STOCHASTIC QUASI-NEWTON METHODS FOR NONCONVEX STOCHASTIC OPTIMIZATION

XIAO WANG *, SHIQIAN MA †, DONALD GOLDFARB ‡, AND WEI LIU §

Abstract. In this paper we study stochastic quasi-Newton methods for nonconvex stochastic optimization, where we assume that noisy information about the gradients of the objective function is available via a stochastic first-order oracle (SFO). We propose a general framework for such methods, and prove the almost sure convergence of them to stationary points and analyze their worst-case iteration complexity. When a randomly chosen iterate is returned as the output of such an algorithm, we prove that in the worst-case, the SFO-calls complexity is $O(\epsilon^{-2})$ to ensure that the expectation of the squared norm of the gradient is smaller than the given accuracy tolerance $\epsilon$. We also propose a specific algorithm, namely a stochastic damped L-BFGS method, that falls under the proposed framework. Numerical results on a nonconvex classification problem are reported for both synthetic and real data, that demonstrate the promising potential of the proposed method.

Keywords: Stochastic Optimization, Nonconvex Optimization, Stochastic Approximation, Quasi-Newton Method, L-BFGS Method, Complexity

Mathematics Subject Classification 2010: 90C15; 90C30; 62L20; 90C60

1. Introduction. In this paper, we consider the following stochastic optimization problem:

$$\min_{x \in \mathbb{R}^n} f(x) = \mathbb{E}[F(x, \xi)],$$

(1.1)

where $F : \mathbb{R}^n \times \mathbb{R}^d \rightarrow \mathbb{R}$ is continuously differentiable and possibly nonconvex, $\xi \in \mathbb{R}^d$ denotes a random variable with distribution function $P$, and $\mathbb{E}[\cdot]$ denotes the expectation taken with respect to the random variable $\xi$. In many cases the function $F(\cdot, \xi)$ is not given explicitly or (and) the distribution function $P$ is unknown, or the function values and gradients of $f$ cannot be easily obtained and only noisy gradient information of $f$ is available. In this paper we assume that noisy gradients of $f$ can be obtained via calls to a stochastic first-order oracle (SFO). Problem (1.1) arises in many applications in statistics and machine learning [34, 50], mixed logit modeling problems in economics and transportation [6, 3, 24] and so on.

The idea of employing stochastic approximation (SA) to solve stochastic programming problems can be traced back to the seminal work by Robbins and Monro [45]. The classical SA method mimics the steepest gradient descent method using a stochastic gradient, i.e., it updates iterate $x_k$ via

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

(1.2)

where $g_k$ is an unbiased estimate of the gradient of $f$ at $x_k$, and $\alpha_k$ is the stepsize for the stochastic gradient step. In the literature, the SA method is also referred to as stochastic gradient descent (SGD) method.
The SA method has been further studied extensively in [11, 16, 18, 43, 46, 47, 48], and the main focus in these papers has been the convergence of SA in different settings. Recently, there has been a lot of interest in analyzing the worst-case complexity of SA methods. Work along this direction was mainly stimulated by the complexity theory developed by Nesterov for first-order methods for solving convex optimization problems [40, 41]. Nemirovski et al. [39] proposed a mirror descent SA method for solving the nonsmooth convex stochastic programming problem \( x^* := \arg\min \{ f(x) \mid x \in X \} \) and analyzed its worst-case iteration complexity, where \( f \) is nonsmooth and convex and \( X \) is a convex set. Specifically, it was shown in [39] that for any given \( \epsilon > 0 \), the proposed mirror descent SA method needs \( O(\epsilon^{-2}) \) iterations to obtain an \( \bar{x} \) such that \( \mathbb{E}[f(\bar{x}) - f(x^*)] \leq \epsilon \). Other SA methods with provable complexities for solving convex stochastic optimization problems were also studied in [19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35].

The SA methods mentioned above all focused on convex problems. Recently there has been a lot of interest in SA methods for stochastic optimization problem (1.1) in which \( f \) is a nonconvex function. In [5], an SA method to minimize a general cost function was proposed by Bottou and proved to be convergent to stationary points. Ghadimi and Lan [20] proposed a randomized stochastic gradient (RSG) method that returns an iterate from a randomly chosen iteration as an approximate solution. It is shown in [20] that to return an \( \epsilon \)-solution \( \bar{x} \), i.e., \( \mathbb{E}[\|\nabla f(\bar{x})\|^2] \leq \epsilon \), the total number of \( \mathcal{SFO} \)-calls needed by RSG is of the order of \( O(\epsilon^{-2}) \). Ghadimi and Lan [21] also studied an accelerated SA method for solving (1.1) based on Nesterov’s accelerated gradient method [40, 41], which improved the \( \mathcal{SFO} \)-call complexity for convex cases from \( O(\epsilon^{-2}) \) to \( O(\epsilon^{-4/3}) \). In [22], Ghadimi, Lan and Zhang proposed a mini-batch SA method for solving a class of nonconvex stochastic optimization problems, in which the objective function is a composition of a nonconvex function \( f \) and a convex nonsmooth function \( h \), i.e., \( x^* := \arg\min \{ f(x) + h(x) : x \in \mathbb{R}^n \} \), and analyzed its worst-case \( \mathcal{SFO} \)-call complexity. In [12], a stochastic block mirror descent method, that incorporates a block-coordinate decomposition scheme into stochastic mirror-descent methodology, was proposed by Dang and Lan for a nonconvex stochastic optimization problem \( x^* = \arg\min \{ f(x) : x \in X \} \) in which the convex set \( X \) has a block structure. More recently, Wang, Ma and Yuan [53] proposed a penalty method for nonconvex stochastic optimization problems with nonconvex constraints, and analyzed its \( \mathcal{SFO} \)-call complexity.

In this paper, we study stochastic quasi-Newton method for solving the nonconvex stochastic optimization problem (1.1). In the deterministic optimization setting, quasi-Newton methods are more robust and achieve higher accuracy than gradient methods, because they use approximate second order derivative information. Quasi-Newton methods usually employ the following updates for solving (1.1):

\[
x_{k+1} = x_k - \alpha_k B_k^{-1} \nabla f(x_k), \quad \text{or} \quad x_{k+1} = x_k - \alpha_k H_k \nabla f(x_k)
\]

(1.3)

where \( B_k \) is an approximation to the Hessian matrix \( \nabla^2 f(x_k) \) of \( f \) at \( x_k \), and \( H_k \) is an approximation to \( [\nabla^2 f(x_k)]^{-1} \). The most widely-used quasi-Newton method is the BFGS method [7, 17, 23, 52], which updates \( B_k \) via

\[
B_k = B_{k-1} + \frac{y_k y_k^\top - B_{k-1} s_{k-1} s_{k-1}^\top B_{k-1}}{s_{k-1}^\top B_{k-1} s_{k-1}}
\]

(1.4)

where \( s_{k-1} := x_k - x_{k-1} \) and \( y_{k-1} := \nabla f(x_k) - \nabla f(x_{k-1}) \). By using the Sherman-Morrison-Woodbury formula, it is easy to derive that the equivalent update to \( H_k = B_k^{-1} \) is

\[
H_k = (I - \rho_{k-1} s_{k-1} y_{k-1}^\top) H_{k-1} (I - \rho_{k-1} s_{k-1} y_{k-1}^\top) + \rho_{k-1} s_{k-1} s_{k-1}^\top
\]

(1.5)
where \( \rho_{k-1} := 1/(s_{k-1}^\top y_{k-1}) \). For stochastic optimization, there has been some work in designing stochastic quasi-Newton methods that update the iterates via

\[
x_{k+1} = x_k - \alpha_k B_k^{-1} g_k, \quad \text{or} \quad x_{k+1} = x_k - \alpha_k H_k g_k.
\]

Specific examples include the following. The adaptive subgradient (AdaGrad) method proposed by Duchi, Hazan and Singer [14], which takes the form of (1.6) with \( B_k \) being a diagonal matrix that estimates the diagonal of the square root of the uncentered covariance matrix of the gradients, has been proven to be quite efficient in practice. In [4], Bordes, Bottou and Gallinari studied SGD with a diagonal rescaling matrix based on the secant condition associated with quasi-Newton methods. Roux and Fitzgibbon [46] discussed the necessity of including both Hessian and covariance matrix information in a stochastic Newton type method. Byrd et al. [8] proposed a quasi-Newton method that uses the sample average approximation (SAA) approach to estimate Hessian-vector multiplications. In [9], Byrd et al. proposed a stochastic limited-memory BFGS (L-BFGS) [32] method based on SA, and convergence of this method was proved for strongly convex problem. Stochastic BFGS and L-BFGS methods were also studied for online convex optimization by Schraudolph, Yu and Günter in [49]. Mokhtari and Ribeiro [36] proposed a regularized stochastic BFGS method (RES) for solving (1.1) with strongly convex \( f \) and analyzed its convergence. In more recent work [37], Mokhtari and Ribeiro studied an online L-BFGS method for strongly convex problem. Recently, Moritz, Nishihara and Jordan [38] studied a stochastic L-BFGS algorithm for minimizing a finite sum of convex functions. This method integrates the L-BFGS method in [9] with a variance reduction technique proposed by Johnson and Zhang in [25] to alleviate the effect of noisy gradients. A related method that incorporates the variance reduction technique in [25] into a quasi-Newton method was studied by Lucchi, McWilliams and Hofmann in [33]. It should be noted that all of the stochastic quasi-Newton methods discussed above are for solving convex or even strongly convex problems.

**Challenges.** The key challenge in designing stochastic quasi-Newton methods for nonconvex problem lies in the difficulty in preserving the positive-definiteness of \( B_k \) (and \( H_k \)), due to the non-convexity of the problem and the presence of noise in gradient estimation. It is known that the BFGS update (1.4) can preserve the positive-definiteness of \( B_k \) as long as the curvature condition

\[
s_{k-1}^\top y_{k-1} > 0
\]

holds, which can be guaranteed for strongly convex problem. For nonconvex problem, the curvature condition (1.7) can be satisfied by performing a line search. However, doing this is no longer possible for (1.4) in the stochastic setting, because exact function value and gradient information is not available. As a result, an important issue in designing stochastic quasi-Newton methods for nonconvex problem is how to preserve the positive-definiteness of \( B_k \) (or \( H_k \)) without line search.

**Our contributions.** Our contributions in this paper are as follows.

1. We propose a general framework for stochastic quasi-Newton methods (SQN) for solving the nonconvex stochastic optimization problem (1.1). We analyze its almost sure convergence to a stationary point when the step size \( \alpha_k \) is diminishing. We also prove that its iteration complexity to obtain

\[
\frac{1}{N} \sum_{k=1}^N \mathbb{E}[\|\nabla f(x_k)\|^2] \leq \epsilon,
\]

for \( \alpha_k \) chosen proportional to \( k^{-\beta} \), where \( N \) is the iteration number and \( \beta \in (0.5, 1) \) is a constant.

2. When an iterate \( x_R \) from a randomly chosen iteration is returned as the output of SQN, we prove that the worst-case SFO-calls complexity is \( O(\epsilon^{-2}) \) to guarantee \( \mathbb{E}[\|\nabla f(x_R)\|^2] \leq \epsilon \).
3. We propose a stochastic damped L-BFGS method that fits into the proposed framework. This method adaptively generates a positive definite matrix $H_k$ that approximates the inverse Hessian matrix at the current iterate $x_k$. Convergence and complexity results for this method are provided. Moreover, our method does not generate $H_k$ explicitly, and only its multiplication with vectors is computed directly.

**Notation.** The gradient of $f$ is denoted as $\nabla f$. Without specification, $\|x\|$ represents the Euclidean norm of vector $x$. Both $\langle x, y \rangle$ and $x^\top y$ with $x, y \in \mathbb{R}^n$ denote the Euclidean inner product of $x$ and $y$. We denote by $\lambda_{\text{max}}(A)$, the largest eigenvalue of a symmetric matrix $A$, and by $\|A\|$, the operator norm of matrix $A$. The expression $A \succeq B$ with $A, B \in \mathbb{R}^{n \times n}$ means that $A - B$ is positive semidefinite. $\text{tr}(A)$ denotes the trace of the matrix $A$.

**Organization.** The rest of this paper is organized as follows. In Section 2, we present a general framework for stochastic quasi-Newton methods for nonconvex optimization (1.1) and prove almost sure convergence to stationary points and analyze the iteration complexity of methods that fall under this framework under the condition that the step size is diminishing. In Section 2.2, we analyze the SFO-calls complexity of such methods when a randomly chosen iterate is returned as the output. A specific method, namely the stochastic damped limited memory BFGS (SdLBFGS) method, which falls under the proposed framework, is proposed in Section 3. In Section 4 we apply our SdLBFGS method to solving a nonconvex support vector machine problem, and report the results for both synthetic and real data arising from text mining. Finally, we draw some conclusion in Section 5.

2. A general framework for stochastic quasi-Newton methods for nonconvex optimization.

In this section, we study SQN methods for the (possibly nonconvex) stochastic optimization problem (1.1). We assume that an SFO outputs a stochastic gradient $g(x, \xi)$ of $f$ for a given $x$, where $\xi$ is a random variable whose distribution is supported on $\Xi \subseteq \mathbb{R}^d$. Here we assume that $\Xi$ does not depend on $x$.

We now give some assumptions that are required throughout this paper.

**AS.1** $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable. $f(x)$ is lower bounded by a real number $f_{\text{low}}$ for any $x \in \mathbb{R}^n$. $\nabla f$ is globally Lipschitz continuous with Lipschitz constant $L$; namely for any $x, y \in \mathbb{R}^n$,

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|.$$ 

**AS.2** For any iteration $k$, we have

\[a) \quad \mathbb{E}_{\xi_k} [g(x_k, \xi_k)] = \nabla f(x_k),\] 
\[b) \quad \mathbb{E}_{\xi_k} [\|g(x_k, \xi_k) - \nabla f(x_k)\|^2] \leq \sigma^2,\]

where $\sigma > 0$ is the noise level of the gradient estimation, and $\xi_k, k = 1, 2, \ldots$, are independent samples, and for a given $k$ the random variable $\xi_k$ is independent of $\{x_j\}_{j=1}^k$.

**Remark 2.1.** Note that the stochastic BFGS methods studied in [30, 42, 37] require that the noisy gradient is bounded, i.e.,

$$\mathbb{E}_{\xi_k} [\|g(x_k, \xi_k)\|^2] \leq M_g,$$ 

where $M_g > 0$ is a constant. Our assumption 2.2 is weaker than (2.3).
Analogous to deterministic quasi-Newton methods, our SQN takes steps 
\[ x_{k+1} = x_k - \alpha_k H_k g_k, \]  
(2.4)
where \( g_k \) is defined as a mini-batch estimate of the gradient: 
\[ g_k = \frac{1}{m_k} \sum_{i=1}^{m_k} g(x_k, \xi_{k,i}), \]  
(2.5)
and \( \xi_{k,i} \) denotes the random variable generated by the \( i \)-th sampling in the \( k \)-th iteration. From AS.2 we can see that \( g_k \) has the following properties:
\[ E[g_k | x_k] = \nabla f(x_k), \quad E[\|g_k - \nabla f(x_k)\|^2 | x_k] \leq \frac{\sigma^2}{m_k}. \]  
(2.6)
The following assumption ensures that \( H_k \) is positive definite. Note that this can be satisfied by our stochastic L-BFGS update in Section 3, and this assumption does not require the original function \( f \) in (1.1) to be convex.

**AS.3** There exist two positive constants \( C_l, C_u \) such that 
\[ C_l I \preceq H_k \preceq C_u I, \quad \text{for all } k. \]

We denote by \( \xi_k = (\xi_{k,1}, \ldots, \xi_{k,m_k}) \), the random samplings in the \( k \)-th iteration, and denote by \( \xi_{[k]} := (\xi_1, \ldots, \xi_k) \), the random samplings in the first \( k \) iterations. Since \( H_k \) is generated iteratively based on historical gradient information by a random process, we make the following assumption on \( H_k (k \geq 2) \) to control the randomness (note that \( H_1 \) is given in the initialization step).

**AS.4** For any \( k \geq 2 \), the random variable \( H_k \) depends only on \( \xi_{[k-1]} \).
It then follows directly from AS.4 and (2.6) that 
\[ E[H_k g_k | \xi_{[k-1]}] = H_k \nabla f(x_k), \]  
(2.7)
where the expectation is taken with respect to \( \xi_k \) generated in the computation of \( g_k \).
We will not specify how to compute \( H_k \) until Section 3 where a specific updating scheme for \( H_k \) satisfying both assumptions AS.3 and AS.4 will be proposed.
We now present our SQN for solving (1.1) as Algorithm 2.1.

**Algorithm 2.1 SQN: Stochastic quasi-Newton method for nonconvex stochastic optimization (1.1)**

**Input:** Given \( x_1 \in \mathbb{R}^n \), a positive definite matrix \( H_1 \in \mathbb{R}^{n \times n} \), batch sizes \( \{m_k\}_{k \geq 1} \), and stepsizes \( \{\alpha_k\}_{k \geq 1} \)

1. for \( k = 1, 2, \ldots \) do
2. Calculate \( g_k = \frac{1}{m_k} \sum_{i=1}^{m_k} g(x_k, \xi_{k,i}) \).
3. Generate a positive definite Hessian inverse approximation \( H_k \).
4. Calculate \( x_{k+1} = x_k - \alpha_k H_k g_k \).
5. end for

### 2.1. Convergence and complexity of SQN with diminishing step size.
In this subsection, we analyze the convergence and complexity of SQN under the condition that the step size \( \alpha_k \) in (2.3) is dimin-
ishing. Specifically, in this subsection we assume \( \alpha_k \) satisfies the following condition:

\[
\sum_{k=1}^{+\infty} \alpha_k = +\infty, \quad \sum_{k=1}^{+\infty} \alpha_k^2 < +\infty, \tag{2.8}
\]

which is a standard assumption in stochastic approximation algorithms (see, e.g., [9, 37, 39]). One very simple choice of \( \alpha_k \) that satisfies (2.8) is \( \alpha_k = O(1/k) \).

The following lemma shows that a descent property in terms of the expected objective value holds for SQN. Our analysis is similar to analyses that have been used in [5, 36].

**Lemma 2.1.** Suppose that \( \{x_k\} \) is generated by SQN and assumptions **AS.1-4** hold. We further assume that (2.8) holds, and \( \alpha_k \leq \frac{C_1}{k} \) for all \( k \). (Note that this can be satisfied if \( \alpha_k \) is non-increasing and the initial step size \( \alpha_1 \leq \frac{C_1}{\epsilon C_u^2} \)). Then the following inequality holds

\[
\mathbb{E}[f(x_{k+1})|x_k] \leq f(x_k) - \frac{1}{2} \alpha_k C_l \|\nabla f(x_k)\|^2 + \frac{L \sigma^2 C_u^2 \alpha_k^2}{2 m_k}, \quad \forall k \geq 1, \tag{2.9}
\]

where the conditional expectation is taken with respect to \( \xi_k \).

**Proof.** Define \( \delta_k = g_k - \nabla f(x_k) \). From (2.4), assumptions **AS.1** and **AS.3**, we have

\[
\begin{align*}
f(x_{k+1}) & \leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2} \|x_{k+1} - x_k\|^2 \\
& = f(x_k) - \alpha_k \langle \nabla f(x_k), H_k g_k \rangle + \frac{L}{2} \alpha_k^2 \|H_k g_k\|^2 \\
& \leq f(x_k) - \alpha_k \langle \nabla f(x_k), H_k \nabla f(x_k) \rangle - \alpha_k \langle \nabla f(x_k), H_k \delta_k \rangle + \frac{L}{2} \alpha_k^2 C_u^2 \|g_k\|^2. \tag{2.10}
\end{align*}
\]

Taking expectation with respect to \( \xi_k \) on both sides of (2.10) conditioned on \( x_k \), we obtain,

\[
\mathbb{E}[f(x_{k+1})|x_k] \leq f(x_k) - \alpha_k \langle \nabla f(x_k), H_k \nabla f(x_k) \rangle + \frac{L}{2} \alpha_k^2 C_u^2 \mathbb{E}[\|g_k\|^2|x_k], \tag{2.11}
\]

where we used (2.7) and the fact that

\[
\mathbb{E}[\delta_k|x_k] = 0. \tag{2.12}
\]

From (2.10) and (2.12), it follows that

\[
\mathbb{E}[\|g_k\|^2|x_k] = \mathbb{E}[\|g_k - \nabla f(x_k) + \nabla f(x_k)\|^2|x_k] \\
= \mathbb{E}[\|\nabla f(x_k)\|^2|x_k] + \mathbb{E}[\|g_k - \nabla f(x_k)\|^2|x_k] + 2 \mathbb{E}[\langle \delta_k, \nabla f(x_k) \rangle|x_k] \\
= \|\nabla f(x_k)\|^2 + \mathbb{E}[\|g_k - \nabla f(x_k)\|^2|x_k] \\
\leq \|\nabla f(x_k)\|^2 + \frac{\sigma^2}{m_k}, \tag{2.13}
\]

which together with (2.11) and **AS.3** yields that

\[
\mathbb{E}[f(x_{k+1})|x_k] \leq f(x_k) - \left( \alpha_k C_l - \frac{L}{2} \alpha_k^2 C_u^2 \right) \|\nabla f(x_k)\|^2 + \frac{L \sigma^2 C_u^2}{2 m_k} \alpha_k^2. \tag{2.14}
\]

Then (2.14) combined with the assumption \( \alpha_k \leq \frac{C_1}{\epsilon C_u^2} \) implies (2.9). \( \Box \)
Before proceeding with our analysis, we introduce the definition of a supermartingale (see [15] for more details).

**Definition 2.1.** Let \( \{\mathcal{F}_k\} \) be an increasing sequence of \( \sigma \)-algebras. If \( \{X_k\} \) is a stochastic process satisfying (i) \( \mathbb{E}[|X_k|] < \infty \); (ii) \( X_k \in \mathcal{F}_k \) for all \( k \); and (iii) \( \mathbb{E}[X_{k+1}|\mathcal{F}_k] \leq X_k \) for all \( k \), then \( \{X_k\} \) is called a supermartingale.

**Proposition 2.1** (see, e.g., Theorem 5.2.9 in [15]). If \( \{X_k\} \) is a nonnegative supermartingale, then \( \lim_{k \to \infty} X_k \to X \) almost surely and \( \mathbb{E}[X] \leq \mathbb{E}[X_0] \).

We are now ready to give convergence results for SQN (Algorithm 2.1).

**Theorem 2.1.** Suppose that assumptions AS.1-4 hold for \( \{x_k\} \) generated by SQN with batch size \( m_k = m \) for all \( k \). If the stepsize \( \alpha_k \) satisfies (2.8) and \( \alpha_k \leq \frac{C}{\gamma f(x_k)} \) for all \( k \), then it holds that

\[
\liminf_{k \to \infty} \|\nabla f(x_k)\| = 0, \quad \text{with probability 1.} \tag{2.15}
\]

Moreover, there exists a positive constant \( M_f \) such that

\[
\mathbb{E}[f(x_k)] \leq M_f, \quad \forall k. \tag{2.16}
\]

**Proof.** Define

\[
\beta_k := \frac{\alpha_k C_i}{2} \|\nabla f(x_k)\|^2, \quad \gamma_k := f(x_k) + \frac{L \sigma^2 C_u^2}{2m} \sum_{i=k}^{\infty} \alpha_i^2.
\]

Let \( \mathcal{F}_k \) be the \( \sigma \)-algebra measuring \( \beta_k, \gamma_k \) and \( x_k \). From (2.9) we know that for any \( k \), it holds that

\[
\mathbb{E}[\gamma_{k+1}|\mathcal{F}_k] = \mathbb{E}[f(x_{k+1})|\mathcal{F}_k] + \frac{L \sigma^2 C_u^2}{2m} \sum_{i=k+1}^{\infty} \alpha_i^2 \leq f(x_k) - \frac{\alpha_k C_i}{2} \|\nabla f(x_k)\|^2 + \frac{L \sigma^2 C_u^2}{2m} \sum_{i=k}^{\infty} \alpha_i^2 = \gamma_k - \beta_k, \quad \tag{2.17}
\]

which implies that \( \mathbb{E}[\gamma_{k+1} - f^{low}|\mathcal{F}_k] \leq \gamma_k - f^{low} - \beta_k \). Since \( \beta_k \geq 0 \), we have \( 0 \leq \mathbb{E}[\gamma_k - f^{low}] \leq \gamma_1 - f^{low} < +\infty \), which implies (2.16). According to Definition 2.1, \( \{\gamma_k - f^{low}\} \) is a supermartingale. Therefore, Proposition 2.1 shows that there exists a \( \gamma \) such that \( \lim_{k \to \infty} \gamma_k = \gamma \) with probability 1, and \( \mathbb{E}[\gamma] \leq \mathbb{E}[\gamma_1] \). Note that from (2.17) we have \( \mathbb{E}[\beta_k] \leq \mathbb{E}[\gamma_k] - \mathbb{E}[\gamma_{k+1}] \). Thus,

\[
\mathbb{E}\left[\sum_{k=1}^{\infty} \beta_k\right] \leq \sum_{k=1}^{\infty} \left(\mathbb{E}[\gamma_k] - \mathbb{E}[\gamma_{k+1}]\right) < +\infty,
\]

which further yields that

\[
\sum_{k=1}^{\infty} \beta_k = \frac{C_i}{2} \sum_{k=1}^{\infty} \alpha_k \|\nabla f(x_k)\|^2 < +\infty \quad \text{with probability 1.} \tag{2.18}
\]

Since \( \sum_{k=1}^{\infty} \alpha_k = +\infty \), it follows that (2.15) holds. \( \square \)

In the following, with the standard assumption (2.8) that has been used in [36, 9, 37], we prove a stronger convergence result showing that any limit point of \( \{x_k\} \) generated by SQN is a stationary point of (1.1) with
probability 1.

**Theorem 2.2.** Assume the same assumptions hold as in Theorem 2.1 and that (2.3) holds. Then

\[
\lim_{k \to \infty} \| \nabla f(x_k) \| = 0, \quad \text{with probability 1.} \tag{2.19}
\]

**Proof.** For any given \( \epsilon > 0 \), according to (2.15), there exist infinitely many iterates \( x_k \) such that \( \| \nabla f(x_k) \| < \epsilon \). Then if (2.19) does not hold, there must exist two infinite indices sequences \( \{ m_i \}, \{ n_i \} \) with \( n_i > m_i \), such that for \( i = 1, 2, \ldots \),

\[
\| \nabla f(x_{m_i}) \| \geq \epsilon, \quad \| \nabla f(x_{n_i}) \| < \epsilon, \quad \| \nabla f(x_k) \| \geq \epsilon, \quad k = m_i + 1, \ldots, n_i - 1. \tag{2.20}
\]

Then from (2.18) it follows that

\[
+\infty > \sum_{k=1}^{+\infty} \alpha_k \| \nabla f(x_k) \|^2 \geq \sum_{i=1}^{+\infty} \sum_{k=m_i}^{n_i-1} \alpha_k \| \nabla f(x_k) \|^2 \geq \epsilon^2 \sum_{i=1}^{+\infty} \sum_{k=m_i}^{n_i-1} \alpha_k, \quad \text{with probability 1},
\]

which implies that

\[
\sum_{k=m_i}^{n_i-1} \alpha_k \to 0, \quad \text{with probability 1, as } i \to +\infty. \tag{2.21}
\]

According to (2.13), we have that

\[
\mathbb{E}[\| x_{k+1} - x_k \| | x_k ] = \alpha_k \mathbb{E}[\| H_k g_k \| | x_k ] \leq \alpha_k \mathbb{C}_u \mathbb{E}[\| g_k \| | x_k ] \leq \alpha_k \mathbb{C}_u (\mathbb{E}[\| g_k \|^2 | x_k ])^{\frac{1}{2}} \leq \alpha_k \mathbb{C}_u (M_g / m)^{\frac{1}{2}}, \tag{2.22}
\]

where the last inequality is due to (2.3) and the convexity of \( \| \cdot \|^2 \). Then it follows from (2.22) that

\[
\mathbb{E}[\| x_{n_i} - x_{m_i} \|] \leq \mathbb{C}_u (M_g / m)^{\frac{1}{2}} \sum_{k=m_i}^{n_i-1} \alpha_k,
\]

which together with (2.21) implies that \( \| x_{n_i} - x_{m_i} \| \to 0 \) with probability 1, as \( i \to +\infty \). Hence, from the Lipschitz continuity of \( \nabla f \), it follows that \( \| \nabla f(x_{n_i}) - \nabla f(x_{m_i}) \| \to 0 \) with probability 1 as \( i \to +\infty \). However, this contradicts (2.20). Therefore, the assumption that (2.19) does not hold is not true. \( \square \)

**Remark 2.2.** Note that our result in Theorem 2.2 is stronger than the ones given in existing works such as \([36]\) and \([37]\). Moreover, although Bottou [5] also proves that the SA method for nonconvex stochastic optimization with diminishing stepsize is almost surely convergent to stationary point, our analysis requires weaker assumptions. For example, [5] assumes that the objective function is three times continuously differentiable, while our analysis does not need this assumption. Furthermore, we are able to analyze the iteration complexity of SQN, which is not provided in [5].

We now analyze the iteration complexity of SQN for a specifically chosen step size \( \alpha_k \).

**Theorem 2.3.** Suppose that assumptions **AS.1-4** hold for \( \{ x_k \} \) generated by SQN with batch size \( m_k = m \) for all \( k \). We also assume that \( \alpha_k \) is specifically chosen as

\[
\alpha_k = \frac{C_1}{LC_2^\beta} k^{-\beta} \tag{2.23}
\]
with $\beta \in (0.5, 1)$. Note that this choice satisfies (2.8) and $\alpha_k \leq \frac{\sigma}{\lambda x_k}$ for all $k$. Then
\[
\frac{1}{N} \sum_{k=1}^{N} \mathbb{E}[\|\nabla f(x_k)\|^2] \leq \frac{2L(M_f - f^{\text{low}})C_u^2}{C_i^2} N^{\beta - 1} + \frac{\sigma^2}{(1 - \beta)m}(N^{-\beta} - N^{-1}),
\] (2.24)
where $N$ denotes the iteration number. Moreover, for a given $\epsilon \in (0, 1)$, to guarantee that $\frac{1}{N} \sum_{k=1}^{N} \mathbb{E}[\|\nabla f(x_k)\|^2] < \epsilon$, the number of iterations $N$ needed is at most $O\left(\epsilon^{-\frac{1}{1-\beta}}\right)$.

Proof. Taking expectation on both sides of (2.9) and summing over $k = 1, \ldots, N$ yields
\[
\frac{1}{2} C_l \sum_{k=1}^{N} \mathbb{E}[\|\nabla f(x_k)\|^2] \leq \sum_{k=1}^{N} \frac{1}{\alpha_k} (\mathbb{E}[f(x_k)] - \mathbb{E}[f(x_{k+1})]) + \frac{L\sigma^2 C_u^2}{2m} \sum_{k=1}^{N} \alpha_k
\]
\[= \sum_{k=1}^{N} \frac{\mathbb{E}[f(x_k)]}{\alpha_k} - \sum_{k=2}^{N+1} \frac{\mathbb{E}[f(x_{k-1})]}{\alpha_{k-1}} + \frac{L\sigma^2 C_u^2}{2m} \sum_{k=1}^{N} \alpha_k
\]
\[= \frac{1}{\alpha_1} f(x_1) + \sum_{k=2}^{N} \left( \frac{1}{\alpha_k} - \frac{1}{\alpha_{k-1}} \right) \mathbb{E}[f(x_k)] - \frac{\mathbb{E}[f(x_{N+1})]}{\alpha_N} + \frac{L\sigma^2 C_u^2}{2m} \sum_{k=1}^{N} \alpha_k
\]
\[\leq \frac{M_f}{\alpha_1} + M_f \sum_{k=2}^{N} \left( \frac{1}{\alpha_k} - \frac{1}{\alpha_{k-1}} \right) + \frac{f^{\text{low}}}{\alpha_N} + \frac{L\sigma^2 C_u^2}{2m} \sum_{k=1}^{N} \alpha_k
\]
\[\leq \frac{L(M_f - f^{\text{low}})C_u^2}{C_i} N^{\beta} + \frac{\sigma^2 C_l}{2(1 - \beta)m}(N^{1-\beta} - 1),
\]
which results in (2.24), where the second inequality is due to (2.10) and the last inequality is due to (2.23).

Then for a given $\epsilon > 0$, to guarantee that $\frac{1}{N} \sum_{k=1}^{N} \mathbb{E}[\|\nabla f(x_k)\|^2] \leq \epsilon$, it suffices to require that
\[
\frac{2L(M_f - f^{\text{low}})C_u^2}{C_i^2} N^{\beta - 1} + \frac{\sigma^2}{(1 - \beta)m}(N^{-\beta} - N^{-1}) < \epsilon.
\]
Since $\beta \in (0.5, 1)$, it follows that the number of iterations $N$ needed is at most $O(\epsilon^{-\frac{1}{1-\beta}})$. \[\]

Remark 2.3. Note that Theorem 2.3 also provides iteration complexity analysis for the classic SGD method, which can be regarded as a special case of SQN with $H_k$ being the identity. To the best of our knowledge, our complexity result in Theorem 2.3 is new for both stochastic gradient and stochastic quasi-Newton methods.

2.2. Complexity of SQN with random output and constant step size. In this subsection, we analyze the $\mathcal{SFO}$-calls complexity of SQN when the output is randomly chosen from $\{x_i\}_{i=1}^{N}$, where $N$ is the maximum iteration number. Our results in this subsection are motivated by the randomized stochastic gradient (RSG) method proposed by Ghadimi and Lan [20]. RSG runs the standard SGD with $g_k$ defined in (2.20), i.e.,
\[
x_{k+1} = x_k - \frac{1}{m_k} \sum_{i=1}^{m_k} g(x_k, \xi_{k,i})
\]\ (2.25)
for $R$ iterations, where $R$ is a randomly chosen integer from $\{1, \ldots, N\}$ with a specifically defined probability mass function $P_R$. Ghadimi and Lan [20] proved that under certain conditions on $\alpha_k$ and $P_R$, the number of SFO-calls needed by SGD (2.25) to guarantee $E[\|\nabla f(x_R)\|^2] \leq \epsilon$ is in the order of $O(1/\epsilon^2)$. In this subsection, we show that under similar conditions, the same complexity holds for our SQN.

**Theorem 2.4.** Suppose that assumptions AS.1-4 hold, and that $\alpha_k$ in SQN (Algorithm 2.1) is chosen such that $0 < \alpha_k \leq 2C_l/(LC_u^2)$ for all $k$ with $\alpha_k < 2C_l/(LC_u^2)$ for at least one $k$. Moreover, for a given integer $N$, let $R$ be a random variable with the probability mass function

$$P_R(k) := \text{Prob}\{R = k\} = \frac{\alpha_k C_l - \alpha_k^2 LC_u^2/2}{\sum_{k=1}^N (\alpha_k C_l - \alpha_k^2 LC_u^2/2)}, \quad k = 1, \ldots, N.$$  

(2.26)

Then we have

$$E[\|\nabla f(x_R)\|^2] \leq D_f + \frac{(\sigma^2 LC_u^2)/2 \sum_{k=1}^N (\alpha_k^2/m_k)}{\sum_{k=1}^N (\alpha_k C_l - \alpha_k^2 LC_u^2/2)},$$

(2.27)

where $D_f := f(x_1) - f_{\text{low}}$ and the expectation is taken with respect to $R$ and $\xi[N]$. Moreover, if we choose $\alpha_k = C_l/(LC_u^2)$ and $m_k = m$ for all $k = 1, \ldots, N$, then (2.27) reduces to

$$E[\|\nabla f(x_R)\|^2] \leq \frac{2LC_u^2 D_f}{NC_l^2} + \frac{\sigma^2}{m}.$$  

(2.28)

**Proof.** From (2.11) it follows that

$$f(x_{k+1}) \leq f(x_k) - \alpha_k \langle \nabla f(x_k), H_k \nabla f(x_k) \rangle - \alpha_k \langle \nabla f(x_k), H_k \delta_k \rangle + \frac{L}{2} \alpha_k^2 C_l^2 \|\nabla f(x_k)\|^2 + 2 \langle \nabla f(x_k), \delta_k \rangle + \|\delta_k\|^2$$

$$\leq f(x_k) - \left(\alpha_k C_l - \frac{L}{2} \alpha_k^2 C_l^2 \right) \|\nabla f(x_k)\|^2 + \frac{1}{2} \alpha_k^2 LC_u^2 \|\delta_k\|^2 + \alpha_k^2 LC_u^2 \langle \nabla f(x_k), \delta_k \rangle$$

$$- \alpha_k \langle \nabla f(x_k), H_k \delta_k \rangle,$$

where $\delta_k = g_k - \nabla f(x_k)$. Summing the above inequality over $k = 1, \ldots, N$ and noticing that $\alpha_k \leq 2C_l/(LC_u^2)$, we have

$$\sum_{k=1}^N \left(\alpha_k C_l - \frac{L}{2} C_u^2 \alpha_k^2 \right) \|\nabla f(x_k)\|^2$$

$$\leq f(x_1) - f_{\text{low}} + \frac{LC_u^2}{2} \sum_{k=1}^N \alpha_k^2 \|\delta_k\|^2 + \sum_{k=1}^N (\alpha_k^2 LC_u^2 \langle \nabla f(x_k), \delta_k \rangle - \alpha_k \langle \nabla f(x_k), H_k \delta_k \rangle).$$  

(2.29)

By AS.2 and AS.4 we have that

$$E_{\xi_k}[\langle \nabla f(x_k), \delta_k \rangle \xi[k-1]] = 0, \quad E_{\xi_k}[\langle \nabla f(x_k), H_k \delta_k \rangle | \xi[k-1]] = 0.$$
Moreover, from (2.16) it follows that \( \mathbb{E}[\delta^2_k | \xi_{[k-1]}] \leq \sigma^2/m_k \). Therefore, taking the expectation on both sides of (2.29) with respect to \( \xi_{[N]} \) yields

\[
\sum_{k=1}^{N} (\alpha_k C_l - \alpha_k^2 L C_a^2/2) \mathbb{E}[\xi_{[N]}][\| \nabla f(x_k) \|^2] \leq f(x_1) - f^{\text{low}} + \frac{LC_a^2 \sigma^2 \alpha}{2} \sum_{k=1}^{N} \frac{\alpha_k^2}{m_k}. \tag{2.30}
\]

It follows from the definition of \( P_R \) in (2.30) that

\[
\mathbb{E}[|| \nabla f(x_R) ||^2] = \mathbb{E}_{R, \xi_{[N]}}[|| \nabla f(x_R) ||^2] = \frac{\sum_{k=1}^{N} (\alpha_k C_l - \alpha_k^2 L C_a^2/2) \mathbb{E}[\xi_{[N]}][\| \nabla f(x_k) \|^2]}{\sum_{k=1}^{N} (\alpha_k C_l - \alpha_k^2 L C_a^2/2)}, \tag{2.31}
\]

which together with (2.30) implies (2.27). \( \Box \)

**Remark 2.4.** Note that in Theorem 2.4, \( \alpha_k \)'s are not required to be diminishing, and they can be constant as long as they are upper bounded by \( 2C_l/(LC_a^2) \).

We now give the following complexity result for SQN with random output and constant step size.

**Corollary 2.5.** Assume the conditions in Theorem 2.4 hold, and \( \alpha_k = C_l/(LC_a^2) \) and \( m_k = m \) for all \( k = 1, \ldots, N \). We denote \( \tilde{N} \) as the total number of \( SFO \)-calls needed to calculate stochastic gradient \( g_k \) in SQN (Algorithm 2.1). For a given accuracy tolerance \( \epsilon > 0 \), we assume that

\[
\tilde{N} \geq \max \left\{ \frac{C_l^2}{\sigma^2}, \frac{4C_l^2}{\epsilon}, \frac{\sigma^2}{L^2D} \right\}, \quad \text{where} \quad C_1 = \frac{4\sigma C_l^2 D_f}{C_l^2 \sqrt{D}} + \sigma L \sqrt{D}, \quad C_2 = \frac{4LC_a^2 D_f}{C_l^2}. \tag{2.32}
\]

where \( \tilde{D} \) is a problem-independent positive constant. Moreover, we assume that the batch size satisfies

\[
m_k = m := \left[ \min \left\{ \tilde{N}, \max \left\{ 1, \frac{\sigma}{L \sqrt{\tilde{D}}} \right\} \right\} \right]. \tag{2.33}
\]

Then it holds that

\[
\mathbb{E}[\| \nabla f(x_R) \|^2] \leq \epsilon,
\]

where the expectation is taken with respect to \( R \) and \( \xi_{[N]} \). That is to say, to achieve \( \mathbb{E}[\| \nabla f(x_R) \|^2] \leq \epsilon \), the number of \( SFO \)-calls needed to compute \( g_k \) in SQN is \( O(\epsilon^{-2}) \).

**Proof.** Note that the number of iterations of SQN is at most \( N = \lceil \tilde{N}/m \rceil \). Obviously, \( N \geq \tilde{N}/(2m) \). From (2.28) we have that

\[
\mathbb{E}[\| \nabla f(x_R) \|^2] \leq \frac{2LC_a^2 D_f}{NC_l^2} + \frac{\sigma^2}{m} \leq \frac{4LC_a^2 D_f}{NC_l^2} m + \frac{\sigma^2}{m} \leq \frac{4LC_a^2 D_f}{NC_l^2} \left( 1 + \frac{\sigma}{L \sqrt{\tilde{D}}} \right) + \max \left\{ \frac{\sigma^2}{\tilde{N}}, \frac{\sigma L \sqrt{\tilde{D}}}{\sqrt{\tilde{N}}} \right\}. \tag{2.34}
\]

(2.32) indicates that

\[
\sqrt{\tilde{N}} \geq \frac{\sqrt{C_l^2 + 4\sigma C_l^2}}{\epsilon} \geq \frac{\sqrt{C_l^2 + 4\epsilon C_l^2 + C_l}}{2\epsilon}.
\]
Note that if \( \frac{\sigma^2}{N} \leq \sigma L \sqrt{D}/\sqrt{N} \). Then (2.34) yields that
\[
E[\|\nabla f(x_R)\|^2] \leq \frac{ALC^2 D\|I\|}{NC_1^2} \left( 1 + \frac{\sigma}{L} \sqrt{\frac{N}{D}} \right) + \frac{\sigma L \sqrt{D}}{\sqrt{N}} = \frac{C_1}{\sqrt{N}} + \frac{C_2}{N} \leq \epsilon,
\]
which completes the proof. \( \square \)

Remark 2.5. In Corollary 2.5, we did not consider the SFO-calls that are involved in updating \( H_k \) in line 3 of SQN. In the next section, we consider a specific updating scheme to generate \( H_k \), and analyze the total SFO-calls complexity of SQN including the generation of the \( H_k \).

3. Stochastic damped L-BFGS method. In this section, we propose a specific way, namely a damped L-BFGS method, to generate \( H_k \) in SQN (Algorithm 2.1) that satisfies assumptions AS.3 and AS.4. We also provide an efficient way to compute \( H_k g_k \) without generating \( H_k \) explicitly.

Before presenting our stochastic damped L-BFGS method (SdLBFGS), we first describe a stochastic damped BFGS method as follows. We generate an auxiliary stochastic gradient at \( x_k \) using the sample from the \( (k-1) \)-st iteration:
\[
\bar{g}_k := \frac{1}{m_{k-1}} \sum_{i=1}^{m_{k-1}} g(x_k, \xi_{k-1,i}).
\]
The stochastic gradient difference is defined as
\[
y_{k-1} := \bar{g}_k - g_{k-1} = \frac{\sum_{i=1}^{m_{k-1}} g(x_k, \xi_{k-1,i}) - g(x_{k-1}, \xi_{k-1,i})}{m_{k-1}}.
\]
The iterate difference is still defined as \( s_{k-1} = x_k - x_{k-1} \). We then define
\[
\bar{y}_{k-1} = \hat{\theta}_{k-1} y_{k-1} + (1 - \hat{\theta}_{k-1}) B_{k-1} s_{k-1},
\]
where
\[
\hat{\theta}_{k-1} = \begin{cases} 
0.75 s_{k-1}^T B_{k-1} s_{k-1}, & \text{if } s_{k-1}^T y_{k-1} < 0.25 s_{k-1}^T B_{k-1} s_{k-1}, \\
1, & \text{otherwise}.
\end{cases}
\]
Note that if \( B_{k-1} > 0 \), then \( 0 < \hat{\theta}_{k-1} \leq 1 \). Our stochastic damped BFGS approach updates \( B_{k-1} \) as
\[
B_k = B_{k-1} + \frac{\bar{y}_{k-1} \bar{y}_{k-1}^T s_{k-1}^T}{s_{k-1}^T \bar{y}_{k-1}} - \frac{B_{k-1} s_{k-1}^T s_{k-1}^T}{s_{k-1}^T B_{k-1} s_{k-1}},
\]
where \( \bar{y}_{k-1} \) is defined in (3.2). According to the Sherman-Morrison-Woodbury formula, this corresponds to updating \( H_k = B_k^{-1} \) as
\[
H_k = (I - \rho_{k-1} s_{k-1}^T \bar{y}_{k-1}) H_{k-1} (I - \rho_{k-1} \bar{y}_{k-1} s_{k-1}^T) + \rho_{k-1} s_{k-1}^T s_{k-1}^T,
\]
where \( \rho_{k-1} = (s_{k-1}^T \bar{y}_{k-1})^{-1} \). The following lemma shows that the damped BFGS updates (3.4) and (3.5) preserve the positive definiteness of \( B_k \) and \( H_k \).

Lemma 3.1. For \( \bar{y}_{k-1} \) defined in (3.2), it holds that \( s_{k-1}^T \bar{y}_{k-1} \geq 0.25 s_{k-1}^T B_{k-1} s_{k-1} \). Moreover, if
B_{k-1} = H_{k-1}^{-1} > 0, then B_k and H_k generated by the damped BFGS updates (3.4) and (3.5) are both positive definite.

Proof. From (3.2) and (3.3) we have that

\[
s_{k-1}^T y_{k-1} = \hat{\theta}_{k-1}(s_{k-1}^T y_{k-1} - s_{k-1}^T B_{k-1} s_{k-1}) + s_{k-1}^T B_{k-1} s_{k-1}
\]

\[
= \begin{cases} 
0.25 s_{k-1}^T B_{k-1} s_{k-1}, & \text{if } s_{k-1}^T y_{k-1} < 0.25 s_{k-1}^T B_{k-1} s_{k-1}, \\
 s_{k-1}^T y_{k-1}, & \text{otherwise},
\end{cases}
\]

which implies \( s_{k-1}^T y_{k-1} \geq 0.25 s_{k-1}^T B_{k-1} s_{k-1} \). Therefore, if \( B_{k-1} > 0 \), it follows that \( \rho_{k-1} > 0 \). As a result, for \( H_k \) defined in (3.5) and any nonzero vector \( z \in \mathbb{R}^n \), we have

\[
z^T H_k z = z^T (I - \rho_{k-1} s_{k-1} y_{k-1}^T)H_{k-1}(I - \rho_{k-1} y_{k-1} s_{k-1}^T)z + \rho_{k-1} (s_{k-1}^T z)^2 > 0,
\]

given that \( H_{k-1} > 0 \). Therefore, both \( H_k \) and \( B_k \) defined in (3.5) and (3.4) are positive definite. 

Computing \( H_k \) by the stochastic damped BFGS update (3.6), and computing the step direction \( H_k y_k \) requires \( O(n^2) \) multiplications. This is costly if \( n \) is large. The L-BFGS method originally proposed by Liu and Nocedal [32] can be adopted here to reduce this computational cost. The L-BFGS method can be described as follows for deterministic optimization problems. Given an initial estimate \( H_k \) and any nonzero vector \( z \in \mathbb{R}^n \), we have

\[
\bar{z} \in \arg\min_{z \in \mathbb{R}^n} \frac{1}{2} z^T H_k z + \rho_{k-1} z^T y_{k-1}, \quad \text{subject to } z^T y_{k-1} = 1.
\]

Therefore, both \( H_k \) and \( B_k \) defined in (3.5) and (3.4) are positive definite.

Recently, stochastic L-BFGS methods have been proposed for solving strongly convex problems in [9, 37, 38]. However, the theoretical convergence analyses in these papers do not apply to nonconvex problems. In the following, we show how to design a stochastic damped L-BFGS formula for nonconvex problems.

Suppose that in the past iterations the algorithm generated \( s_j \) and \( \bar{y}_j \) that satisfy

\[
s_j^T \bar{y}_j \geq 0.25 s_j^T H_{j+1,0}^{-1} s_j, \quad j = k - p, \ldots, k - 2.
\]

Then at the current iterate, we compute \( s_{k-1} = x_k - x_{k-1} \) and \( y_{k-1} \) by (3.1). Since \( s_{k-1}^T y_{k-1} \) may not be positive, motivated by the stochastic damped BFGS update (3.2) and (3.6), we define a new vector \( \{\bar{y}_{k-1}\} \) as

\[
\bar{y}_{k-1} = \theta_{k-1} y_{k-1} + (1 - \theta_{k-1}) H_{k,0}^{-1} s_{k-1},
\]

where

\[
\theta_{k-1} = \begin{cases} 
0.75 s_{k-1}^T H_{k,0}^{-1} s_{k-1}, & \text{if } s_{k-1}^T y_{k-1} < 0.25 s_{k-1}^T H_{k,0}^{-1} s_{k-1}, \\
1, & \text{otherwise}.
\end{cases}
\]
Similar to Lemma 3.1, we can prove that
\[ s_{k-1}^\top \tilde{y}_{k-1} \geq 0.25 s_{k-1}^\top H_{k,0}^{-1} s_{k-1}. \]

Using \( s_j \) and \( \tilde{y}_j, j = k - p, \ldots, k - 1 \), we define the stochastic damped L-BFGS formula as
\[ H_{k,i} = (I - \rho_j s_j \tilde{y}_j^\top) H_{k,i-1} (I - \rho_j \tilde{y}_i s_j^\top) + \rho_j s_j s_j^\top, \quad j = k - (p - i + 1); i = 1, \ldots, p, \tag{3.9} \]
where \( \rho_j = (s_j^\top \tilde{y}_j)^{-1} \). Similar to the analysis in Lemma 3.1 by induction we can show that \( H_{k,i} \succ 0 \), \( i = 1, \ldots, p \). Note that when \( k < p \), we use \( s_j \) and \( \tilde{y}_j, j = 1, \ldots, k \) to execute the stochastic damped L-BFGS update.

We next discuss the choice of \( H_{k,0} \). A popular choice in the standard L-BFGS method is to set \( H_{k,0} = \frac{s_{k-1}^\top y_{k-1}}{y_{k-1}^\top y_{k-1}} I \). However, this choice is not necessarily positive definite for nonconvex problems. So we modify this formula as
\[ H_{k,0} = \gamma_k^{-1} I, \quad \text{where } \gamma_k = \max \left\{ \frac{y_{k-1}^\top y_{k-1}}{s_{k-1}^\top y_{k-1}}, \delta \right\} \geq \delta, \tag{3.10} \]
where \( \delta > 0 \) is a given constant.

To prove that \( H_k = H_{k,p} \) generated by (3.9)-(3.10) satisfies assumptions AS.3 and AS.4, we need to make the following assumption.

**AS.5** The function \( F(x, \xi) \) is twice continuously differentiable with respect to \( x \). The stochastic gradient \( g(x, \xi) \) is computed as \( g(x, \xi) = \nabla_x F(x, \xi) \), and there exists a positive constant \( \kappa \) such that \( \| \nabla_x^2 F(x, \xi) \| \leq \kappa \), for any \( x, \xi \).

Note that AS.5 is equivalent to requiring that \( -\kappa I \preceq \nabla_x^2 F(x, \xi) \preceq \kappa I \), rather than the strong convexity assumption \( 0 \prec \kappa I \preceq \nabla_x^2 F(x, \xi) \preceq \kappa I \) required in [9, 37]. The following lemma shows that the eigenvalues of \( H_k \) are bounded below away from zero under assumption AS.5.

**Lemma 3.2.** Suppose that the assumption AS.5 holds. Given \( H_{k,0} \) defined in (3.10), suppose that \( H_k = H_{k,p} \) is updated through the stochastic damped L-BFGS formula (3.9). Then all the eigenvalues of \( H_k \) satisfy
\[ \lambda(H_k) \geq \left( \frac{4p \kappa^2}{\delta} + (4p + 1)(\kappa + \delta) \right)^{-1}. \tag{3.11} \]

**Proof.** According to Lemma 3.1, \( H_{k,i} \succ 0, i = 1, \ldots, p \). To prove that the eigenvalues of \( H_k \) are bounded below away from zero, it suffices to prove that the eigenvalues of \( B_k = H_k^{-1} \) are bounded from above. From the damped L-BFGS formula (3.9), \( B_k = B_{k,p} \) can be computed recursively as
\[ B_{k,i} = B_{k,i-1} + \frac{\tilde{y}_j s_j^\top}{s_j^\top \tilde{y}_j} - \frac{B_{k,i-1} s_j s_j^\top B_{k,i-1}}{s_j^\top B_{k,i-1} s_j}, \quad j = k - (p - i + 1); i = 1, \ldots, p, \]
starting from \( B_{k,0} = H_{k,0}^{-1} = \gamma_k I \). Since \( B_{k,0} \succ 0 \), Lemma 3.1 indicates that \( B_{k,i} \succ 0 \) for \( i = 1, \ldots, p \).
Moreover, the following inequalities hold:

\[
\|B_{k,i}\| \leq \left\| B_{k,i-1} - \frac{B_{k,i-1}s_js_j^T B_{k,i-1}}{s_j^T B_{k,i-1}s_j} \right\| + \left\| \frac{\bar{y}_j\bar{y}_j^T}{s_j} \right\| \leq \|B_{k,i-1}\| + \left\| \frac{\bar{y}_j\bar{y}_j^T}{s_j} \right\| = \|B_{k,i-1}\| + \frac{\bar{y}_j^T \bar{y}_j}{s_j}.
\]

(3.12)

From the definition of \(\bar{y}_j\) in (3.7) and the facts that \(s_j^T \bar{y}_j \geq 0.25s_j^T B_{j+1,0} s_j\) and \(B_{j+1,0} = \gamma_{j+1} I\) from (3.10), we have that for any \(j = k-1, \ldots, k-p\)

\[
\frac{\bar{y}_j^T \bar{y}_j}{s_j} \leq 4\left\| \theta_j y_j + (1 - \theta_j) B_{j+1,0} s_j \right\|^2 = 4\theta_j^2 y_j^T y_j + 8\theta_j(1 - \theta_j) y_j^T s_j + 4(1 - \theta_j)^2 \gamma_{j+1}.
\]

(3.13)

Note that from (3.1) we have

\[
y_j = \sum_{i=1}^{m_j} \frac{g(x_{j+1}, \xi_{j,i}) - g(x_j, \xi_{j,i})}{m_j} = \frac{1}{m_j} \left( \sum_{i=1}^{m_j} \nabla_{xx}^2 F(x_{j+1}, \xi_{j,i}, s_j) \right) s_j,
\]

where \(\nabla_{xx}^2 F(x_{j+1}, \xi_{j,i}, s_j) = \int_0^1 \nabla_{xx}^2 F(x_j + ts_j, \xi_{j,i}, s_j) dt\), because \(g(x_{j+1}, \xi_{j,i}) - g(x_j, \xi_{j,i}) = \int_0^1 \frac{dg}{dt}(x_j + ts_j, \xi_{j,i}) dt = \int_0^1 \nabla_{xx}^2 F(x_j + ts_j, \xi_{j,i}, s_j) dt\). Therefore, for any \(j = k-1, \ldots, k-p\), from (3.10), and the facts that \(0 < \theta_j \leq 1\) and \(\delta \leq \gamma_{j+1} \leq \kappa + \delta\), and the assumption AS.5 it follows that

\[
\frac{\bar{y}_j^T \bar{y}_j}{s_j} \leq \frac{4\theta_j^2 \kappa^2}{\gamma_{j+1}} + 8\theta_j(1 - \theta_j) \kappa + 4(1 - \theta_j)^2 \gamma_{j+1} \leq \frac{4\theta_j^2 \kappa^2}{\delta} + 4[(1 - \theta_j^2) \kappa + (1 - \theta_j)^2 \delta] \leq \frac{4\kappa^2}{\delta} + 4(\kappa + \delta).
\]

(3.14)

Combining (3.12) and (3.14) yields

\[
\|B_{k,i}\| \leq \|B_{k,i-1}\| + 4 \left( \frac{\kappa^2}{\delta} + \kappa + \delta \right).
\]

By induction, we have that

\[
\|B_k\| = \|B_{k,p}\| \leq \|B_{k,0}\| + 4p \left( \frac{\kappa^2}{\delta} + \kappa + \delta \right) \leq \frac{4p\kappa^2}{\delta} + (4p + 1)(\kappa + \delta),
\]

which implies (3.11). □

We now prove that \(H_k\) is uniformly upper bounded.

**Lemma 3.3.** Suppose that the assumption AS.5 holds. Given \(H_{k,0}\) defined in (3.10), suppose that \(H_k = H_{k,p}\) is updated through the stochastic damped L-BFGS formula (3.9). Then \(H_k\) satisfies

\[
\lambda_{\text{max}}(H_k) = \|H_k\| \leq \left( \frac{\alpha^{2p} - 1}{\alpha^2 - 1} \right) \frac{4}{\delta} + \frac{\alpha^{2p}}{\delta},
\]

(3.15)

where \(\alpha = (4\kappa + 5\delta)/\delta\).

**Proof.** For notational simplicity, let \(H = H_{k,i-1}, H^+ = H_{k,i}, s = s_j, \bar{y} = \bar{y}_j, \rho = (s_j^T \bar{y}_j)^{-1} = (s^T \bar{y})^{-1}\). Now (3.3) can be written as

\[
H^+ = H - \rho(H \bar{y} s^T + s \bar{y}^T H) + \rho ss^T + \rho^2(s^T H \bar{y}) ss^T.
\]
Using the facts that

- \( \| u u^T \| = \| u \| \cdot \| v \| \) for any vectors \( u \) and \( v \);
- \( \rho s^T s = \rho \| s \|^2 = \frac{s^T s}{y} \leq \frac{4}{\delta} \);
- \( \| \frac{y_j y_j}{s_j} \| \leq 4 \left( \frac{\kappa^2}{\delta} + \kappa + \frac{\delta}{4} \right) < \frac{4}{\delta} (\kappa + \delta)^2 \), which follows from (3.14),

we have that

\[
\| H^+ \| \leq \| H \| + \frac{2 \| H \| \cdot \| y \| \cdot \| s \|}{s^T y} + \frac{s^T s}{s^T y} + \frac{s^T s}{s^T y} \frac{\| H \| \cdot \| y \|^2}{s^T y}.
\]

Noting that \( \frac{\| y \|}{s^T y} = \left[ \frac{\| y \|^2}{s^T y} \cdot \frac{s^T y}{s^T y} \right]^{1/2} \), it follows that

\[
\| H^+ \| \leq \left( 1 + 2 \cdot \frac{4}{\delta} (\kappa + \delta) + \left( \frac{4}{\delta} (\kappa + \delta) \right)^2 \right) \| H \| + \frac{4}{\delta} = (1 + (4 \kappa + 4 \delta) / \delta^2) \| H \| + \frac{4}{\delta}.
\]

Hence, by induction we obtain (3.15). \( \square \)

Lemmas 3.2 and 3.3 indicate that \( H_k \) generated by the stochastic damped L-BFGS formula (3.9) satisfies the assumption \( \text{AS.3} \) with \( C_1 = \left( \frac{4 \rho s^2}{\delta} + (4 p + 1) (\kappa + \delta) \right)^{-1} \) and \( C_\kappa = \left( \frac{\alpha^2 - 1}{\alpha - 1} \right) \frac{4}{\delta} + \frac{\alpha^2}{\delta} \). Moreover, since \( y_{k-1} \) defined in (3.11) does not depend on random samplings in the \( k \)-th iteration, it follows that \( H_k \) depends only on \( \xi_{[k-1]} \) and the assumption \( \text{AS.4} \) is satisfied.

We next analyze the computational cost of step direction \( H_k g_k \). Note that from (3.9), \( H_k \) can be equivalently represented as

\[
H_k = V_{k-1}^T \cdots V_{k-p}^T H_{k,0} V_{k-p} \cdots V_{k-1} + \rho_{k-p} V_{k-1}^T \cdots V_{k-p+1}^T s_{k-p} \cdots V_{k-p+1}^T V_{k-p} \cdots V_{k-1} + \cdots + \rho_{k-2} V_{k-1}^T s_{k-2} V_{k-2} + \rho_{k-1} s_{k-1} V_{k-1}^T
\]

(3.16)

where \( V_j = I - \rho_j s_j y_j^T \). Note that (3.16) is the same as the classical L-BFGS formula in (3.6), except that \( y_j \) is replaced by \( \bar{y}_j \). Thus the mechanism for both updates for computing the step direction is the same. Based on the analysis in (3.2), computing the step direction corresponds to the following two-loop recursion. Given \( s_j, \bar{y}_j, j = k - p, \ldots, k - 1 \) and \( u_0 = g_k \), compute the vector \( u_i \) through

\[
u_{i+1} = u_i - \mu_i \bar{y}_{k-i-1}, \quad i = 0, \ldots, p - 1,
\]

where \( \mu_i = \rho_{k-i-1} u_i^T s_{k-i-1} \). Further setting \( v_0 = H_{k,0} u_p \), recursively compute the vector \( v_i \) through

\[
u_{i+1} = v_i + (\mu_{i-1} - \nu_i) s_{k-p+i}, \quad i = 0, \ldots, p - 1,
\]

where \( \nu_i = \rho_{k-p+i} v_i^T \bar{y}_{k-p+i} \). This procedure gives \( H_k g_k = v_p \). We refer to (3.2) for more details. We now summarize this computational process as Procedure 3.1.

We now analyze the computational cost of Procedure 3.1. In Step 2, the computation of \( \gamma_k \) involves \( y_{k-1} \bar{y}_{k-1} \) and \( s_{k-1} \bar{y}_{k-1} \), which take \( 2n \) multiplications. In Step 3, from the definition of \( \bar{y}_k \) in (3.7), since \( s_{k-1} \bar{y}_{k-1} \) has been obtained in a previous step, one only needs to compute \( s_{k-1}^T s_{k-1} \) and some scalar-vector
Procedure 3.1 Step computation using stochastic damped L-BFGS

Input: Let \( x_k \) be current iterate. Given the stochastic gradient \( g_{k-1} \) at iterate \( x_{k-1} \), the random variable \( \xi_{k-1} \) and the batch size \( m_{k-1} \), calculate \( \bar{y}_{k-1} \) through (3.11)

Output: \( H_k g_k = v_p \)

1. Set \( s_{k-1} = x_k - x_{k-1} \) and calculate \( y_{k-1} \) through (3.11)
2. Calculate \( \gamma_k \) through (3.10)
3. Calculate \( \bar{y}_{k-1} \) through (3.11) and \( p_{k-1} = (s_{k-1}^\top \bar{y}_{k-1})^{-1} \)
4. for \( i = 0, \ldots, \min\{p, k-1\} \) - 1 do
5. Calculate \( \mu_i = \rho_{k-1} - 1 \)
6. Calculate \( u_{i+1} = u_i - \mu_i \bar{y}_{k-1} \)
7. end for
8. Calculate \( v_0 = \gamma_k^{-1} u_p \)
9. for \( i = 0, \ldots, \min\{p, k-1\} \) - 1 do
10. Calculate \( v_i = \rho_{k-1} v_{i+1} \bar{y}_{k-1} \)
11. Calculate \( v_{i+1} = v_i + (\mu_i - \mu_i - \nu_i) s_{k-1} \)
12. end for

products, thus the computation of \( \bar{y}_{k-1} \) takes \( 3n \) multiplications. Due to the fact that

\[
\rho_{k-1}^{-1} = s_{k-1}^\top \bar{y}_{k-1} = \begin{cases} 0.25 \gamma_k s_{k-1}^\top s_{k-1}, & \text{if } s_{k-1}^\top y_{k-1} < 0.25 \gamma_k s_{k-1}^\top s_{k-1}, \\ s_{k-1}^\top y_{k-1}, & \text{otherwise,} \end{cases}
\]

all involved computations have been done for \( p_{k-1} \). Furthermore, the first loop Steps 4-7 involves \( p \) scalar-vector multiplications and \( p \) vector inner products. So does the second loop Steps 9-12. Including the product \( \gamma_k^{-1} u_p \), the whole procedure takes \((4p + 6)n\) multiplications.

Notice that in Step 1 of Procedure 3.1 the computation of \( y_{k-1} \) involves the evaluation of \( \sum_{i=1}^{m_{k-1}} g(x_k, \xi_{k-1,i}) \), which requires \( m_{k-1} \) \textit{SFO}-calls. As a result, when Procedure 3.1 is plugged into SQN (Algorithm 2.1), the total number of \textit{SFO}-calls needed in the \( k \)-th iteration becomes \( m_k + m_{k-1} \). This leads to the following overall \textit{SFO}-calls complexity result for our stochastic damped L-BFGS method.

**Theorem 3.1.** Suppose that \textit{AS.1}, \textit{AS.2} and \textit{AS.5} hold. Let \( N_{\text{fso}} \) denote the total number of \textit{SFO}-calls in SQN (Algorithm 2.1) in which Procedure 3.1 is used to compute \( H_k g_k \). Under the same conditions as in Corollary 2.3 to achieve \( E[\|\nabla f(x_k)\|^2] \leq \epsilon \), \( N_{\text{fso}} \) is at most \( 2\hat{N} \) where \( \hat{N} \) satisfies (2.32), i.e., is of the order of \( O(\epsilon^{-2}) \).

**4. Numerical Experiments.** In this section, we report the results of numerical experiments that test the performance of the proposed SdLBFGS method, i.e., SQN (Algorithm 2.1) with Procedure 3.1 incorporated to generate \( H_k \). We mainly focus on the comparison of SdLBFGS with SGD (1.2) with \( g_k \) given by (2.5) for solving the following nonconvex support vector machine (SVM) problem with a sigmoid loss function, which has been considered in [23] [35]:

\[
\min_{x \in \mathbb{R}^n} f(x) := \mathbb{E}_{u,v}[1 - \tanh(v(x,u))] + \lambda\|x\|^2_2,
\]

(4.1)

where \( \lambda > 0 \) is a regularization parameter, \( u \in \mathbb{R}^n \) denotes the feature vector, and \( v \in \{-1, 1\} \) refers to the corresponding label. In our experiments, \( \lambda \) was chosen as \( 10^{-4} \). All the algorithms were implemented in Matlab R2013a on a PC with a 2.60 GHz Intel microprocessor and 8GB of memory. We restate here some notation used in the algorithms.

(1) \( m \): The number of training samples that are randomly chosen to define the stochastic gradient (2.5)
with \( m_k = m \).

(2) \( \alpha_k \): The stepsize used in both SGD and SdLBFGS, which is defined as \( \alpha_k = \frac{\beta}{k} \) with \( \beta > 0 \).

(3) \( \delta \): The parameter used in (3.10), which is set as \( \delta = 1 \) in our experiments.

(4) \( p \): The memory size used in SdLBFGS (3.9).

(5) \( \mathcal{SFO}\)-calls: The number of individual gradient evaluations \( g(x_k, \xi_{k,i}) \), which corresponds to the number of training samples accessed.

4.1. Experiments on a synthetic dataset. In this subsection, we report numerical comparison results for SdLBFGS and SGD for solving (4.1) on synthetic data for problems of dimension \( n = 500 \). We set the initial point for both SdLBFGS and SGD as \( x_1 = 5 \cdot \bar{x}_1 \), where \( \bar{x}_1 \) was drawn from the uniform distribution over \([0, 1]^n\). Every time when we computed a stochastic gradient, we generated a training point \((u, v)\) in the following manner. We first generated a sparse vector \( u \) with 5\% nonzero components following the uniform distribution on \([0, 1]^n\), and then set \( v = \text{sign}(\langle \bar{x}, u \rangle) \) for some \( \bar{x} \in \mathbb{R}^n \) drawn from the uniform distribution on \([-1, 1]^n\). Every time we computed a stochastic gradient of the sigmoid loss function in (4.1), we accessed \( m \) data points \((u, v)\) from the training data set without replacement.

In Figure 4.1 we compare the performance of SGD and SdLBFGS with various memory sizes \( p \). The batch size was set to \( m = 100 \) and the stepsize to both \( \alpha_k = 10^k / k \) and \( \alpha_k = 20^k / k \) for SGD and \( 10^k / k \) for SdLBFGS. In Figure 4.1 (a) we plot the squared norm of gradient (SNG) versus the number of iterations, up to a total of 1000. The SNG was computed using \( \bar{x} \) as:

\[
\text{SNG} = \left\| \frac{1}{N} \sum_{i=1}^{N} \nabla_x F(\bar{x}; u_i, v_i) + \lambda \bar{x} \right\|^2, \tag{4.2}
\]

where \( \bar{x} \) is the output of the algorithm and \( F(x; u, v) = 1 - \tanh(v(x, u)) \). In Figure 4.1 (b) we plot the percentage of correctly classified testing data. From Figure 4.1 we can see that increasing the memory size improves the performance of SdLBFGS. When the memory size \( p = 0 \), we have \( H_k = \gamma_k^{-1} I \) and SdLBFGS reduces to SGD with an adaptive stepsize. SdLBFGS with memory size \( p = 1 \) oscillates quite a lot, but to a lesser degree for \( p = 3, 5, 10, 20 \). The performance of the variants of SdLBFGS with memory size \( p = 3, 5, 10, 20 \) are all quite similar and they all outperform significantly SdLBFGS with \( p = 0 \) and \( p = 1 \).

In Figure 4.2 we report the effect of the batch size \( m \) on the performance of SGD and SdLBFGS with memory size \( p = 20 \). We tested SGD and SdLBFGS with three different batch sizes \( m = 50, 100, 500 \). Figure 4.2 (a) plots the squared norm of the gradient versus the number of iterations, and Figure 4.2 (b) plots the squared norm of the gradient versus the number of \( \mathcal{SFO}\)-calls, up to \( 2 \times 10^4 \). From Figure 4.2 we see that the performance of SGD for the three batch sizes is quite similar. For SdLBFGS, Figure 4.2 (a) shows that \( m = 500 \) gives the best performance among the three choices with respect to the total number of iterations taken. This is because a larger batch size leads to gradient estimation with lower variance. Figure 4.2 (b) shows that if the total number of \( \mathcal{SFO}\)-calls is fixed, then because of the tradeoff between the number of iterations and the batch size, i.e., because in this case the number of iterations is proportional to the reciprocal of the batch size, the SdLBFGS variant corresponding to \( m = 100 \) slightly outperforms the \( m = 500 \) variant.

In Figure 4.3 we report the percentage of correctly classified data for 5000 randomly generated testing points. The results are consistent with the one shown in Figure 4.2 (a), i.e., the ones with a lower squared norm of the gradient give a higher percentage of correctly classified data.
In Figure 4.4, we report the number of “damped steps” taken by SdLBFGS. Here slightly different from (3.8), we count the number of iterations in which $s_k^T y_{k-1} < 0$ as the number of “damped steps”. We set the total number of iterations to 1000 and report the effect of the memory size and batch size of SdLBFGS on the number of damped steps. From Figure 4.4 we see that the number of damped steps decreases as the memory size $p$ and the batch size $m$ increase. This is to be expected because as $p$ increases, there is less negative effect caused by “limited-memory”; and as $m$ increases, the gradient estimation has lower variance.

4.2. RCV1 dataset. In this subsection, we compare SGD and SdLBFGS for solving (4.1) on a real dataset: RCV1 [31], which is a collection of newswire articles produced by Reuters in 1996-1997. In our tests, we used a subset of RCV1 that is used in [10]. This subset contains 9625 articles with 29992 distinct words. The articles are classified into four categories “C15”, “ECAT”, “GCAT”, and “MCAT”, each with 2022, 2064, 2901 and 2638 articles respectively. We consider the binary classification problem of predicting whether or not an article is in the second and fourth category, i.e., “MCAT” and “ECAT”. As a result, the entry of each label vector is 1 if a given article appears in category “MCAT” or “ECAT”, and -1 otherwise.

We used 60% of the articles as training data and the remaining 40% as testing data. As a result, there were 5776 articles in the training data and 3849 articles in the testing data. We again used the nonconvex SVM model (4.1), with a problem dimension of 29992. In SGD and SdLBFGS, every time we computed a stochastic gradient, we randomly chose one data point from the training set without replacement.

In Figure 4.5, we compare SdLBFGS with various memory sizes and SGD on the RCV1 dataset. For SGD and SdLBFGS, we use the stepsize: $\alpha_k = 10/k$ and the batch size $m = 100$. We also used a second stepsize of $20/k$ for SGD. Note that the squared norm of the gradient is computed via (4.2) using $N = 3849$ testing data. Figure 4.5 (a) shows that for the RCV1 data set, increasing the memory size improves the performance of SdLBFGS. The performance of SdLBFGS with memory sizes $p = 10, 20$ was similar, although for $p = 10$ it was slightly better. Figure 4.5 (b) also shows that larger memory sizes can achieve higher correct classification percentages.

Figure 4.6 presents the comparison of SGD and SdLBFGS with different batch sizes. The step size of SGD was set to $\alpha_k = 20/k$, while the step size of SdLBFGS was set to $\alpha_k = 10/k$. The memory size of SdLBFGS was chosen as $p = 10$. We tested SGD with batch size $m = 1, 50, 100$, and SdLBFGS with batch size $m = 1, 50, 75, 100$. From Figure 4.6 we can see that SGD performs worse than SdLBFGS. For SdLBFGS, from Figure 4.6 (a) we observe that larger batch sizes give better results in terms of SNG. If we fix the total number of $SFO$-calls to $2 \times 10^4$, SdLBFGS with $m = 1$ performs the worst among the different batch sizes and exhibits dramatic oscillation. The performance gets much better when the batch size becomes larger. In this set of tests, the performance with $m = 50, 75$ was slightly better than $m = 100$. One possible reason for that is that for the same number of $SFO$-calls, a smaller batch size leads to larger number of iterations and thus gives better results.

In Figure 4.7, we report the percentage of correctly classified data points for both SGD and SdLBFGS with different batch sizes. The step size of SGD was $\alpha_k = 20/k$, while the step size of SdLBFGS was $\alpha_k = 10/k$. The memory size of SdLBFGS was $p = 10$. Results shown in Figure 4.7 are consistent with the ones in Figure 4.6. Roughly speaking, the algorithm that gives a lower SNG leads to a higher percentage of correctly classified data points.

We also tested the effect of memory size and batch size of SdLBFGS on the number of damped steps. Here the total number of iterations was 1000. In Figure 4.8, we report the number of damped steps in SdLBFGS for different values of memory size and batch size. Figure 4.8 is qualitatively similar to Figure 4.4.
except that for the fixed batch size $m = 50$, a fewer number of damped steps were required by the SdLBFGS variants with memory sizes $p = 1$ and $p = 3$ compared with $p = 5$ and $p = 10$.

5. Conclusion and Future Work. In this paper we proposed a general framework for stochastic quasi-Newton methods for nonconvex stochastic optimization. Global convergence, iteration complexity, and $SFO$-calls complexity were analyzed under different conditions on the step size and the output of the algorithm. Specifically, a stochastic damped limited memory BFGS method was proposed, which falls under the proposed framework and does not generate $H_k$ explicitly. The damping technique was used to preserve the positive definiteness of $H_k$, without requiring the original problem to be convex. Encouraging numerical results were reported for solving nonconvex machine learning problems on both synthetic and real data arising from text mining and classification. Future work will focus on developing variants of our SdLBFGS method that incorporate techniques like those developed in [25] and used in [38] and [33].

REFERENCES

[1] F. Bach. Adaptivity of averaged stochastic gradient descent to local strong convexity for logistic regression. *Journal of Machine Learning Research*, 15:595–627, 2014.

[2] F. Bach and E. Moulines. Non-strongly-convex smooth stochastic approximation with convergence rate $O(1/n)$. In *NIPS*, 2013.

[3] F. Bastin, C. Cirillo, and P. L. Toint. Convergence theory for nonconvex stochastic programming with an application to mixed logit. *Math. Program.*, 108:207–234, 2006.

[4] A. Bordes, L. Bottou, and P. Gallinari. SGD-QN: Careful quasi-Newton stochastic gradient descent. *J. Mach. Learn. Res.*, 10:1737–1754, 2009.

[5] L. Bottou. Online algorithms and stochastic approximations. *Online Learning and Neural Networks*, Edited by David Saad, Cambridge University Press, Cambridge, UK, 1998.

[6] D. Brownstone, D. S. Bunch, and K. Train. Joint mixed logit models of stated and revealed preferences for alternative-fuel vehicles. *Transport. Res. B*, 34(5):315–338, 2000.

[7] C. G. Broyden. The convergence of a class of double-rank minimization algorithms. *J. Inst. Math. Appl.*, 6(1):76–90, 1970.

[8] R.H. Byrd, G. Chin, W. Neveitt, and J. Nocedal. On the use of stochastic hessian information in optimization methods for machine learning. *SIAM J. Optim.*, 21(3):977–995, 2011.

[9] R.H. Byrd, S.L. Hansen, J. Nocedal, and Y. Singer. A stochastic quasi-Newton method for large-scale optimization. http://arxiv.org/pdf/1401.7020v2.pdf, 2014.

[10] D. Cai and X. He. Manifold adaptive experimental design for text categorization. *IEEE Transactions on Knowledge and Data Engineering*, 4:707–719, 2012.

[11] K. L. Chung. On a stochastic approximation method. *Annals of Math. Stat.*, pages 463–483, 1954.

[12] C. D. Dang and G. Lan. Stochastic block mirror descent methods for nonsmooth and stochastic optimization. *SIAM Journal on Optimization*, 25(2):856–881, 2015.

[13] A. Defazio, F. Bach, and S. Lacoste-Julien. SAGA: A fast incremental gradient method with support for non-strongly convex composite objectives. In *NIPS*, 2014.

[14] J. C. Duchi, E. Hazan, and Y. Singer. Adaptive subgradient methods for online learning and stochastic optimization. *J. Mach. Learn. Res.*, 999999:2121–2159, 2011.

[15] R. Durrett. *Probability: Theory and Examples*. Cambridge University Press, London, 2010.

[16] Y. Ermoliev. Stochastic quasigradient methods and their application to system optimization. *Stochastics*, 9:1–36, 1983.

[17] R. Fletcher. A new approach to variable metric algorithms. *Comput. J.*, 13(3):317–322, 1970.

[18] A. A. Gavurin. Nonstationary stochastic programming problems. *Kibernetika*, 4:89–92, 1978.

[19] S. Ghadimi and G. Lan. Optimal stochastic approximation algorithms for strongly convex stochastic composite optimization, I: a generic algorithmic framework. *SIAM J. Optim.*, 22:1469–1492, 2012.

[20] S. Ghadimi and G. Lan. Stochastic first- and zeroth-order methods for nonconvex stochastic programming. *SIAM J. Optim.*, 15(6):2341–2368, 2013.

[21] S. Ghadimi and G. Lan. Accelerated gradient methods for nonconvex nonlinear and stochastic programming. *Mathematical Programming*, 2015.
Fig. 4.1. Comparison on a synthetic data set of SGD and SdLBFGS variants with different memory size $p$, with respect to the squared norm of the gradient and the percent of correctly classified data, respectively. A stepsize of $\alpha_k = 10/k$ and batch size of $m = 100$ was used for all SdLBFGS variants. Step sizes of $10/k$ and $20/k$ were used for SGD.
Fig. 4.2. Comparison of SGD and SdLBFGS variants with different batch size $m$ on a synthetic data set. The memory size of SdLBFGS was $p = 20$ and the step size of SdLBFGS was $\alpha_k = 10/k$, while the step size of SGD was $\alpha_k = 20/k$. 
Fig. 4.3. Comparison of correct classification percentage on a synthetic dataset by SGD and SdLBFGS with different batch sizes. The memory size of SdLBFGS was $p = 20$ and the stepsize of SdLBFGS was $\alpha_k = 10/k$. The step size of SGD was $\alpha_k = 20/k$.

Fig. 4.4. The average number of damped steps over 10 runs of SdLBFGS on a synthetic data set. Here the maximum number of iterations was set to 1000 and step size was $10/k$.

[22] S. Ghadimi, G. Lan, and H. Zhang. Mini-batch stochastic approximation methods for nonconvex stochastic composite optimization. *Math. Program.*, November, 2014.

[23] D. Goldfarb. A family of variable metric updates derived by variational means. *Math. Comput.*, 24(109):23–26, 1970.

[24] D. A. Hensher and W. H. Greene. The mixed logit model: The state of practice. *Transportation*, 30(2):133–176, 2003.

[25] R. Johnson and T. Zhang. Accelerating stochastic gradient descent using predictive variance reduction. *NIPS*, 2013.

[26] A. Juditsky, A. Nazin, A. B. Tsybakov, and N. Vayatis. Recursive aggregation of estimators via the mirror descent algorithm with average. *Probl. Inform. Transm.*, 41(4):78–96, 2005.
Fig. 4.5. Comparison of SdLBFGS variants with different memory sizes on the RCV1 dataset. The step size of SdLBFGS was $\alpha_k = 10/k$ and the batch size was $m = 100$. 
Fig. 4.6. Comparison of SGD and SdLBFGS with different batch sizes on the RCV1 dataset. For SdLBFGS the step size was $\alpha_k = 10/k$ and the memory size was $p = 10$. For SGD the step size was $\alpha_k = 20/k$. 
Fig. 4.7. Comparison of correct classification percentage by SGD and SdLBFGS with different batch sizes on the RCV1 dataset. For SdLBFGS the step size was $\alpha_k = \frac{10}{k}$ and the memory size was $p = 10$. For SGD the step size was $\alpha_k = \frac{20}{k}$.

Fig. 4.8. The average number of damped steps over 10 runs of SdLBFGS on the RCV1 data set. Here the maximum number of iterations was set to 1000 and step size was $10/k$.

[27] A. Juditsky, P. Rigollet, and A. B. Tsybakov. Learning by mirror averaging. *Annals of Stat.*, 36:2183–2206, 2008.
[28] G. Lan. An optimal method for stochastic composite optimization. *Math. Program.*, 133(1):365–397, 2012.
[29] G. Lan, A. S. Nemirovski, and A. Shapiro. Validation analysis of mirror descent stochastic approximation method. *Math. Program.*, 134:425–458, 2012.
[30] N. Le Roux, M. Schmidt, and F. Bach. A stochastic gradient method with an exponential convergence rate for strongly-convex optimization with finite training sets. In *NIPS*, 2012.
[31] D. Lewis, Y. Yang, T. Rose, and F. Li. RCV1: A new benchmark collection for text categorization research. *Journal of Mach. Learn. Res.*, 5(361-397), 2004.
D. C. Liu and J. Nocedal. On the limited memory BFGS method for large scale optimization. *Math. Program.*, Ser. B, 45(3):503–528, 1989.

A. Lucchi, B. McWilliams, and T. Hofmann. A variance reduced stochastic Newton method. *preprint available at http://arxiv.org/abs/1503.08316*, 2015.

J. Mairal, F. Bach, J. Ponce, and G. Sapiro. Online dictionary learning for sparse coding. In *ICML*, 2009.

L. Mason, J. Baxter, P. Bartlett, and M. Frean. Boosting algorithms as gradient descent in function space. In *NIPS*, volume 12, pages 512–518, 1999.

A. Mokhtari and A. Ribeiro. RES: Regularized stochastic BFGS algorithm. *IEEE Trans. Signal Process.*, no. 10, 2014.

A. Mokhtari and A. Ribeiro. Global convergence of online limited memory BFGS. *to appear in J. Mach. Learn. Res.*, 2015.

P. Moritz, R. Nishihara, and M.I. Jordan. A linearly-convergent stochastic L-BFGS algorithm. *arXiv: 1508.02087v1 [math.OC]*, 9 Aug 2015.

A. S. Nemirovski, A. Juditsky, G. Lan, and A. Shapiro. Robust stochastic approximation approach to stochastic programming. *SIAM J. Optim.*, 19:1574–1609, 2009.

Y. E. Nesterov. A method for unconstrained convex minimization problem with the rate of convergence $\mathcal{O}(1/k^2)$. *Dokl. Akad. Nauk SSSR*, 269:543–547, 1983.

Y. E. Nesterov. *Introductory lectures on convex optimization: A basic course*. Applied Optimization. Kluwer Academic Publishers, Boston, MA, 2004.

J. Nocedal and S. J. Wright. *Numerical Optimization*. Springer, New York, USA, 2006.

B. T. Polyak. New stochastic approximation type procedures. *Automat. i Telemech.*, 7:98–107, 1990.

B. T. Polyak and A. B. Juditsky. Acceleration of stochastic approximation by averaging. *SIAM J. Control and Optim.*, 30:838–855, 1992.

H. Robbins and S. Monro. A stochastic approximatin method. *Annals of Math. Stat.*, 22:400–407, 1951.

N.L. Roux and A.W. Fitzgibbon. A fast natural Newton method. In *Proceedings of the 27th International Conference on Machine Learning (ICML-10)*, pages 623–630, 2010.

A. Ruszczynski and W. Syski. A method of aggregate stochastic subgradients with on-line stepsize rules for convex stochastic programming problems. *Math. Prog. Stud.*, 28:113–131, 1986.

J. Sacks. Asymptotic distribution of stochastic approximation. *Annals of Math. Stat.*, 29:373–409, 1958.

N. N. Schraudolph, J. Yu, and S. Günter. A stochastic quasi-Newton method for online convex optimization. In *Proc. 11th Intl. Conf. Artificial Intelligence and Statistics (AISTATS)*, pages 436–443, San Juan, Puerto Rico, 2007.

S. Shalev-Shwartz and S. Ben-David. *Understanding Machine Learning: From Theory to Algorithms*. Cambridge University Press, 2014.

O. Shamir and T. Zhang. Stochastic gradient descent for non-smooth optimization: Convergence results and optimal averaging schemes. In *ICML*, 2013.

D. F. Shanno. Conditioning of quasi-Newton methods for function minimization. *Math. Comput.*, 24(111):647–656, 1970.

X. Wang, S. Ma, and Y. Yuan. Penalty methods with stochastic approximation for stochastic nonlinear programming. *arXiv:1312.2690*, 2013.

L. Xiao and T. Zhang. A proximal stochastic gradient method with progressive variance reduction. *SIAM Journal on Optimization*, 24:2057–2075, 2014.