = k_{\hat{\ell}},\ell(x,x')^T = k_{\hat{\ell}},\hat{\ell}(x,x') + \begin{bmatrix} \sigma_c^2 & 0 & 0 \\ 0 & \Sigma_g & 0 \\ 0 & 0 & \Sigma_h \end{bmatrix}.
\] (35)

The utility of this model is that if we have a collection of observations \( \{\hat{\ell}(x_1), \ldots, \hat{\ell}(x_N)\} \) then we can infer the cost function (and its associated gradient and Hessian) at any \( x \) value based on the standard conditional formulas

\[
\ell(x) = \mu_\ell(x) + K_{\ell,\hat{\ell}} K^{-1}_{\hat{\ell},\hat{\ell}} \begin{bmatrix} \hat{\ell}(x_1) - \mu_{\hat{\ell}}(x_1) \\ \vdots \\ \hat{\ell}(x_N) - \mu_{\hat{\ell}}(x_N) \end{bmatrix},
\] (36)
Require: A termination threshold value \( \epsilon > 0 \).
1: Set \( k = 1 \), and initialise \( x_k \).
2: Based on \( x_k \), estimate the cost function noise covariance \( \nu_e \) and the gradient covariance \( \Sigma_g \) empirically.
3: while \( \| g(x_k) \| > \epsilon \) do
4:  Obtain the cost and gradient measurements \( \ell(x_k) \).
5:  Use a gradient-based search algorithm to minimise \( f(x) \) from \( \ell(x) \) in (36) and set \( x_{k+1} \) to be the minimising argument.
   Note: \( \ell(x) \) must be updated for each new iterate generated within the search algorithm.
6:  Set \( k \rightarrow k + 1 \).
7: end while

where

\[
K_{\ell,\ell} = \begin{bmatrix}
k_{\ell,\ell}(x_1, x_1) & k_{\ell,\ell}(x_1, x_2) & \cdots & k_{\ell,\ell}(x_1, x_N) \\
k_{\ell,\ell}(x_2, x_1) & k_{\ell,\ell}(x_2, x_2) & \cdots & k_{\ell,\ell}(x_2, x_N) \\
\vdots & \vdots & \ddots & \vdots \\
k_{\ell,\ell}(x_N, x_1) & k_{\ell,\ell}(x_N, x_2) & \cdots & k_{\ell,\ell}(x_N, x_N)
\end{bmatrix}
\]

(37)

\[
K_{\ell,\ell} = [k_{\ell,\ell}(x_1, x_1) \quad k_{\ell,\ell}(x_1, x_2) \quad \cdots \quad k_{\ell,\ell}(x_1, x_N)].
\]

(38)

Therefore, the function \( \ell(x) \) in (36) can be considered a surrogate for the true cost function \( f(x) \), its gradient \( g(x) \) and its Hessian \( h(x) \). Importantly, the smoothness properties of \( \ell(x) \) are now controlled by the choice of which covariance function \( k(\cdot, \cdot) \) to use, which acts as a filtering mechanism. This is critical, since it allows us to make use of standard optimisation routines for smooth cost functions in optimising \( \ell(x) \). For example, classical Newton’s method algorithms (or quasi-Newton methods) can be employed. Importantly, observations of the cost function and its gradient that are collected during the search procedure can be rolled into the model so that \( \ell(x) \) more accurately models \( f(x) \). These ideas are formalised in Algorithm 2.

By way of a pedagogical example, consider a very simple problem where the cost function is given by the following quadratic function

\[
f(x) = \frac{5}{2} (x - 5)^2, \quad x \in \mathbb{R}.
\]

(39)

Assume that we only have access to noisy measurements of the cost function and its gradient according to (30a)–(30b) with \( \sigma_c = 20 \) and \( \Sigma_g = 1 \). Assuming that the mean function \( \mu_\ell(x) \) is zero everywhere, then Figure 1 shows the true cost function and the GP estimate as a standard gradient-based search algorithm proceeds based on the surrogate \( \ell(x) \) starting at \( x_1 = -10 \). Here, we have used a squared-exponential kernel \( k(x, x') = \sigma^2 e^{-0.5(x-x')^2} \), with \( \sigma = 10 \) and \( l = 0.01 \). This sequence of plots shows that the GP approach manages to capture the global shape of the cost function, while at the same time remaining largely un-affected by the noise. More interesting and challenging examples are provided in the subsequent section.

5 System identification experiments

As a testing ground for the probabilistic optimisation algorithms developed and reviewed above we have chosen to study the problem of identifying a nonlinear state-space model of the form

\[
\begin{align*}
x_{t+1} &= f(x_t, \theta) + w_t, \\
y_t &= g(x_t, \theta) + e_t.
\end{align*}
\]

(40a)

(40b)

Note that we will in this section switch to the standard notation used within system identification. Here \( x_t \in X \subseteq \mathbb{R}^n_x \) and \( y_t \in Y \subseteq \mathbb{R}^n_y \) denotes the state and the measurement, respectively. The dynamics and the measurements are modeled by the nonlinear functions \( f(\cdot) \) and \( g(\cdot) \) parameterised by the unknown parameters \( \theta \in \Theta \subseteq \mathbb{R}^n_\theta \). Finally, \( w_t \) and \( e_t \) denotes the process noise and measurement noise, respectively.
More specifically we will study the maximum likelihood formulation of the nonlinear system identification problem, which amounts to finding a point estimate of the unknown parameter $\theta$ in (40a) by solving the following optimisation problem

$$\hat{\theta}_{\text{ML}} = \arg \max_{\theta \in \Theta} p_\theta(y_{1:N}),$$

where $y_{1:N} = \{y_1, \ldots, y_N\}$. The likelihood function $L(\theta) = p_\theta(y_{1:N})$ is not available in closed form, however using sequential Monte Carlo methods (a.k.a. particle filters) [20, 21] we can compute unbiased estimates of the likelihood, by solving the following integral

$$L(\theta) = p_\theta(y_{1:N}) = \int p_\theta(y_{1:N}, x_{1:N}) dx_{1:N},$$

where the accuracy depends on the computational power we have available. For recent overviews and links into the rapidly expanding literature on the use of particle filters for nonlinear system identification we refer to [22, 23]. The idea of using a global GP model for the cost function in the nonlinear system identification problem has previously been explored in [24], but only using noisy observations of the Likelihood, not its gradients.

We will in Section 5.1 show the performance on a simple and controlled example where we can compute true cost function and the true optimal solution using alternative methods. This is to instill confidence in that both methods do
Based on these positive results, we conducted a further Monte–Carlo simulation, again comprising 100 runs, where each run involves the generation of a new dataset for each Monte–Carlo run. The top–left plot in Figure 2 shows the results for the Monte–Carlo runs. Perhaps not surprisingly, all algorithms made possible because the GP approximation is smooth. This is not true of Algorithm 1, which ran to the maximum number of iterations for every run.

For this simulation study, the GP hyperparameters used in Algorithm 1 were chosen as $B_1 = 100I$, $C_1 = I$, $V = 10^{-3}I$ and $\sigma^2 = 1$. For Algorithm 2 we employed a squared exponential covariance function $k(\theta, \theta') = \sigma^2 \exp(-0.5(\theta - \theta')^T V(\theta - \theta'))$ with $\sigma = 200$ and $V$ chosen as a diagonal matrix with diagonal entries $\{2, 2, 2, 20\}$.

The top–left plot in Figure 2 shows the results for the Monte–Carlo runs. Perhaps not surprisingly, all algorithms produced identical transfer function estimates for the noise-free case, so we have shown only one plot.

Based on these positive results, we conducted a further Monte–Carlo simulation, again comprising 100 runs, where noise was deliberately added to both the Likelihood and gradient. Specifically, we are interested in estimating the parameters $\theta = \{a, c, q, r\}$ for the following system

$$
x_{t+1} = ax_t + w_t, \quad w_t \sim \mathcal{N}(0, q),
$$

$$
y_t = cx_t + e_t, \quad e_t \sim \mathcal{N}(0, r).
$$

The true values for the system are $a^* = 0.9$, $c^* = 1.0$, $q^* = 0.1$ and $r^* = 0.5$. The initial state is given by $x_1 \sim \mathcal{N}(0, 1)$.

For a given set of measurements $y_1:N$ it is possible to calculate the likelihood $L(\theta)$ and its gradient $\nabla_{\theta} L(\theta)$ via standard Kalman filter equations and then employ standard gradient-based search algorithms to obtain $\hat{\theta}$ that maximises the Likelihood. In this regard, the problem does not suffer from noisy Likelihood and gradient calculations, which serves the purpose of profiling Algorithms 1 and 2 in the noise-free case.

To that end, we generated a Monte–Carlo simulation with 100 runs, where each run involves the generation of a new dataset $Y_N$ according to system (43). Furthermore, the initial parameter vector $\theta_0$ was selected at random via moving each element within a range of 50% of the true value. A standard gradient-based search algorithm and Algorithms 1 and 2 were all provided with the same initial conditions and dataset for each Monte–Carlo run.

For this simulation study, the GP hyperparameters used in Algorithm 1 were chosen as $B_1 = 100I$, $C_1 = I$, $V = 10^{-3}I$ and $\sigma^2 = 1$. For Algorithm 2 we employed a squared exponential covariance function $k(\theta, \theta') = \sigma^2 \exp(-0.5(\theta - \theta')^T V(\theta - \theta'))$ with $\sigma = 200$ and $V$ chosen as a diagonal matrix with diagonal entries $\{2, 2, 2, 20\}$.

The top–left plot in Figure 2 shows the results for the Monte–Carlo runs. Perhaps not surprisingly, all algorithms produced identical transfer function estimates for the noise-free case, so we have shown only one plot.

Based on these positive results, we conducted a further Monte–Carlo simulation, again comprising 100 runs, where noise was deliberately added to both the Likelihood and gradient. Specifically,

$$
\tilde{L}(\theta) = L(\theta) + v_c, \quad v_c \sim (0, 10^5),
$$

$$
\nabla_{\theta} \tilde{L}(\theta) = \nabla_{\theta} L(\theta) + v_g, \quad v_g \sim (0, 25I).
$$

Again, each run involved the generation of a new dataset and this time the initial parameters were chosen as $\theta_0 = \{a^*/10, c^*/10, q^*/10, r^*/10\}$, in order to ensure that the results were not just a function of randomly chosen initial parameters. Again, we ran both a standard gradient-based search algorithm and Algorithms 1 and 2 for each run.

The right-hand column of plots in Figure 2 shows the Bode responses for each estimated system. As possibly expected, the standard gradient-search algorithm often fails to converge due to the presence of noisy cost and gradient evaluations hence resulting in a large variation of estimated transfer functions. In many cases it is impossible to know if the search direction is actually a descent direction, and at the same time a line-search algorithm often fails to find a suitable scaling parameter since it is based on noisy function evaluations.

Contrasting this, Algorithms 1 and 2 appear to generate estimates that have a similar distribution to the noise-free case. It is difficult to discern which of these two algorithms that performs best. One notable difference between them is that Algorithm 2 was able to terminate based on standard stopping criteria (small gradient norm for example), which is made possible because the GP approximation is smooth. This is not true of Algorithm 1, which ran to the maximum allowed (100) iterations for every run.

While we recognise that it is dangerous to draw definitive conclusions from this limited study, it is nevertheless very encouraging results.
5.2 More Challenging Nonlinear Example

Encouraged by the results obtained above for the noisy linear case, here we consider a more challenging problem of identifying the parameters $b$ and $q$ for the following nonlinear and time-varying state-space model,

\[ x_{t+1} = 0.5x_t + b \frac{x_t}{1 + x_t^2} + 8 \cos(1.2t) + qw_t, \]
\[ y_t = 0.05x_t^2 + e_t, \]

where

\[ \begin{bmatrix} w_t \\ e_t \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 0.1 \end{bmatrix} \right) \]

and the true parameters are $b^* = 25$ and $q^* = 0.1^{1/2}$. This example has previously been investigated by the current authors [25] and is profiled again here due to it being acknowledged as a challenging problem [26, 27].

Algorithms 1 and 2 were employed to estimate $b$ and $q$ based on 100 Monte–Carlo runs using $N = 100$ data points for each run as generated by (45) with the true parameter values. The initial parameter values were chosen randomly in each simulation where the value was chosen uniformly within a 50% range of the true value. The algorithms were allowed to iterate for no more than 100 iterations.
In this case, Algorithm 1 was employed with exactly the same hyperparameter choices as for the linear example. Algorithm 2 was employed using the covariance function used above, but with $\sigma = 10^3$ and $V$ chosen as a diagonal matrix with entries $\{0.01, 1\}$.

In the case of Algorithm 2 we employed the availability of the Hessian approximation from the GP in order to employ a Newton type algorithm, rather than a quasi-Newton algorithm as before. While this is not strictly necessary, it highlights the flexibility of that approach.

The likelihood and its gradient cannot be calculated exactly in this case and we therefore employed sequential Monte Carlo methods and Fisher’s identity [28, 29] to provide noisy estimates of both. The number of particles used to calculate these terms was 500 in all cases. Note that each simulation required no more than 8 seconds of computation time on a MacBook Pro 2.8GHz Intel i7.

The results of this Monte–Carlo simulation can be observed in Figure 3. For Algorithm 2 we have removed 19 of the 100 simulation results due to convergence to a local minima, which resulted in a final parameter value that was greater than 5% in error relative true parameter value. For Algorithm 1 we removed only 1 simulation result due to the same criteria.

Again, it is dangerous to draw too many conclusions from these results. At the same time, the performance of Algorithm 1 appears to be slightly better than Algorithm 2, which may be related to the choice of hyperparameters for the latter method.

![Figure 3: Iterations of parameter values using the GP Hessian approximation in Algorithm 1 (left column) and the global GP of Algorithm 2 (right column) with estimates in red and true value shown as solid blue.](image)
It is interesting to visually observe the effect of using the global GP model offered by Algorithm 2 in terms of smoothing the cost function. The current example is known to exhibit erratic likelihood behaviour at extreme points in the parameter space [29]. This is perhaps best visualised by restricting to just one parameter, in this case the $b$ parameter. Figure 4 shows a sequence of plots where progressively more samples are used to model the underlying likelihood. It can be verified in these plots that the likelihood changes rapidly at the extremities of the $b$ range, and yet the GP approximation remains smooth and captures the global behaviour.

Figure 4: The surrogate cost function modeled as a global GP according to Algorithm 2 (red solid line with grey shading to indicate uncertainty) and the true cost function given by the likelihood (solid blue). Sample points are shown as black circles.

6 Discussion

Minimising a nonlinear cost function $f(x)$ is a challenging problem in general, and as verified again here, is made even more difficult if the cost function and its derivatives cannot be evaluated without unknown errors. These latter types of stochastic problems have been considered for some time now, and yet very recent results in [30] show that this is still an active area of research. The main thrust of current activities is to capture the curvature information available from noisy gradient measurements. In the current paper, we have developed a new approach and reviewed an existing approach for capturing this curvature information that both rely on Bayesian non-parametric estimates of the unknown functions. The first treats the Hessian matrix as an unknown function and employs integral observations of the gradient.
vector in order to form the curvature estimate. The second approach employs a GP for the entire cost function and is based on noisy observations of the cost, its gradient and possibly even Hessian matrix.

Both approaches appear to have merit and we believe that these approaches deserve further attention. Specifically, to the best of our knowledge, the choice of covariance functions and the corresponding selection of hyperparameters has not been explored in a rigorous manner. For example, Student-t processes [31] might be a natural way to reduce the effect of spurious large errors in the function or gradient. The question of adaptively tuning the hyperparameters as these algorithms progress also deserves more attention. Other areas to explore include suitable stopping criteria for problems involving stochastic cost functions, and the problem of reducing computational load by employing GP approximations.

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A Derivation of the standard quasi-Newton equations

Recall the optimisation problem outlined in (9),

$$B_k = \min_B \|B - B_{k-1}\|_W^2 \quad \text{s.t.} \quad B = B^T \quad \text{and} \quad Bs_k = y_k.$$  \hfill (46)

Note that

$$\|B - B_{k-1}\|_W^2 \equiv \text{trace} \, W(B - B_{k-1})^T W(B - B_{k-1}) = (\overrightarrow{B} - \overrightarrow{B}_{k-1})^T (W \otimes W)(\overrightarrow{B} - \overrightarrow{B}_{k-1})$$  \hfill (47)

and where $\overrightarrow{B}$ is the usual vectorization operator that stacks the columns of $B$ on top of one another to form a column vector, and $\otimes$ is the Kronecker product.

Another way to write the optimisation problem is in terms of the column vector $\overrightarrow{B}$ so that $\overrightarrow{B}_k$ is the solution to the following constrained optimization problem

$$\max_{\overrightarrow{B}} (\overrightarrow{B} - \overrightarrow{B}_{k-1})^T (W \otimes W)(\overrightarrow{B} - \overrightarrow{B}_{k-1}),$$  \hfill (48)

s.t. \hspace{1em} $\Gamma \overrightarrow{B} = 0$,

$$\hspace{1em} (s_k^T \otimes I)\overrightarrow{B} = y_k,$$

where $\Gamma \equiv I - P$, and $P$ is the vec-permutation matrix that has the property $P \overrightarrow{B} = \overrightarrow{B^T}$. Therefore, $\Gamma \overrightarrow{B} = 0$ is equivalent to $B = B^T$. If we define some new variables

$$b \equiv \overrightarrow{B},$$  \hfill (49a)

$$b_k \equiv \overrightarrow{B}_k,$$  \hfill (49b)

$$V \equiv W \otimes W,$$  \hfill (49c)

$$S_k \equiv s_k^T \otimes I,$$  \hfill (49d)

then we can rewrite the minimisation problem as

$$b_k = \min_b \, (b - b_{k-1})^T V (b - b_{k-1}),$$  \hfill (50)

s.t. \hspace{1em} $\Gamma b = 0$,

$$S_k b = y_k.$$
A suitable Lagrangian for this problem is

\[ L(b, \lambda, \eta) = \frac{1}{2} b^T V b - b^T V b_{k-1} + \frac{1}{2} b_{k-1}^T V b_{k-1} - \lambda^T (\Gamma b) + \eta^T (y_k - S_k b). \]  

(51)

Note that the first order necessary conditions of optimality require that

\[ \nabla_b L = V b - V b_{k-1} - \Gamma^T \lambda - S_k^T \eta = 0. \]  

(52)

This implies that

\[ \Gamma^T \lambda = V (b - b_{k-1}) - S_k^T \eta. \]  

(53)

Recall that \( \Gamma = \Gamma^T \) and that if we define

\[ \lambda \triangleq \bar{\lambda}, \]  

(54)

then

\[ \Gamma^T \lambda = \Lambda - \Lambda^T. \]  

(55)

So from (53) and the inverse vec operator

\[ \Lambda - \Lambda^T = W(B - B_{k-1}) W - \eta s_k^T. \]  

(56)

We can add \((\Lambda - \Lambda^T)^T\) to the left hand side to reveal that

\[ \Lambda - \Lambda^T + (\Lambda - \Lambda^T)^T = 0, \]  

(57)

so that

\[ 0 = W(B - B_{k-1}) W - \eta s_k^T + W(B - B_{k-1}) W - s_k \eta^T. \]  

(58)

In the above we have exploited the fact that \( W, B \) and \( B_{k-1} \) are symmetric. This implies that

\[ B = B_{k-1} + \frac{1}{2} W^{-1} (\eta s_k^T + s_k \eta^T) W^{-1}. \]  

(59)

From the constraints we have that

\[ B s_k = y_k = B_{k-1} s_k + \frac{1}{2} W^{-1} (\eta s_k^T + s_k \eta^T) W^{-1} s_k. \]  

(60)

So that

\[ W^{-1} (\eta s_k^T + s_k \eta^T) W^{-1} s_k = 2(y_k - B_{k-1} s_k). \]  

(61)

This implies that

\[ \eta = \frac{2W(y_k - B_{k-1} s_k) - s_k \eta^T W^{-1} s_k}{s_k^T W^{-1} s_k} \]  

(62)

Post multiplying \( \eta^T \) by \( W^{-1} s_k \) results in

\[ \eta^T W^{-1} s_k = \frac{2(y_k - B_{k-1} s_k)^T W W^{-1} s_k - s_k^T W^{-1} \eta s_k W^{-1} s_k}{s_k^T W^{-1} s_k} \]

\[ = \frac{2(y_k - B_{k-1} s_k)^T W W^{-1} s_k}{s_k^T W^{-1} s_k} - s_k^T W^{-1} \eta \]

\[ = \frac{2(y_k - B_{k-1} s_k)^T W W^{-1} s_k}{s_k^T W^{-1} s_k} - \eta^T W^{-1} s_k \]  

(63)
Therefore
\[ 2\eta^T W^{-1} s_k = \frac{2(y_k - B_{k-1}s_k)^T W W^{-1}s_k}{s_k^T W^{-1} s_k} \] (64)

Cancelling the common 2 factor and substituting this into (62) provides
\[ \eta = \frac{2W(y_k - B_{k-1}s_k) - s_k(y_k - B_{k-1}s_k)^T s_k}{s_k^T W^{-1} s_k} = \frac{2W(y_k - B_{k-1}s_k)}{s_k^T W^{-1} s_k} - \frac{s_k(y_k - B_{k-1}s_k)^T s_k}{(s_k^T W^{-1} s_k)^2} \] (65)

Recall from (59) that
\[ B = B_{k-1} + \frac{1}{2} W^{-1}(\eta s_k^T + s_k \eta^T)W^{-1} \] (66)

Substituting (65) into (66) results in
\[
B = B_{k-1} + \frac{(y_k - B_{k-1}s_k)s_k^T W^{-1}}{s_k^T W^{-1} s_k} - \frac{1}{2} W^{-1} s_k(y_k - B_{k-1}s_k)^T s_k s_k^T W^{-1} - \frac{W^{-1} s_k(y_k - B_{k-1}s_k)^T s_k}{2(s_k^T W^{-1} s_k)^2}
\]
(67)

Noting that \(s_k^T (y_k - B_{k-1}s_k) = (y_k - B_{k-1}s_k)^T s_k\) and collecting like terms gives
\[
B = B_{k-1} + \frac{W^{-1} s_k(y_k - B_{k-1}s_k)^T + (y_k - B_{k-1}s_k)s_k^T W^{-1}}{s_k^T W^{-1} s_k} - \frac{W^{-1} s_k(y_k - B_{k-1}s_k)^T s_k s_k^T W^{-1}}{(s_k^T W^{-1} s_k)^2}
\] (68)

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