Stochastic quasi-Newton with adaptive step lengths for large-scale problems

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Abstract

We provide a numerically robust and fast method capable of exploiting the local geometry when solving large-scale stochastic optimisation problems. Our key innovation is an auxiliary variable construction coupled with an inverse Hessian approximation computed using a receding history of iterates and gradients. It is the Markov chain nature of the classic stochastic gradient algorithm that enables this development. The construction offers a mechanism for stochastic line search adapting the step length. We numerically evaluate and compare against current state-of-the-art with encouraging performance on real-world benchmark problems where the number of observations and unknowns is in the order of millions.

1 Introduction

We are interested in the unconstrained stochastic non-convex optimisation problem

\[
\min_{x \in \mathbb{R}^d} f(x),
\]

when the cost function \( f(x) \) is on the form

\[
f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x) + R(x),
\]

where \( d \) denotes the dimension of the unknown variable \( x \) and \( n \) denotes the number of available observations, i.e. the size of the dataset. Here, \( f_i(x) \) denotes a loss function and \( R(x) \) denotes a regularizer. The stochasticity of the problem is due to the fact that we only have access to noisy evaluations of the cost function \( f(x) \) and its gradient \( \nabla f(x) \) according to

\[
f_k = f(x_k) + e_k, \quad g_k = \nabla f(x)|_{x=x_k} + v_k.
\]

Here \( e_k \) and \( v_k \) denotes the noise on the function and gradient evaluations, respectively. We take a particular interest in situations where the number of data \( n \) and/or the number of unknowns \( d \) are very large.

The stochastic optimisation problem (1) is one of the most commonly encountered problems within supervised machine learning. The stochastic nature of the problem arises in different ways. First we mention large-scale problems where it is prohibitive to evaluate the cost function and its gradient on the entire dataset. Instead it is divided into several mini-batches via a subsampling procedure, which also explains where the noise arises. As a second example we mention the use of numerical algorithms in approximately computing the cost function and its gradients, inevitably resulting in stochastic optimisation problems. We illustrate the result of our new developments on a problem of the first kind in Figure 1, namely the optimisation problem arising in training a deep convolutional neural network.
Figure 1: Solving the optimisation problem used in training a state-of-the-art deep convolutional neural network (CNN) used for recognizing images of handwritten digits from the MNIST data. Alg1 refers to our new developments in this paper, SG refers to basic stochastic gradient and Adam refers to Kingma and Ba (2015). For a full account of these experiments, see Section 6.

The first stochastic optimisation algorithm was introduced almost 70 years ago by Robbins and Monro (1951). They made use of first-order information only, motivating the name stochastic gradient (SG) which is the contemporary machine learning term for these algorithms originally referred to as stochastic approximation. Interestingly most SG algorithms are not decent methods, since the stochastic nature of the update can easily produce a new iterate corresponding to an increase in the cost function, which is illustrated in Figure 1. Instead they are in fact Markov chain methods, due to the fact that their update rule actually defines a particular Markov chain. This was indeed also clearly acknowledged already in the seminal paper by Robbins and Monro (1951).

Contributions and key properties: We will heavily build upon the Markov chain nature of SG and our key contribution is a new construction enabled via an auxiliary variable trick allowing us to define an extended Markov chain. The key feature of this construction is that we can efficiently make use of second-order (curvature) information in computing the search direction. This curvature information stems from an estimate of the inverse Hessian that we compute using a bounded history of previous iterates and stochastic gradients. The computational cost and memory footprint of this computation scales linearly in the number of data. Another important contribution is a stochastic line search capable of adapting the step length. From our numerical experiments we can see that this capability seems beneficial, especially in the beginning. A practical feature is that our method only requires the user to select three tuning parameters, the size of the mini-batch, the size of the memory and the weight of a regulariser. We also develop a method for updating a Cholesky factor given the new measurement pair making our approach computationally cheap and numerically robust, which we illustrate using extensive numerical experiments comparing against current state-of-the-art methods on challenging large-scale real-world problems.

2 Background and related work

Many numerical optimisation algorithms can be interpreted as learning algorithms, where the first step is to build a local model of the cost function $f(x)$. This local model is then used to compute the next iterate, a new model is learned around this new iterate and the procedure is repeated. The so-called second-order methods make use of quadratic Taylor series approximations $q_k(x)$ of $f(x)$ around the current iterate $x_k$

$$q_k(x) = f(x_k) + g_k^T(x-x_k) + \frac{1}{2}(x-x_k)^TH_k^{-1}(x-x_k),$$  

(3)
where $g_k$ denotes an approximation of the gradient $\nabla f(x_k)$ and $H_k$ denotes an approximation of the inverse Hessian $(\nabla^2 f(x_k))^{-1}$. Direct minimisation of the quadratic model (3) suggests the following update of the iterates

$$
x_{k+1} = x_k - \alpha_k H_k g_k,
$$

where $\alpha_k$ denotes the step length. The matrix $H_k$ will be referred to as the scaling matrix since it scales the gradient approximation $g_k$. Many algorithms (including our present developments) update the iterates according to (4), but they differ greatly in how the components are found. Choosing the scaling matrix to be the identity $H_k = I$ we are back at the basic first-order gradient methods and with $H_k = (\nabla^2 f(x_k))^{-1}$ we have Newton’s method. The quasi-Newton methods sit somewhere in between these two extremes, in that they employ a scaling matrix $H_k$ that is a tractable approximation of the inverse Hessian. It is indeed this partial use of second-order information (curvature) that makes the quasi-Newton methods more robust and capable of reaching higher accuracy compared to pure gradient-based methods. The standard quasi-Newton method is the BFGS method, named after its inventors (Broyden, 1967; Fletcher, 1970; Goldfarb, 1970; Shanno, 1970). In its basic form this algorithm does not scale to the large-scale settings we are interested in. The idea of only making use of the most recent iterates and gradients in forming the inverse Hessian approximation was later suggested by Nocedal (1980) and Liu and Nocedal (1989). The result is a computationally cheaper method with a significantly reduced memory footprint, explaining the name L-BFGS, where the L stands for limited memory. Due to its simplicity and good performance this has become one of the most commonly used second-order methods for large-scale problems. Our developments make use of the same trick underlying L-BFGS, but it is carefully tailored to the stochastic setting. After this background let us now turn our attention to the most relevant related work when it comes to solving the stochastic problems we are interested in.

The basic first-order SG algorithms have recently been significantly improved by the introduction of various noise reduction techniques, including the following methods; stochastic variance reduced gradient (SVRG) by Johnson and Zhang (2013), Stochastic average gradient (SAG) (Schmidt et al., 2013), Semi-Stochastic Gradient Descent (S2GD) (Konečný and Richtárik, 2017), and SAGA (Defazio et al., 2014). They all compute the gradient approximation via subsampling. There has recently also been some developments for non-convex settings, see e.g. Reddi et al. (2016) and Allen-Zhu and Hazan (2016). A thorough and forward-looking overview of the SG algorithm and its use within a modern machine learning context is provided by Bottou et al. (2017). It also includes interesting accounts of possible improvements along the lines of first-order noise reduction techniques and second-order methods.

The well-known drawback of all first-order methods is that they do not make use of any curvature information. Analogously to the deterministic setting we can assemble methods that are numerically more robust and achieve better performance in general by also extracting and using second-order information, i.e. the curvature that is maintained in the form of the Hessian matrix or an approximation of it. Over the past decade we have witnessed increasing capabilities of these so-called stochastic quasi-Newton methods. There is still scope for significant developments when it comes to methods in this class and in this paper we aim to push the current boundaries.

The work by Schraudolph et al. (2007) developed modifications of BFGS and its limited memory version applicable to online stochastic optimisation problems. There has also been a series of papers approximating the scaling matrix $H_k$ with a diagonal matrix, see e.g. Bordes et al. (2009) and Duchi et al. (2011). The idea of exploiting regularization together with BFGS was successfully introduced by Mokhtari and Ribeiro (2014), where the scaling matrix $H_k$ was modified using regularization. Later they (Mokhtari and Ribeiro, 2015) also developed a stochastic L-BFGS algorithm without regularization. The idea of replacing the stochastic gradient difference in the BFGS update with a subsampled Hessian-vector product was recently introduced by Byrd et al. (2016) and Wang et al. (2017) introduced a damped L-BFGS method.

Over the past five years we have also seen quite a lot of fruitful activity in combining the stochastic quasi-Newton algorithms with various first-order noise reduction methods. Moritz et al. (2016) successfully showed that it is possible to combine the L-BFGS methods by Byrd et al. (2016) with the SVRG noise reduction algorithm by Johnson and Zhang (2013) to reduce the problem with noisy gradients. Along this line of work we also find Gower et al. (2016) where the authors introduced a stochastic block BFGS update that they then combined with the SVRG method.

Contrary to almost all of the existing work mentioned above we make explicit use of and build upon the fact that the SG algorithm is a particular Markov chain designed specifically to solve the stochastic optimisation problem.

Related to the Markov chain theme, the highly innovative work by Welling and Teh (2011) has recently sparked a relevant parallel development within the Markov chain Monte Carlo (MCMC) literature for the case when $f(x)$ can
be interpreted as a likelihood function. The aim is to exploit the geometry of the target distribution (the posterior) by using constructions from stochastic optimisation and Langevin diffusion dynamics. The use of a carefully designed local curvature estimate was enabled by Simsekli et al. (2016) when they incorporated ideas from L-BGFS within an MCMC setting. The main focus of this MCMC work has been directed towards exploring the posterior distribution when the chain is initialised at a “good” initial point (e.g. Teh et al. (2016) assume a MAP estimate to start the chain). In contrast, here we are primarily interested in rapid convergence towards an area of minimum cost from any initial point and for a more general class of cost functions.

3 Algorithm summary

The key innovation in our solution lies in an auxiliary variable construction allowing for line search within a stochastic quasi-Newton setting. Hence, we are no longer forced to make use of decreasing step lengths in solving stochastic optimisation problems. As can be seen in Algorithm 1 the overall structure of our solution is similar to most existing solutions, but all details have been carefully tailored to the stochastic setting. We start by describing how the search direction is calculated (rows 4-5) in Section 4. Here, we take care to derive a numerically robust and fast update of the inverse Hessian approximation. The auxiliary variables construction (rows 7-9) described in Section 5 allows for the use of step lengths that adapt according to the local geometry, resulting in a functionality very similar to standard deterministic second-order algorithms with line search.

4 Search direction computation

In this section we address the problem of computing a search direction based on having a limited memory available for storing previous gradients and associated iterates. The approach we adopt is similar to limited memory quasi-Newton methods, but here we employ a direct least-squares estimate of the inverse Hessian matrix rather than more well-known methods such as damped L-BFGS and L-SR1. The main reason for considering the least-squares approach is that it appears to perform quite well against the alternative methods for the class of problems considered in this paper. We construct a limited-memory inverse Hessian approximation in Section 4.1 and show how to update this representation in Section 4.2. Section 4.3 provides a means to ensure that a descent direction is calculated.

4.1 Inverse Hessian approximation

According to the Secant condition (see e.g. Fletcher (1987)), the inverse Hessian matrix $H_k$ should satisfy

$$ H_k y_k = s_k, \quad (9) $$

where $y_k = g_k - g_{k-1}$ and $s_k = x_k - x_{k-1}$. Since there are generally more unknown values in $H_k$ than can be determined from $y_k$ and $s_k$ alone, quasi-Newton methods update $H_k$ from a previous estimate by solving problems of the type

$$ H_k = \arg \min_H \| H - H_{k-1} \|_{F,W}^2 $$

subject to $H = H^T$, $H y_k = s_k$, \quad (10)

where $\|X\|_{F,W}^2 = \|XW\|_F^2 = \text{trace}(W^T X^T X W)$ and the choice of weighting matrix $W$ results in different algorithms (see Hennig (2015) for an interesting perspective on this).

Here we employ a similar approach and determine $H_k$ as the solution to the following regularised least-squares problem

$$ H_k = \arg \min_H \| H Y_k - S_k \|_F^2 + \lambda \| H - \bar{H}_k \|_F^2, \quad (11) $$

where $Y_k$ and $S_k$ hold a limited number of past $y_k$’s and $s_k$’s according to

$$ Y_k \triangleq [y_k-m+1, \ldots, y_k], \quad (12a) $$

$$ S_k \triangleq [s_k-m+1, \ldots, s_k], \quad (12b) $$
Algorithm 1 Stochastic quasi-Newton with line search

Require: An initial estimate $x_1$, a maximum number of iterations $k_{\text{max}}$ and maximum step-length $0 < \alpha_k \leq 1$. Choose $\rho \in \{0, 1\}$, where $\rho = 1$ provides SG decay rate on step length $\alpha_k$, and $\rho = 0$ guarantees that the step-length will not exceed $\bar{\alpha}_k$. Choose a step-length scaling factor $\kappa \in (0, 1)$.

1: Set $k = 1$ and $\alpha_k = \bar{\alpha}_k$ and perform the following.
2: while $k < k_{\text{max}}$ do
3: Search direction calculation:
4: Obtain a measurement of the cost function and its gradient
   \begin{align*}
   f_k &= f(x_k) + e_k, \tag{5a} \\
   g_k &= \nabla f(x_k) + v_k. \tag{5b}
   \end{align*}
5: Calculate a search direction $p_k$ such that
   \begin{align*}
   \begin{cases}
   p_k^T g_k < 0, & \|g_k\| > 0, \\
   p_k = 0, & \text{otherwise.}
   \end{cases} \tag{6}
   \end{align*}
6: New iterate calculation:
7: Compute proposal $\xi_{k+1} = x_k + \alpha_k p_k$.
8: Calculate the acceptance indicator variable
   \begin{align*}
   c_k = \begin{cases}
   1, & \text{w.p. } \max\{\rho, a(\xi_{k+1} | x_k)\}, \\
   0, & \text{otherwise.}
   \end{cases} \tag{7}
   \end{align*}
9: Update the variables
   \begin{align*}
   x_{k+1} &= x_k + c_k \alpha_k p_k, \tag{8a} \\
   p_{k+1} &= p_k, \tag{8b} \\
   \alpha_{k+1} &= c_k \left(\frac{1}{k}\right)^{\rho} \bar{\alpha}_k + (1 - c_k) \kappa \alpha_k. \tag{8c}
   \end{align*}
10: if $c_k = 0$ then
11: Set $k \leftarrow k + 1$ and return to step 7.
12: else
13: Set $k \leftarrow k + 1$ and return to step 2.
14: end if
15: end while

and $m << n$ is the memory limit. The regulator matrix $\tilde{H}_k$ acts as a prior on $H$ and can be modified at each iteration $k$. The parameter $\lambda > 0$ is used to control the relative cost of the two terms in (11). It can be verified that the solution to the above least-squares problem (11) is given by
\begin{equation}
H_k = \left(\lambda I + Y_k Y_k^T\right)^{-1} \left(\lambda \tilde{H}_k + Y_k S_k^T\right), \tag{13}
\end{equation}
where $I$ denotes the identity matrix. The above inverse Hessian estimate can be used to generate a search direction in the standard manner by scaling the negative gradient, that is
\begin{equation}
p_k = -H_k g_k. \tag{14}
\end{equation}
However, for large-scale problems this is not practical since it involves the inverse of a large matrix. To ameliorate this difficulty, we adopt the standard approach by storing only a minimal (limited memory) representation of the inverse Hessian estimate $\tilde{H}_k$. To describe this, note that the dimensions of the matrices involved are
\begin{equation}
H_k \in \mathbb{R}^{d \times d}, \quad Y_k \in \mathbb{R}^{d \times m}, \quad S_k \in \mathbb{R}^{d \times m}. \tag{15}
\end{equation}
We can employ the Sherman–Morrison–Woodbury formula to arrive at the following equivalent expression for $H_k$

$$H_k = \left[ I - Y_k \left( \lambda I + Y_k^T Y_k \right)^{-1} Y_k^T \right] \left( H_k + \lambda^{-1} Y_k S_k^T \right). \quad (16)$$

Importantly, the matrix inverse $(\lambda I + Y_k^T Y_k)^{-1}$ is now by construction a positive definite matrix of size $m \times m$. Therefore, we will construct and maintain a Cholesky factor of $I + Y_k^T Y_k$ since this leads to efficient solutions. In particular, if we express this matrix via a Cholesky decomposition

$$R_k^T R_k = \lambda I + Y_k^T Y_k, \quad (17)$$

where $R_k \in \mathbb{R}^{m \times m}$ is an upper triangular matrix, then the search direction $p_k = -H_k g_k$ can be computed via

$$p_k = -z_k + Y_k w_k, \quad (18a)$$

$$z_k = \tilde{H}_k g_k + \lambda^{-1} Y_k (S_k^T g_k), \quad (18b)$$

$$w_k = R_k^{-1} \left( R_k^T (Y_k^T s_k) \right). \quad (18c)$$

Constructing $R_k$ can be achieved in several ways. The so-called normal-equation method constructs the (upper triangular) part of $\lambda I + Y_k^T Y_k$ and then employs a Cholesky routine, which produces $R_k$ in $O({m(m+1)}^2 + m^3/3)$ operations. Alternatively, we can compute $R_k$ by applying Givens rotations or Householder reflections to the matrix

$$M_k = \begin{bmatrix} \sqrt{\lambda} I & \vspace{0.3cm} \\ \vspace{0.3cm} Y_k \end{bmatrix}. \quad (19)$$

This costs $O(2m^2((n + m) - m/3)$ operations, and is therefore more expensive, but typically offers better numerical accuracy (Golub and Van Loan, 2012).

### 4.2 Fast and robust inclusion of new measurements

In order to maximise the speed, we have developed a method for updating a Cholesky factor given the new measurement pair $(s_{k+1}, y_{k+1})$. Suppose we start with a Cholesky factor $R_k$ at iteration $k$ such that

$$R_k^T R_k = \lambda I + Y_k^T Y_k \quad (20)$$

and that we are given a new measurement pair $(s_{k+1}, y_{k+1})$. Assume, without loss of generality, that $Y_k$ and $S_k$ are ordered in the following manner

$$Y_k \triangleq [Y_1, y_{k-m+1}, Y_2], \quad (21a)$$

$$S_k \triangleq [S_1, s_{k-m+1}, S_2], \quad (21b)$$

where $Y_1$, $Y_2$, $S_1$ and $S_2$ are defined as

$$Y_1 \triangleq [y_{k-m+\ell+1}, \ldots, y_k], \quad (22a)$$

$$Y_2 \triangleq [y_{k-m+2}, \ldots, y_{k-m+\ell}], \quad (22b)$$

$$S_1 \triangleq [s_{k-m+\ell+1}, \ldots, s_{k}], \quad (22c)$$

$$S_2 \triangleq [s_{k-m+2}, \ldots, s_{k-m+\ell}], \quad (22d)$$

and $\ell$ is an appropriate integer so that $Y_k$ and $S_k$ have $m$ columns. The above ordering arises from “wrapping-around” the index when storing the measurements. We create the new $Y_{k+1}$ and $S_{k+1}$ by replacing the oldest column entries, $y_{k-m+1}$ and $s_{k-m+1}$, with the latest measurements $y_{k+1}$ and $s_{k+1}$, respectively, so that

$$Y_{k+1} \triangleq [Y_1, y_{k+1}, Y_2], \quad (23a)$$

$$S_{k+1} \triangleq [S_1, s_{k+1}, S_2], \quad (23b)$$
The aim is to generate a new Cholesky factor $R_{k+1}$ such that

$$R_{k+1}^{T} R_{k+1} = \lambda I + Y_{k+1}^{T} Y_{k+1}. \quad (24)$$

To this end, let the upper triangular matrix $R_k$ be written conformally with the columns of $Y_k$ as

$$R_k = \begin{bmatrix} \mathcal{R}_1 & r_1 & \mathcal{R}_2 \\ r_2 & r_3 & \mathcal{R}_4 \end{bmatrix} \quad (25)$$

so that $\mathcal{R}_1$ and $\mathcal{R}_2$ have the same number of columns as $Y_1$ and $Y_2$, respectively. Furthermore, $r_1$ is a column vector, $r_2$ is a scalar and $r_3$ is a row vector. Therefore,

$$R_k^{T} R_k = \begin{bmatrix} \mathcal{R}_1^{T} \mathcal{R}_1 & \mathcal{R}_1^{T} r_1 & \mathcal{R}_1^{T} \mathcal{R}_2 \\ \cdot & r_2^2 + r_1^2 r_1 & r_1^{T} \mathcal{R}_2 + r_2 r_3 \\ \cdot & \cdot & \mathcal{R}_4^{T} \mathcal{R}_4 + \mathcal{R}_2^{T} \mathcal{R}_2 + r_3^{T} r_3 \end{bmatrix}$$

$$= \begin{bmatrix} \lambda I + Y_1^{T} Y_1 & Y_1^{T} y_{k-m+1} & Y_1^{T} Y_2 \\ \cdot & \lambda + y_{k-m+1}^{T} y_{k-m+1} & y_{k-m+1}^{T} Y_2 \\ \cdot & \cdot & \lambda I + Y_2^{T} Y_2 \end{bmatrix}$$

(26)

By observing a common structure for the update $\lambda I + Y_{k+1}^{T} Y_{k+1}$ it is possible to write

$$\lambda I + Y_{k+1}^{T} Y_{k+1}$$

$$= \begin{bmatrix} \lambda I + Y_1^{T} Y_1 & Y_1^{T} y_{k-m+1} & Y_1^{T} Y_2 \\ \cdot & \lambda + y_{k-m+1}^{T} y_{k-m+1} & y_{k-m+1}^{T} Y_2 \\ \cdot & \cdot & \lambda I + Y_2^{T} Y_2 \end{bmatrix}$$

$$= \begin{bmatrix} \mathcal{R}_1^{T} \mathcal{R}_1 & \mathcal{R}_1^{T} r_1 & \mathcal{R}_1^{T} \mathcal{R}_2 \\ \cdot & r_2^2 + r_1^2 r_1 & r_1^{T} \mathcal{R}_2 + r_2 r_3 \\ \cdot & \cdot & \mathcal{R}_4^{T} \mathcal{R}_4 + \mathcal{R}_2^{T} \mathcal{R}_2 + r_3^{T} r_3 \end{bmatrix}$$

(27)

where $r_4$, $r_5$ and $r_6$ are determined by

$$r_4 = \mathcal{R}_4^{T} (Y_1^{T} y_{k+1}), \quad (28a)$$

$$r_5 = (\lambda + y_{k-m+1}^{T} y_{k-m+1} - r_4^{T} r_4)^{1/2}, \quad (28b)$$

$$r_6 = \frac{1}{r_5} (y_{k-m+1}^{T} Y_2 - r_4^{T} \mathcal{R}_2). \quad (28c)$$

The final term $\mathcal{R}_6$ can be obtained by noticing that

$$\mathcal{R}_6^{T} \mathcal{R}_6 + \mathcal{R}_2^{T} \mathcal{R}_2 + r_6^{T} r_6 = \mathcal{R}_4^{T} \mathcal{R}_4 + \mathcal{R}_2^{T} \mathcal{R}_2 + r_3^{T} r_3, \quad (29)$$

implies

$$\mathcal{R}_6^{T} \mathcal{R}_6 = \mathcal{R}_4^{T} \mathcal{R}_4 - r_6^{T} r_6 + r_3^{T} r_3. \quad (30)$$

Therefore $\mathcal{R}_6$ can be obtained in a computationally very efficient manner by down-dating and updating the Cholesky factor $\mathcal{R}_4$ with the rank-1 matrices $r_6^{T} r_6$ and $r_3^{T} r_3$, respectively (see e.g. Section 12.5.3 in Golub and Van Loan (2012)).

### 4.3 Ensuring a descent direction

In Algorithm 1 we stipulate that the search direction $p_k$ must be chosen to mimic a descent direction such that $p_k^{T} g_k < 0$. Due to the fact that the gradient is not exact, then this descent condition does not strictly enforce a descent direction, but it is nonetheless useful to satisfy the descent condition in practice. The search direction $p_k$ as determined by (14)
will not be a descent direction in general since the approximation \( H_k \) of the inverse Hessian is not necessarily positive definite. Nevertheless, by observing that
\[
g_k^T (p_k + \beta g_k) = g_k^T p_k - \beta g_k^T g_k,
\]
we can always choose a \( \beta \geq 0 \) such that \( p_k + \beta g_k \) is a descent direction with respect to the inexact gradient \( g_k \). For example, we can choose
\[
\beta = 2 \max \left\{ 0, \frac{p_k^T g_k}{g_k^T g_k} \right\}.
\]

It is also worth pointing out that this situation occurred very infrequently during all of the experiments reported in Section 6. The above is by no means an optimal strategy, but it appears to perform very well in practice.

5 Auxiliary variable construction

Algorithm 1 offers two distinct variants. If the parameter \( \rho = 1 \), then the algorithm will mimic a classical SG approach in that we accept every proposal \( \xi_{k+1} \) according to (7) and we are free to choose \( \bar{\alpha}_k \) as a decaying sequence
\[
\bar{\alpha}_k \triangleq \frac{\bar{\alpha}_0}{k}, \text{ for some fixed } \bar{\alpha}_0 > 0.
\]

Therefore, \( \alpha_{k+1} = \bar{\alpha}_0 / k \), which is a typical choice for many SG algorithms. In this case we can employ all the analysis from SG methods, see Bottou et al. (2017).

The alternative \( \rho = 0 \), offers a different approach, which is our main focus in this work as detailed in Section 5.1. Our algorithm produces a Markov chain and in Section 5.2 it is briefly described how we can use it to extract a competitive point estimate.

5.1 Adaptive step lengths

When we set \( \rho = 0 \) in Algorithm 1 it will generate an \( m \)-th order Markov chain \( \{x_{k-m+1:k}, \alpha_{k-m+1:k}, u_{k-m+1:k}\}_{k \geq 1} \) where the notation \( x_{k-m+1:k} \triangleq \{x_{k-m+1}, \ldots, x_k\} \) is used to represent the past \( m \) iterates. The first auxiliary variable \( \alpha_k \) is the step length from Algorithm 1 and the second auxiliary variable \( u_k \) represents the information required to evaluate the approximate (noisy) cost and gradient. For example, in the case of subsampling, \( u_k \) represents the subset of integers from \( \{1, \ldots, n\} \) used to approximate the subsampled cost and associated gradient. In Sequential Monte Carlo (SMC) methods (used in Section 6.4), the auxiliary variable \( u_k \) represents the selection of modes that propagate through the filter in order to again estimate the likelihood and its gradient (see Andrieu et al. (2010) for details).

In what follows, we make the dependence on the auxiliary variable \( u_k \) explicit by using the notation that \( f(x_k, u_k) \) is the cost approximation and \( g(x_k, u_k) \) is the gradient of \( f(x_k, u_k) \) with respect to \( x \).

The Markov chain evolves according to
\[
x_{k+1} = x_k + c_k \alpha_k p_k,
\]
\[
p_k = -H_k g_k - 2 \max \left\{ 0, \frac{g_k^T H_k g_k}{g_k^T g_k} \right\} g_k,
\]
\[
g_k = g(x_k, u_k),
\]
\[
H_k = H(x_{k-m+1:k}, \alpha_{k-m+1:k}, u_{k-m+1:k}),
\]
\[
\alpha_{k+1} = c_k + (1 - c_k) \kappa \alpha_k,
\]

where \( H(x_{k-m+1:k}, \alpha_{k-m+1:k}, u_{k-m+1:k}) \) is defined as \( H_k \) in (13), but here we highlight that the inverse Hessian approximation is a function of the past \( m \) iterates \( x_{k-m+1:k} \) and of the auxiliary variables \( u_{k-m+1:k} \) and \( \alpha_{k-m+1:k} \).
over this same window. The variable $c_k$ is determined by

$$c_k = \begin{cases} 1, & \text{w.p. } a(x_k + \alpha_k p_k \mid x_k), \\ 0, & \text{otherwise}, \end{cases} \quad (35)$$

where the acceptance probability is calculated as

$$a(\xi_{k+1}, x_k) = \begin{cases} 1, & \epsilon_k < 0, \\ C(-\epsilon_k, \sigma^2), & \text{otherwise}, \end{cases} \quad (36a)$$

$$\epsilon_k \triangleq f(\xi_{k+1}) - f(x_k), \quad (36b)$$

where $C(-\epsilon_k, \sigma^2)$ denotes the cumulative distribution function for a Gaussian with mean $-\epsilon_k$ and variance $\sigma^2$. The acceptance probability in (36) has the effect of strictly accepting proposals that decrease the cost, while accepting those that increase the cost with a probability $C(-\epsilon_k, \sigma^2)$. Therefore, a proposed $\xi_{k+1}$ that causes a large increase in the cost, relative to the uncertainty of the cost, is very unlikely to be accepted. Note that it is possible to readily calculate an unbiased estimate of the cost function variance $\sigma^2$, and this can be re-evaluated as the algorithm progresses.

Should a proposal be rejected then the step length is reduced according to $\alpha_{k+1} = \kappa \alpha_k$ and the algorithm returns to proposing a new $\xi_{k+1}$ with reduced step length in Step 7 without calculating a new search direction (the intent is similar to stochastic line search algorithms (Mahsereci and Hennig, 2017)). In the event that the proposal is accepted then $\alpha_{k+1} = \bar{\alpha}_k$, which for this variant of the algorithm was chosen as $\bar{\alpha}_k = 1$ for all $k$.

**Comments:** A natural question to ask is that of convergence of the proposed algorithm. Convergence of a Markov chain to an invariant distribution has been the subject of intense research within statistics and related communities, see e.g. Meyn and Tweedie (2009) for a solid textbook account. Essentially, if it can be shown that the Markov transition kernel is invariant, that the chain is irreducible, and that it is also aperiodic, then it will converge to a stationary distribution. However, it is not immediately obvious (or indeed possibly correct) to assert that the transition kernel devised in Algorithm 1 is invariant.

### 5.2 Extracting estimates

As discussed above, Algorithm 1 produces iterates $\{x_k\}_{k \geq 1}$ that are distributed according to some underlying distribution $p(x)$, that in accordance with the acceptance probability, favours reductions in the cost function. As with standard Markov chain methods, we can then utilise these samples via a law of large numbers argument to form expectations of the type

$$h = \int h(x)p(x)dx = \lim_{M \to \infty} \frac{1}{M} \sum_{k=1}^{M} h(x_k), \quad (37)$$

where $h(\cdot)$ refers to a test function. The utility of this approach is that we can produce as many samples from the target distribution as required in order to compute a desired expectation.

In the experiments presented in Section 6, we employed a very simple strategy of computing the expected value of $x$, so that $h(x) = x$, which results in the following estimate

$$\hat{x} = \frac{1}{M} \sum_{k=k_{\min}}^{M+k_{\min}-1} x_k \quad (38)$$

where $k_{\min} > 0$ defines a minimum number of transient iterations to ignore in the calculation. The results summarised in Table 2 were calculated according to (38) by using the final 20% of the iterations.
6  Numerical experiments

Let us now put our new developments to test on a suite of problems from four different categories carefully chosen to exhibit different properties and challenges. In Section 6.1 we study a synthetic example to gauge the performance in a controlled setting. We then move on to more interesting and challenging problems involving large-scale and real-world data. In particular we will in Section 6.2 consider an optimisation problem arising from the use of deep learning to solve the classical machine learning benchmark MNIST\textsuperscript{1}, where the task is to classify images of handwritten digits. Another commonly used benchmark is considered in Section 6.3, namely the collection of logistic classification problems described by Chang and Lin (2011) in the form of their library for support vector machines (LIBSVM). Finally we study a class of problems of much smaller scale, posing a different challenge in that for these problems it is inherently impossible to compute the cost function and the gradient exactly despite their small-scale nature. In our experiments we compare against relevant state-of-the-art methods. All experiments were run on a MacBook Pro 2.8GHz laptop with 16GB of RAM using Matlab 2017b. More details about some of the experiments and their background are available in the supplemental material.

6.1 Synthetic example – Rosenbrock’s banana function

Let us start by demonstrating our proposed algorithm on a simple and possibly familiar problem, namely, that of minimising the Rosenbrock banana function (a contour plot of the Rosenbrock function is provided in Figure 2a). To emulate the stochastic nature of the problems considered in this paper, we have added artificial noise (standard deviation of $\sigma = 0.1$) to both the cost function and gradient calculations.

The Rosenbrock function is well-known to cause difficulty for first-order methods because the Hessian matrix has disparate eigenvalues along its banana-shaped valley. To compare our approach, we also implemented the Adam algorithm from Kingma and Ba (2015). Figure 2a shows the first 50 iterates of both methods. Clearly the proposed algorithm is converging to a region around the optimal point while Adam is making slower progress along the valley. Figure 2b shows the cost value as a function of iteration, and while both methods converge to a similar cost value, the proposed approach achieves this quite quickly.

While it is difficult and ill-advised to draw strong conclusions from this tiny experiment, it does provide some confidence that the second-order information is indeed captured and exploited by our proposed algorithm.

![Figure 2: Rosenbrock’s banana function. Figure (a) shows the contour lines of the cost function together with 50 iterates from Algorithm 1 and Adam, respectively. Figure (b) shows the cost per iteration for the same two algorithms.](yann.lecun.com/exdb/mnist/)

1\textsuperscript{1}yann.lecun.com/exdb/mnist/
6.2 MNIST

Deep convolutional neural networks (CNNs) with multiple layers of convolution, pooling and nonlinear activation functions are delivering state-of-the-art results on many tasks in computer vision. We are here borrowing the stochastic optimisation problems arising in using such a deep CNN to solve the MNIST benchmark. The particular CNN structure used in this example employs $5 \times 5$ convolution kernels, pooling layers and a fully connected layer at the end. We made use of the publicly available code provided by Zhang (2016), which contains all the implementation details. In Figure 1 we show the average cost versus time for 20 Monte-Carlo trials with Algorithm 1 (with $b = 300$, $m = 30$ and $\lambda = 0.1$), Adam developed by Kingma and Ba (2015) and the basic SG algorithm. Note that the three algorithms all make use of the same gradients.

6.3 Logistic loss and a 2-norm regularizer

The task here is to solve seven different empirical risk minimisation problems using a logistic loss function with an L2 regularizer. The data is taken from Chang and Lin (2011). These problems are commonly used for profiling optimisation algorithms of the kind introduced in this paper, facilitating comparison with existing state-of-the-art algorithms. More specifically, we have used the same set-up as Gower et al. (2016), which inspired this study. A summary of the salient features of each problem is provided in Table 1. Recall that our algorithm only requires the user to select two tuning parameters, namely the mini-batch size used ($b$), and the memory length ($m$). Our choices for these parameters are listed in Table 1.

| Problem | $n$  | $d$  | $b$  | $m$  | $\lambda$ |
|---------|-----|-----|-----|-----|-----------|
| gisette | 6000| 5000| 500 | 20  | 1.0       |
| covtype | 581012| 54  | 763 | 54  | 0.04      |
| HIGGS   | 11000000| 28  | 317 | 28  | 0.04      |
| SUSY    | 3548466| 18  | 5000| 18  | 0.04      |
| epsilon | 400000| 2000| 1000| 20  | 0.2       |
| rcv1    | 20242| 47236| 284 | 2   | 0.2       |
| URL     | 2396130| 3231961| 1798| 50  | 0.04      |

Table 1: List of seven problems (columns 1), the number of data points $n$ (column 2), the number of variables $d$ (column 3), the mini-batch size $b$ (column 4), the memory size $m$ (column 5), and the regulariser $\lambda$ (column 6).

| Problem | Alg1 | MNJ  | GGR  | SVRG |
|---------|------|------|------|------|
| gisette | **0.005** | 0.244 | 0.0176 | 0.172 |
| covtype | **0.514** | 0.684 | **0.514** | 0.667 |
| HIGGS   | **0.638** | **0.638** | **0.638** | **0.638** |
| SUSY    | **0.458** | **0.458** | **0.458** | **0.458** |
| epsilon | **0.282** | **0.282** | **0.282** | 0.421 |
| rcv1    | **0.202** | **0.202** | **0.202** | 0.280 |
| URL     | 0.0196 | **0.0193** | 0.0249 | **0.0639** |

Table 2: Cost function values for each problem (columns 1), and each method Alg1 (column 2), MNJ (column 3), GGR (column 4) and SVRG (column 5). Minimum value in bold face.

We compared Algorithm 1 (denoted as Alg1) against three existing methods from the literature, namely, the limited memory stochastic block BFGS method from Gower et al. (2016) (denoted as GGR) and the limited memory stochastic BFGS method of Moritz et al. (2016) (denoted as MNJ) and the stochastic variance reduced gradient (SVRG) by Johnson and Zhang (2013) (denoted SVRG). For the GGR, MNJ and SVRG approaches we used the recommended tuning of each
algorithm. In the case of GGR we used the prev variant as this performed best across all test problems\(^2\). The result is illustrated in Table 2 and Figure 3.

### 6.4 Nonlinear system identification

Another important application requiring stochastic optimisation problems to be solved is that of nonlinear system identification, where the task is to learn unknown parameters in nonlinear dynamical systems (see Appendix 8 for further details). Here the stochasticity arises due to the fact that it is impossible to exactly evaluate the cost function (provided by maximum likelihood) and its gradients. Instead we have to resort to approximations resulting in noisy evaluations of the kind (2). Consider the problem of learning the parameters \(b\) and \(q\) for the following nonlinear and time-varying state-space model,

\[
x_{t+1} = 0.5x_t + b \frac{x_t}{1 + x_t^2} + 8 \cos(1.2t) + q^{-1}w_t, \tag{39a}
\]

\[
y_t = 0.05x_t^2 + e_t, \tag{39b}
\]

where the true parameters are \(b^* = 25\) and \(q^* = 1/\sqrt{0.5}\). The noise terms are mutually independent and given by \(w_t \sim N(0, 1)\) and \(e_t \sim N(0, 0.1)\). This has been acknowledged as a challenging problem (Doucet et al., 2000; Godsill et al., 2004) within the sequential Monte Carlo (SMC) community. The results using 100 measurements and 200 particles for 100 Monte–Carlo simulations are provided in Figure 3h.

### 7 Conclusion and future work

In this paper we have developed a new approach for solving large-scale stochastic optimisation problems by combining curvature information in computing the search direction with the use of an adaptive step length that is regulated by the cost function. The local curvature information is captured using a limited memory method whose computational cost scales linearly in the data size. We demonstrate our approach on a range of problems from different fields of research including a suite of challenging large-scale problems. The proposed method performs well against state-of-the-art techniques and we believe that this provides some impetus for further research. As a final remark, an interesting situation occurs when we employ Algorithm 1 with \(\rho = 0\) together with a decaying maximum step length \(\bar{\alpha}_k\). In the limit, this mimics SG methods, but in early iterations it regulates the step length in order to reduce the cost. This circumvents the requirement of conservative initial step lengths.

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\(^2\)The implementation for GGR and MNJ was downloaded from www.maths.ed.ac.uk/~prichtar/i_software.html
8 Appendix – Learning nonlinear dynamical systems

8.1 Problem formulation

Consider the following general nonlinear state-space model

\[ x_t = f(x_{t-1}, \theta) + w_t, \]  
\[ y_t = h(x_t, \theta) + e_t, \]  

(40a)  
(40b)

where \( x_t \) denotes the state, \( y_t \) denotes the measurement and \( \theta \) denotes the unknown (static) parameters. The two nonlinear functions \( f(\cdot) \) and \( h(\cdot) \) denotes the nonlinear functions describing the dynamics and the measurements, respectively. The process noise is Gaussian distributed with zero mean and covariance \( Q, w_t \sim \mathcal{N}(0, Q) \) and the measurement noise is given by \( e_t \sim \mathcal{N}(0, R) \). Finally, the initial state is distributed according to \( x_0 \sim p(x_0 | \theta) \).

The problem we are interested in is to estimate the unknown parameters \( \theta \) by making use of the available measurements \( y_{1:n} = \{ y_1, y_2, \ldots, y_n \} \) to maximize the likelihood function \( p(y_{1:n} | \theta) \)

\[ \max_{\theta} p(y_{1:n} | \theta). \]  
(41)

In the supplemental material we provide more background on how to compute approximations of the likelihood function (41) and its gradients using sequential Monte Carlo (SMC) methods (Gordon et al., 1993; Kitagawa, 1993). For a tutorial introduction to SMC methods we refer to Doucet and Johansen (2011) and their use in solving system identification problems is offered by Schön et al. (2015) and Kantas et al. (2015).

8.2 Computing the likelihood and its gradient

The likelihood function can via repeated use of conditional probabilities be rewritten as

\[ p(y_{1:n} | \theta) = \prod_{t=1}^{n} p(y_t | y_{1:t-1}, \theta), \]  
(42)

with the convention that \( y_{1:0} = \emptyset \). The one step ahead predictors are available via marginalization

\[ p(y_t | y_{1:t-1}, \theta) = \int p(y_t, x_t | y_{1:t-1}, \theta) dx_t = \int p(y_t | x_t, \theta) p(x_t | y_{1:t-1}, \theta) dx_t. \]  
(43)

One intuitive interpretation of the above integral is that it corresponds to averaging over all possible values for the state \( x_t \). The challenge is of course how to actually compute this integral. By making use of particle filter (Gordon et al., 1993; Kitagawa, 1993) to approximate the likelihood we are guaranteed to obtain an unbiased estimate (Del Moral, 2004).

The likelihood gradients can also be computed using particle filters, for example by making use of Fisher’s identity (Cappé et al., 2005)

\[ \nabla_\theta \ell(\theta) \big|_{\theta=\theta_k} = \nabla_\theta Q(\theta, \theta_k) \big|_{\theta=\theta_k} \]  
(44)

where we have defined

\[ \ell(\theta) = \ln p(y_{1:n} | \theta), \]  
(45a)

\[ Q(\theta, \theta_k) = \int \ln p(x_{0:n}, y_{1:n} | \theta) p(x_{0:n} | y_{1:n}, \theta_k) dx_{0:n}. \]  
(45b)

The particle filter—which is one member of the family of sequential Monte Carlo (SMC) methods—has a fairly rich history when it comes to solving nonlinear system identification problems. For an introductory overview we refer to Schön et al. (2015); Kantas et al. (2015).

The likelihood and its gradient cannot be calculated exactly in this case and we therefore employed sequential Monte Carlo methods and Fisher’s identity (Cappé et al., 2005; Ninness et al., 2010) 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.
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Figure 3: Performance on seven classification tasks using a logistic loss with a two-norm regulariser (Figures (a)–(g)). In Figure (h) we show the result on a learning parameters in a challenging nonlinear dynamical system.