
A Progressive Batching L-BFGS Method for Machine Learning

Raghu Bollapragada¹ Dheevatsa Mudigere² Jorge Nocedal¹ Hao-Jun Michael Shi¹ Ping Tak Peter Tang³

Abstract

The standard L-BFGS method relies on gradient approximations that are not dominated by noise, so that search directions are descent directions, the line search is reliable, and quasi-Newton updating yields useful quadratic models of the objective function. All of this appears to call for a full batch approach, but since small batch sizes give rise to faster algorithms with better generalization properties, L-BFGS is currently not considered an algorithm of choice for large-scale machine learning applications. One need not, however, choose between the two extremes represented by the full batch or highly stochastic regimes, and may instead follow a progressive batching approach in which the sample size increases during the course of the optimization. In this paper, we present a new version of the L-BFGS algorithm that combines three basic components — progressive batching, a stochastic line search, and stable quasi-Newton updating — and that performs well on training logistic regression and deep neural networks. We provide supporting convergence theory for the method.

1. Introduction

The L-BFGS method (Liu & Nocedal, 1989) has traditionally been regarded as a batch method in the machine learning community. This is because quasi-Newton algorithms need gradients of high quality, as they are designed to produce descent directions and select the steplength through a line search procedure. All of these algorithmic ingredients can be implemented, it seems, only by using very large batch

sizes, resulting in a costly iteration that makes the overall algorithm slow compared with stochastic gradient methods (Robbins & Monro, 1951; Bottou & Cun, 2004).

Even before the recent resurgence of neural networks, many researchers observed that a well-tuned implementation of the stochastic gradient (SG) method was far more effective on large-scale logistic applications than the batch L-BFGS method, even when taking into account the advantages of parallelism offered by the use of large batches. The preeminence of the SG method (and its variants) became more pronounced with the advent of deep neural networks, and some researchers have speculated that SG is endowed with certain regularization properties that are essential in the minimization of such complex nonconvex functions (Hardt et al., 2015; Keskar et al., 2016).

In this paper, we postulate that the most efficient algorithms for machine learning may not reside entirely in the highly stochastic or full batch regimes, but should employ a progressive batching approach in which the sample size is initially small, and is increased as the iteration progresses. This view is consistent with recent numerical experiments on training various deep neural networks (Smith et al., 2017), where the SG method, with increasing sample sizes, yields similar test loss and accuracy as the standard (fixed mini-batch) SG method, while offering significantly greater opportunities for parallelism.

Progressive batching algorithms have received much attention recently from a theoretical perspective; it has been shown that they enjoy good complexity properties and can achieve a fast rate of convergence (Byrd et al., 2012; Friedlander & Schmidt, 2012). The main appeal of these methods is that they inherit the efficient initial behavior of the SG method, achieve a fast rate of convergence, offer greater opportunities to exploit parallelism, and allow for the incorporation of second-order information. The latter can be done efficiently via quasi-Newton updating. This requires a line search procedure that allows for the construction of a convex quadratic model of the objective function at every iteration.

One challenge that immediately arises is how to perform the line search given that the objective function may change from one iteration to the next, and should therefore be considered stochastic. This is an issue that has not received

¹Department of Industrial Engineering and Management Sciences, Northwestern University, Evanston, IL, USA
²Intel Corporation, Bangalore, India ³Intel Corporation, Santa Clara, CA, USA. Correspondence to: Raghu Bollapragada <raghu.bollapragada@u.northwestern.edu>, Dheevatsa Mudigere <dheevatsa.mudigere@intel.com>, Jorge Nocedal <j-nocedal@northwestern.edu>, Hao-Jun Michael Shi <hjmshi@u.northwestern.edu>, Ping Tak Peter Tang <petert.tang@intel.com>.

sufficient attention in the literature, where stochastic line searches have been largely dismissed as inappropriate. In this paper, we propose a formula for estimating the initial steplength (based on statistical considerations) to be used in a backtracking Armijo-style line search.

The paper is organized into five sections. A literature review and our contributions are presented in the rest of this section. In Section 2, we describe the algorithm, and in Section 3 we provide convergence guarantees for it. In Section 4, we provide numerical results on logistic regression and neural networks. Section 5 summarizes our contributions and outlines future work.

1.1. Literature Review

Progressive batching (some referred to as dynamic sampling) has been well studied in the optimization literature, both for stochastic gradient and subsampled Newton-type methods (Byrd et al., 2012; Friedlander & Schmidt, 2012; Cartis & Scheinberg, 2015; Pasupathy et al., 2015; Roosta-Khorasani & Mahoney, 2016a;b; Bollapragada et al., 2016, 2017; De et al., 2017). Friedlander and Schmidt (2012) introduced theoretical conditions under which a progressive batching SG method converges linearly for finite sum problems, and experimented with a quasi-Newton adaptation of their algorithm. Byrd et al. (2012) proposed a progressive batching strategy, based on a *norm test*, that determines when to increase the sample size; they established linear convergence and computational complexity bounds in the case when the batch size grows geometrically. More recently, Bollapragada et al. (2017) introduced a batch control mechanism based on an *inner product* test that improves upon the norm test mentioned above.

There has been a renewed interest in understanding the generalization properties of small-batch and large-batch methods for training neural networks; see (Keskar et al., 2016; Dinh et al., 2017; Goyal et al., 2017; Hoffer et al., 2017). Keskar et al. (2016) empirically observed that large-batch methods converge to solutions with inferior generalization properties; however, Goyal et al. (2017) showed that large-batch methods can match the performance of small-batch methods when a warm-up strategy is used in conjunction with scaling the step length by the same factor as the batch size. Hoffer et al. (2017) and You et al. (2017) also explored larger batch sizes and steplengths to reduce the number of updates necessary to train the network. All of these studies naturally led to an interest in progressive batching techniques. Smith et al. (2017) showed empirically that increasing the sample size and decaying the steplength are quantitatively equivalent for the SG method; hence, steplength schedules could be directly converted to batch size schedules. This approach was parallelized by Devarakonda et al. (2017). De et al. (2017) present numerical results with a

progressive batching method that employs the norm test.

Stochastic second-order methods have been explored within the context of convex and non-convex optimization; see (Schraudolph et al., 2007; Sohl-Dickstein et al., 2014; Mokhtari & Ribeiro, 2015; Berahas et al., 2016; Byrd et al., 2016; Keskar & Berahas, 2016; Curtis, 2016; Berahas & Takáč, 2017; Zhou et al., 2017). Schraudolph et al. (2007) ensured stability of quasi-Newton updating by computing gradients using the same batch at the beginning and end of the iteration. Since this can potentially double the cost of the iteration, Berahas et al. (2016) proposed to achieve gradient consistency by computing gradients based on the overlap between consecutive batches; this approach was further tested by Berahas and Takac (2017). An interesting approach introduced by Martens and Grosse (2015; 2016) approximates the Fisher information matrix to scale the gradient; a distributed implementation of their K-FAC approach is described in (Ba et al., 2016). Another approach approximately computes the inverse Hessian by using the Neumann power series representation of matrices (Krishnan et al., 2017).

Several prominent first-order methods were also introduced for training logistic regression and neural network models. SAG (Schmidt et al., 2017) and SAGA (Defazio et al., 2014) are two algorithms that achieve linear convergence without the need for progressive batching, but at the cost of extra storage. SVRG (Johnson & Zhang, 2013) could be viewed as a hybrid that employs large batches at the beginning of each cycle of variance reduction iterations. Another line of research incorporates per-element adaptive step sizes or diagonal scalings into stochastic first-order algorithms, which is popular for training neural networks (Duchi et al., 2011; Tieleman & Hinton, 2012; Kingma & Ba, 2014).

1.2. Contributions

This paper builds upon three algorithmic components that have recently received attention in the literature — progressive batching, stable quasi-Newton updating, and adaptive steplength selection. It advances their design and puts them together in a novel algorithm with attractive theoretical and computational properties.

The cornerstone of our progressive batching strategy is the mechanism proposed by Bollapragada et al. (2017) in the context of first-order methods. We extend their *inner product* control test to second-order algorithms, something that is delicate and leads to a significant modification of the original procedure. Another main contribution of the paper is the design of an Armijo-style backtracking line search where the initial steplength is chosen based on statistical information gathered during the course of the iteration. We show that this steplength procedure is effective on a wide range of applications, as it leads to well scaled steps and

allows for the BFGS update to be performed most of the time, even for nonconvex problems. We also test two techniques for ensuring the stability of quasi-Newton updating, and observe that the overlapping procedure described by Berahas et al. (2016) is more efficient than a straightforward adaptation of classical quasi-Newton methods (Schraudolph et al., 2007).

We report numerical tests on large-scale logistic regression and deep neural network training tasks that indicate that our method is robust and efficient, and has good generalization properties. An additional advantage is that the method requires almost no parameter tuning, which is possible due to the incorporation of second-order information. All of this suggests that our approach has the potential to become one of the leading optimization methods for training deep neural networks. In order to achieve this, the algorithm must be optimized for parallel execution, something that was only briefly explored in this study.

2. Progressive Batching Quasi-Newton Method

The problem of interest is

$$\min_{x \in \mathbb{R}^d} F(x) = \int f(x; z, y) dP(z, y). \quad (1)$$

where f is the composition of a prediction function (parametrized by x) and a loss function, and (z, y) are random input-output pairs with probability distribution $P(z, y)$. The associated empirical risk problem consists of minimizing

$$R(x) = \frac{1}{N} \sum_{i=1}^N f(x; z^i, y^i) \triangleq \frac{1}{N} \sum_{i=1}^N F_i(x),$$

where we define $F_i(x) = f(x; z^i, y^i)$. A stochastic quasi-Newton method is given by

$$x_{k+1} = x_k - \alpha_k H_k g_k^{S_k}, \quad (2)$$

where the batch (or subsampled) gradient is given by

$$g_k^{S_k} = \nabla F_{S_k}(x_k) = \frac{1}{|S_k|} \sum_{i \in S_k} \nabla F_i(x_k), \quad (3)$$

the set $S_k \subset \{1, 2, \dots\}$ indexes data points (y^i, z^i) sampled from the distribution $P(z, y)$, and H_k is a positive definite quasi-Newton matrix. We now discuss each of the components of the new method.

2.1. Sample Size Selection

The proposed algorithm has the form (2)-(3). Initially, it utilizes a small batch size $|S_k|$, and increases it gradually in

order to attain a fast local rate of convergence and permit the use of second-order information. A challenging question is to determine when, and by how much, to increase the batch size $|S_k|$ over the course of the optimization procedure based on observed gradients — as opposed to using prescribed rules that depend on the iteration number k .

We propose to build upon the strategy introduced by Bollapragada et al. (2017) in the context of first-order methods. Their *inner product test* determines a sample size such that the search direction is a descent direction with high probability. A straightforward extension of this strategy to the quasi-Newton setting is not appropriate since requiring only that a stochastic quasi-Newton search direction be a descent direction with high probability would underutilize the curvature information contained in the search direction.

We would like, instead, for the search direction $d_k = -H_k g_k^{S_k}$ to make an acute angle with the true quasi-Newton search direction $-H_k \nabla F(x_k)$, with high probability. Although this does not imply that d_k is a descent direction for F , this will normally be the case for any reasonable quasi-Newton matrix.

To derive our new inner product quasi-Newton (IPQN) test, we first observe that the stochastic quasi-Newton search direction makes an acute angle with the true quasi-Newton direction in expectation, i.e.,

$$\mathbb{E} \left[(H_k \nabla F(x_k))^T (H_k g_k^{S_k}) \right] = \|H_k \nabla F(x_k)\|^2. \quad (4)$$

We must, however, control the variance of this quantity to achieve our stated objective. Specifically, we select our sample size $|S_k|$ such that the following condition is satisfied:

$$\mathbb{E} \left[\left((H_k \nabla F(x_k))^T (H_k g_k^{S_k}) - \|H_k \nabla F(x_k)\|^2 \right)^2 \right] \leq \theta^2 \|H_k \nabla F(x_k)\|^4, \quad (5)$$

for some $\theta > 0$. The left hand side of (5) is difficult to compute but can be bounded by the true variance of individual search directions, i.e.,

$$\frac{\mathbb{E} \left[\left((H_k \nabla F(x_k))^T (H_k g_k^i) - \|H_k \nabla F(x_k)\|^2 \right)^2 \right]}{|S_k|} \leq \theta^2 \|H_k \nabla F(x_k)\|^4, \quad (6)$$

where $g_k^i = \nabla F_i(x_k)$. This test involves the true expected gradient and variance, but we can approximate these quantities with sample gradient and variance estimates, respectively, yielding the practical inner product quasi-Newton test:

$$\frac{\text{Var}_{i \in S_k^v} \left((g_k^i)^T H_k^2 g_k^{S_k} \right)}{|S_k|} \leq \theta^2 \|H_k g_k^{S_k}\|^4, \quad (7)$$

where $S_k^v \subseteq S_k$ is a subset of the current sample (batch), and the variance term is defined as

$$\frac{\sum_{i \in S_k^v} \left((g_k^i)^T H_k^2 g_k^{S_k} - \|H_k g_k^{S_k}\|^2 \right)^2}{|S_k^v| - 1}. \quad (8)$$

Whenever condition (7) is not satisfied, we increase the sample size $|S_k|$. In order to estimate the increase that would lead to a satisfaction of (7), we reason as follows. If we assume that new sample $|\bar{S}_k|$ is such that

$$\|H_k g_k^{S_k}\| \approx \|H_k g_k^{\bar{S}_k}\|,$$

and similarly for the variance estimate, then a simple computation shows that a lower bound on the new sample size is

$$|\bar{S}_k| \geq \frac{\text{Var}_{i \in S_k^v} \left((g_k^i)^T H_k^2 g_k^{S_k} \right)}{\theta^2 \|H_k g_k^{S_k}\|^4}. \quad (9)$$

In our implementation of the algorithm, we set the new sample size $|S_{k+1}|$ to be equal to the right hand side of (9). When the sample approximation of $F(x_k)$ is not accurate, which can occur when $|S_k|$ is small, the progressive batching mechanism just described may not be reliable. In this case we employ the moving window technique described in Bollapragada et al. (2017), Section 4.2 to produce a sample estimate of $\nabla F(x_k)$.

2.2. The Line Search

In deterministic optimization, line searches are employed to select a steplength that provides sufficient decrease in the objective function and that ensures that the step is not too short (Nocedal & Wright, 1999). Line searches are particularly important in quasi-Newton methods since they improve the robustness and efficiency of the iteration with little additional cost.

In contrast, stochastic line searches are poorly understood and rarely employed in practice because they must make decisions based on sample function values

$$F_{S_k}(x) = \frac{1}{|S_k|} \sum_{i \in S_k} F_i(x), \quad (10)$$

which are noisy approximations to the true objective F . One of the key questions in the design of a stochastic line search is how to ensure, with high probability, that there is a decrease in the true function when one can only observe stochastic approximations $F_{S_k}(x)$. We address this question by proposing a formula for the step size α_k , which has the property that increases in true function values are controlled. Specifically, the first trial steplength in our proposed stochastic backtracking line search is computed so

that the predicted decrease in the expected function value is sufficiently large, as we now explain.

Using Lipschitz continuity of $\nabla F(x)$ and taking the conditional expectation, we can show the following inequality

$$\mathbb{E}_k [F_{k+1}] \leq F_k - \alpha_k \nabla F(x_k)^T H_k^{1/2} W_k H_k^{1/2} \nabla F(x_k) \quad (11)$$

where

$$W_k = \left(I - \frac{L\alpha_k}{2} \left(1 + \frac{\text{Var}\{H_k g_k^i\}}{|S_k| \|H_k \nabla F(x_k)\|^2} \right) H_k \right),$$

$\text{Var}\{H_k g_k^i\} = \mathbb{E}_k [\|H_k g_k^i - H_k \nabla F(x_k)\|^2]$, $F_k = F(x_k)$, and L is the Lipschitz constant. The proof of (11) is given in the supplement.

The only difference in (11) between the deterministic and stochastic quasi-Newton methods is the additional variance term in the matrix W_k . To obtain decrease in the function value in the deterministic case, the matrix $(I - \frac{L\alpha_k}{2} H_k)$ must be positive definite, whereas in the stochastic case the matrix W_k must be positive definite to yield a decrease in the function value *in expectation*. In the deterministic case, for any reasonably good quasi-Newton matrix H_k , one expects that $\alpha_k = 1$ will result in a decrease in the function, and therefore the initial trial steplength parameter should be chosen to be 1. In the stochastic case, if we make a similar assumption about the quality of the Hessian approximation, the analog to the deterministic case suggests that a step length of

$$\hat{\alpha}_k = \left(1 + \frac{\text{Var}\{H_k g_k^i\}}{|S_k| \|H_k \nabla F(x_k)\|^2} \right)^{-1} \quad (12)$$

will result in decrease in the expected function value. However, since formula (12) involves the expensive computation of the individual matrix-vector products $H_k g_k^i$, we approximate the variance-bias ratio as follows:

$$\bar{\alpha}_k = \left(1 + \frac{\text{Var}\{g_k^i\}}{|S_k| \|\nabla F(x_k)\|^2} \right)^{-1}, \quad (13)$$

where $\text{Var}\{g_k^i\} = \mathbb{E}_k [\|g_k^i - \nabla F(x_k)\|^2]$. In our practical implementation, we estimate the population variance and gradient with the sample variance and gradient, respectively, yielding the initial steplength

$$\alpha_k = \left(1 + \frac{\text{Var}_{i \in S_k^v} \{g_k^i\}}{|S_k| \|g_k^{S_k}\|^2} \right)^{-1} \quad (14)$$

where

$$\text{Var}_{i \in S_k^v} \{g_k^i\} = \frac{1}{|S_k^v| - 1} \sum_{i \in S_k^v} \|g_k^i - g_k^{S_k}\|^2 \quad (15)$$

and $S_k^v \subseteq S_k$. With this initial value of α_k in hand, our algorithm performs a backtracking line search that aims to satisfy the sampled Armijo condition

$$\begin{aligned} F_{S_k}(x_k - \alpha_k H_k g_k^{S_k}) \\ \leq F_{S_k}(x_k) - c_1 \alpha_k (g_k^{S_k})^T H_k g_k^{S_k}, \end{aligned} \quad (16)$$

where $c_1 > 0$.

2.3. Stable Quasi-Newton Updates

In the BFGS and L-BFGS methods, the inverse Hessian approximation is updated using the formula

$$\begin{aligned} H_{k+1} &= V_k^T H_k V_k + \rho_k s_k s_k^T \\ \rho_k &= (y_k^T s_k)^{-1} \\ V_k &= I - \rho_k y_k s_k^T \end{aligned} \quad (17)$$

where $s_k = x_{k+1} - x_k$ and y_k is the difference in the gradients at x_{k+1} and x_k . When the batch changes from one iteration to the next ($S_{k+1} \neq S_k$), it is not obvious how y_k should be defined, but it has been observed that when gradient differences are computed using different samples, the updating process may be unstable. Hence it seems natural to use the same sample at the beginning and at the end of the iteration (Schraudolph et al., 2007), and define

$$y_k = g_{k+1}^{S_k} - g_k^{S_k}. \quad (18)$$

However, this requires that the gradient be evaluated twice for every batch S_k at x_k and x_{k+1} . To avoid this additional cost, Berahas et al. (2016) propose to use the overlap between consecutive samples in the gradient differencing. If we denote this overlap as $O_k = S_k \cap S_{k+1}$, then one defines

$$y_k = g_{k+1}^{O_k} - g_k^{O_k}. \quad (19)$$

This requires no extra computation since the two gradients in this expression are subsets of the gradients corresponding to the samples S_k and S_{k+1} . The overlap should not be too small to avoid differencing noise, but this is easily achieved in practice. We test both formulas for y_k in our implementation of the method; see Section 4.

2.4. The Complete Algorithm

The pseudocode of the progressive batching L-BFGS method is given in Algorithm 1. For the batch size control test (7), we choose $\theta = 0.9$ in the logistic regression experiments, and θ is a tunable parameter chosen in the interval $[0.9, 3]$ in the neural network experiments. The constant c_1 in (16) is set to $c_1 = 10^{-4}$. For L-BFGS, we set the memory as $m = 10$. We skip the quasi-Newton update if the following curvature condition is not satisfied:

$$y_k^T s_k > \epsilon \|s_k\|^2, \quad \text{with } \epsilon = 10^{-2}. \quad (20)$$

The initial Hessian matrix H_0^k in the L-BFGS recursion at each iteration is chosen as $\gamma_k I$ where $\gamma_k = y_k^T s_k / y_k^T y_k$.

Algorithm 1 Progressive Batching L-BFGS Method

Input: Initial iterate x_0 , initial sample size $|S_0|$;

Initialization: Set $k \leftarrow 0$

Repeat until convergence:

- 1: Sample $S_k \subseteq \{1, \dots, N\}$ with sample size $|S_k|$
 - 2: **if** condition (7) is not satisfied **then**
 - 3: Compute $|S_k|$ using (9)
 - 4: Choose a new sample S_k with sample size $|S_k|$
 - 5: **end if**
 - 6: Compute $g_k^{S_k}$
 - 7: Compute $p_k = -H_k g_k^{S_k}$ using L-BFGS Two-Loop Recursion in (Nocedal & Wright, 1999)
 - 8: Compute α_k using (14)
 - 9: **while** sampled Armijo condition (16) not satisfied **do**
 - 10: Set $\alpha_k = \alpha_k/2$
 - 11: **end while**
 - 12: Compute $x_{k+1} = x_k + \alpha_k p_k$
 - 13: Compute y_k using (18) or (19)
 - 14: Compute $s_k = x_{k+1} - x_k$
 - 15: **if** $y_k^T s_k > \epsilon \|s_k\|^2$ **then**
 - 16: **if** number of stored (y_j, s_j) exceeds m **then**
 - 17: Discard oldest curvature pair (y_j, s_j)
 - 18: **end if**
 - 19: Store new curvature pair (y_k, s_k)
 - 20: **end if**
 - 21: Set $k \leftarrow k + 1$
 - 22: Set $|S_k| = |S_{k-1}|$
-

3. Convergence Analysis

We now present convergence results for the proposed algorithm, both for strongly convex and nonconvex objective functions. Our emphasis is in analyzing the effect of progressive sampling, and therefore, we follow common practice and assume that the steplength in the algorithm is fixed ($\alpha_k = \alpha$), and that the inverse L-BFGS matrix H_k has bounded eigenvalues, i.e.,

$$\Lambda_1 I \preceq H_k \preceq \Lambda_2 I. \quad (21)$$

This assumption is a well-known result that has already been proven for both convex and nonconvex cases; see (Berahas et al., 2016). We assume that the sample size is controlled by the exact inner product quasi-Newton test (6). This test is designed for efficiency, and in rare situations could allow for the generation of arbitrarily long search directions. To prevent this from happening, we introduce an additional control on the sample size $|S_k|$, by extending (to the quasi-Newton setting) the orthogonality test introduced in (Bollapragada et al., 2017). This additional requirement

states that the current sample size $|S_k|$ is acceptable only if

$$\frac{\mathbb{E} \left[\left\| H_k g_k^i - \frac{(H_k g_k^{S_k})^T (H_k \nabla F(x_k))}{\|H_k \nabla F(x_k)\|^2} H_k \nabla F(x_k) \right\|^2 \right]}{|S_k|} \leq \nu^2 \|H_k \nabla F(x_k)\|^2, \quad (22)$$

for some given $\nu > 0$.

We now establish linear convergence when the objective is strongly convex.

Theorem 3.1. *Suppose that F is twice continuously differentiable and that there exist constants $0 < \mu \leq L$ such that*

$$\mu I \preceq \nabla^2 F(x) \preceq LI, \quad \forall x \in \mathbb{R}^d. \quad (23)$$

Let $\{x_k\}$ be generated by iteration (2), for any x_0 , where $|S_k|$ is chosen by the (exact variance) inner product quasi-Newton test (6). Suppose that the orthogonality condition (22) holds at every iteration, and that the matrices H_k satisfy (21). Then, if

$$\alpha_k = \alpha \leq \frac{1}{(1 + \theta^2 + \nu^2)L\Lambda_2}, \quad (24)$$

we have that

$$\mathbb{E}[F(x_k) - F(x^*)] \leq \rho^k (F(x_0) - F(x^*)), \quad (25)$$

where x^* denotes the minimizer of F , and $\rho = 1 - \mu\Lambda_1\alpha$.

The proof of this result is given in the supplement. We now consider the case when F is nonconvex and bounded below.

Theorem 3.2. *Suppose that F is twice continuously differentiable and bounded below, and that there exists a constant $L > 0$ such that*

$$\nabla^2 F(x) \preceq LI, \quad \forall x \in \mathbb{R}^d. \quad (26)$$

Let $\{x_k\}$ be generated by iteration (2), for any x_0 , where $|S_k|$ is chosen by (6) and (22), and suppose that (21) holds. Then, if α_k satisfies (24), we have

$$\lim_{k \rightarrow \infty} \mathbb{E}[\|\nabla F(x_k)\|^2] \rightarrow 0. \quad (27)$$

Moreover, for any positive integer T we have that

$$\min_{0 \leq k \leq T-1} \mathbb{E}[\|\nabla F(x_k)\|^2] \leq \frac{2}{\alpha T \Lambda_1} (F(x_0) - F_{min}),$$

where F_{min} is a lower bound on F in \mathbb{R}^d .

The proof is given in the supplement. This result shows that the sequence of gradients $\{\|\nabla F(x_k)\|\}$ converges to zero in expectation, and establishes a global sublinear rate of convergence of the smallest gradients generated after every T steps.

4. Numerical Results

In this section, we present numerical results for the proposed algorithm, which we refer to as PBQN for the Progressive Batching Quasi-Newton algorithm.

4.1. Experiments on Logistic Regression Problems

We first test our algorithm on binary classification problems where the objective function is given by the logistic loss with ℓ_2 regularization:

$$R(x) = \frac{1}{N} \sum_{i=1}^N \log(1 + \exp(-z^i x^T y^i)) + \frac{\lambda}{2} \|x\|^2, \quad (28)$$

with $\lambda = 1/N$. We consider the 8 datasets listed in the supplement. An approximation R^* of the optimal function value is computed for each problem by running the full batch L-BFGS method until $\|\nabla R(x_k)\|_\infty \leq 10^{-8}$. Training error is defined as $R(x_k) - R^*$, where $R(x_k)$ is evaluated over the training set; test loss is evaluated over the test set without the ℓ_2 regularization term.

We tested two options for computing the curvature vector y_k in the PBQN method: the multi-batch (MB) approach (19) with 25% sample overlap, and the full overlap (FO) approach (18). We set $\theta = 0.9$ in (7), chose $|S_0| = 512$, and set all other parameters to the default values given in Section 2. Thus, none of the parameters in our PBQN method were tuned for each individual dataset. We compared our algorithm against two other methods: (i) Stochastic gradient (SG) with a batch size of 1; (ii) SVRG (Johnson & Zhang, 2013) with the inner loop length set to N . The steplength for SG and SVRG is constant and tuned for each problem ($\alpha_k \equiv \alpha = 2^j$, for $j \in \{-10, -9, \dots, 9, 10\}$) so as to give best performance.

In Figures 1 and 2 we present results for two datasets, spam and covertype; the rest of the results are given in the supplement. The horizontal axis measures the number of full gradient evaluations, or equivalently, the number of times that N component gradients ∇F_i were evaluated. The left-most figure reports the long term trend over 100 gradient evaluations, while the rest of the figures zoom into the first 10 gradient evaluations to show the initial behavior of the methods. The vertical axis measures training error, test loss, and test accuracy, respectively, from left to right.

The proposed algorithm competes well for these two datasets in terms of training error, test loss and test accuracy, and decreases these measures more evenly than the SG and SVRG. Our numerical experience indicates that formula (14) is quite effective at estimating the steplength parameter, as it is accepted by the backtracking line search for most iterations. As a result, the line search computes very few additional function values.

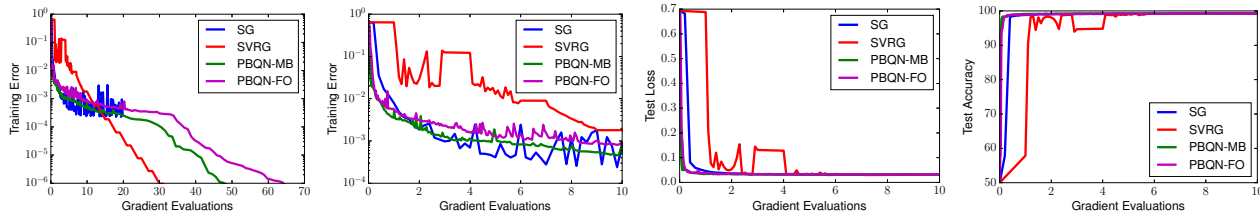


Figure 1. **spam dataset**: Performance of the progressive batching L-BFGS method (PBQN), with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

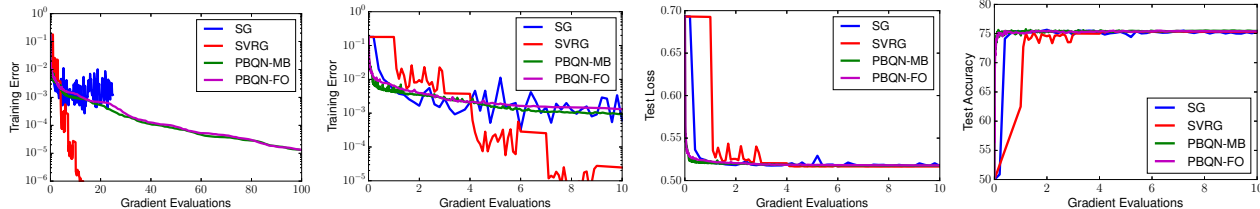


Figure 2. **covertype dataset**: Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

It is interesting to note that SVRG is not as efficient in the initial epochs compared to PBQN or SG, when measured either in terms of test loss and test accuracy. The training error for SVRG decreases rapidly in later epochs but this rapid improvement is not observed in the test loss and accuracy. Neither the PBQN nor SVRG significantly outperforms the other across all datasets tested in terms of training error, as observed in the supplement.

Our results indicate that defining the curvature vector using the MB approach is preferable to using the FB approach. The number of iterations required by the PBQN method is significantly smaller compared to the SG method, suggesting the potential efficiency gains of a parallel implementation of our algorithm.

4.2. Results on Neural Networks

We have performed a preliminary investigation into the performance of the PBQN algorithm for training neural networks. As is well-known, the resulting optimization problems are quite difficult due to the existence of local minimizers, some of which generalize poorly. Thus our first requirement when applying the PBQN method was to obtain as good generalization as SG, something we have achieved.

Our investigation into how to obtain fast performance is, however, still underway for reasons discussed below. Nevertheless, our results are worth reporting because they show that our line search procedure is performing as expected, and that the overall number of iterations required by the PBQN method is small enough so that a parallel implementation could yield state-of-the-art results, based on the theoretical

performance model detailed in the supplement.

We compared our algorithm, as described in Section 2, against SG and Adam (Kingma & Ba, 2014). It has taken many years to design regularizations techniques and heuristics that greatly improve the performance of the SG method for deep learning (Srivastava et al., 2014; Ioffe & Szegedy, 2015). These include batch normalization and dropout, which (in their current form) are not conducive to the PBQN approach due to the need for gradient consistency when evaluating the curvature pairs in L-BFGS. Therefore, we do not implement batch normalization and dropout in any of the methods tested, and leave the study of their extension to the PBQN setting for future work.

We consider three network architectures: (i) a small convolutional neural network on CIFAR-10 (\mathcal{C}) (Krizhevsky, 2009), (ii) an AlexNet-like convolutional network on MNIST and CIFAR-10 ($\mathcal{A}_1, \mathcal{A}_2$, respectively) (LeCun et al., 1998; Krizhevsky et al., 2012), and (iii) a residual network (ResNet18) on CIFAR-10 (\mathcal{R}) (He et al., 2016). The network architecture details and additional plots are given in the supplement. All of these networks were implemented in PyTorch (Paszke et al., 2017). The results for the CIFAR-10 AlexNet and CIFAR-10 ResNet18 are given in Figures 3 and 4, respectively. We report results both against the total number of iterations and the total number of gradient evaluations. Table 1 shows the best test accuracies attained by each of the four methods over the various networks.

In all our experiments, we initialize the batch size as $|S_0| = 512$ in the PBQN method, and fix the batch size to $|S_k| = 128$ for SG and Adam. The parameter θ given in (7), which

controls the batch size increase in the PBQN method, was tuned lightly by choosing among the 3 values: 0.9, 2, 3. SG and Adam are tuned using a development-based decay (dev-decay) scheme, which track the best validation loss at each epoch and reduces the steplength by a constant factor δ if the validation loss does not improve after e epochs.

Table 1. Best test accuracy performance of SG, Adam, multi-batch L-BFGS, and full overlap L-BFGS on various networks over 5 different runs and initializations.

Network	SG	Adam	MB	FO
C	66.24	67.03	67.37	62.46
\mathcal{A}_1	99.25	99.34	99.16	99.05
\mathcal{A}_2	73.46	73.59	73.02	72.74
\mathcal{R}	69.5	70.16	70.28	69.44

We observe from our results that the PBQN method achieves a similar test accuracy as SG and Adam, but requires more gradient evaluations. Improvements in performance can be obtained by ensuring that the PBQN method exerts a finer control on the sample size in the small batch regime — something that requires further investigation. Nevertheless, the small number of iterations required by the PBQN method, together with the fact that it employs larger batch sizes than SG during much of the run, suggests that a distributed version similar to a data-parallel distributed implementation of the SG method (Chen et al., 2016; Das et al., 2016) would lead to a highly competitive method.

Similar to the logistic regression case, we observe that the steplength computed via (14) is almost always accepted by the Armijo condition, and typically lies within $(0.1, 1)$. Once the algorithm has trained for a significant number of iterations using full-batch, the algorithm begins to overfit on the training set, resulting in worsened test loss and accuracy, as observed in the graphs.

5. Final Remarks

Several types of quasi-Newton methods have been proposed in the literature to address the challenges arising in machine learning. Some of these methods operate in the purely stochastic setting (which makes quasi-Newton updating difficult) or in the purely batch regime (which leads to generalization problems). We believe that progressive batching is the right context for designing an L-BFGS method that has good generalization properties and fast convergence. The advantages of our approach are clearly seen in logistic regression experiments. To make the new method competitive with SG and Adam for deep learning, we need to improve several of its components. This includes the design of a more robust progressive batching mechanism, the redesign of batch normalization and dropout heuristics to improve the

generalization performance of our method for training larger networks, and most importantly, the design of a parallelized implementation that takes advantage of the higher granularity of each iteration. We believe that a new alternative to the SG method for deep learning is in sight.

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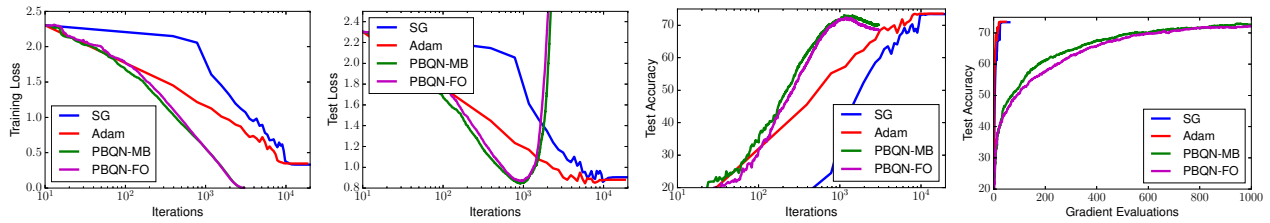


Figure 3. **CIFAR-10 AlexNet (\mathcal{A}_2)**: Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and Adam methods. The best results for L-BFGS are achieved with $\theta = 0.9$.

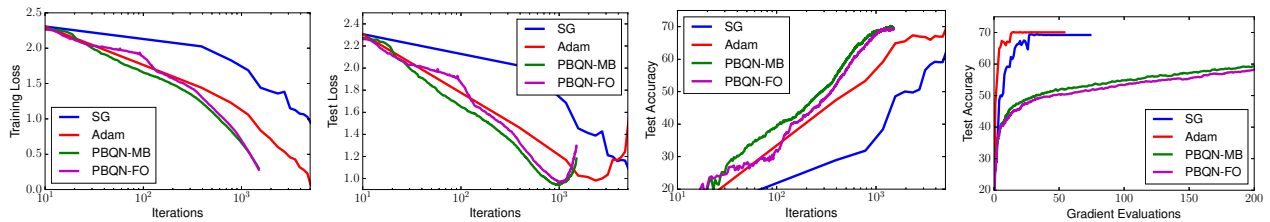


Figure 4. **CIFAR-10 ResNet18 (\mathcal{R})**: Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and Adam methods. The best results for L-BFGS are achieved with $\theta = 2$.

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A. Initial Step Length Derivation

To establish our results, recall that the stochastic quasi-Newton method is defined as

$$x_{k+1} = x_k - \alpha_k H_k g_k^{S_k}, \quad (29)$$

where the batch (or subsampled) gradient is given by

$$g_k^{S_k} = \nabla F_{S_k}(x_k) = \frac{1}{|S_k|} \sum_{i \in S_k} \nabla F_i(x_k), \quad (30)$$

and the set $S_k \subset \{1, 2, \dots\}$ indexes data points (y^i, z^i) . The primary theoretical mechanism for determining batch sizes is the exact variance inner product quasi-Newton (IPQN) test, which is defined as

$$\frac{\mathbb{E} \left[\left((H_k \nabla F(x_k))^T (H_k g_k^i) - \|H_k \nabla F(x_k)\|^2 \right)^2 \right]}{|S_k|} \leq \theta^2 \|H_k \nabla F(x_k)\|^4. \quad (31)$$

We establish the inequality used to determine the initial steplength α_k for the stochastic line search:

Lemma A.1. *Assume that F is continuously differentiable with Lipschitz continuous gradient with Lipschitz constant L . Then*

$$\mathbb{E}_k [F(x_{k+1})] \leq F(x_k) - \alpha_k \nabla F(x_k)^T H_k^{1/2} W_k H_k^{1/2} \nabla F(x_k)$$

where

$$W_k = \left(I - \frac{L\alpha_k}{2} \left(1 + \frac{\text{Var}\{H_k g_k^i\}}{|S_k| \|H_k \nabla F(x_k)\|^2} \right) H_k \right),$$

and $\text{Var}\{H_k g_k^i\} = \mathbb{E}_k [\|H_k g_k^i - H_k \nabla F(x_k)\|^2]$.

Proof. By Lipschitz continuity of the gradient, we have that

$$\begin{aligned} \mathbb{E}_k [F(x_{k+1})] &\leq F(x_k) - \alpha_k \nabla F(x_k)^T H_k \mathbb{E}_k [g_k^{S_k}] + \frac{L\alpha_k^2}{2} \mathbb{E}_k [\|H_k g_k^{S_k}\|^2] \\ &= F(x_k) - \alpha_k \nabla F(x_k)^T H_k \nabla F(x_k) + \frac{L\alpha_k^2}{2} \left(\|H_k \nabla F(x_k)\|^2 + \mathbb{E}_k [\|H_k g_k^{S_k} - H_k \nabla F(x_k)\|^2] \right) \\ &\leq F(x_k) - \alpha_k \nabla F(x_k)^T H_k \nabla F(x_k) + \frac{L\alpha_k^2}{2} \left(\|H_k \nabla F(x_k)\|^2 + \frac{\text{Var}\{H_k g_k^i\}}{|S_k| \|H_k \nabla F(x_k)\|^2} \|H_k \nabla F(x_k)\|^2 \right) \\ &= F(x_k) - \alpha_k \nabla F(x_k)^T H_k^{1/2} \left(I - \frac{L\alpha_k}{2} \left(1 + \frac{\text{Var}\{H_k g_k^i\}}{|S_k| \|H_k \nabla F(x_k)\|^2} \right) H_k \right) H_k^{1/2} \nabla F(x_k) \\ &= F(x_k) - \alpha_k \nabla F(x_k)^T H_k^{1/2} W_k H_k^{1/2} \nabla F(x_k). \end{aligned}$$

□

B. Convergence Analysis

For the rest of our analysis, we make the following two assumptions:

Assumptions B.1. *We assume that the orthogonality condition is satisfied, i.e.*

$$\frac{\mathbb{E} \left[\left\| H_k g_k^i - \frac{(H_k g_k^i)^T (H_k \nabla F(x_k))}{\|H_k \nabla F(x_k)\|^2} H_k \nabla F(x_k) \right\|^2 \right]}{|S_k|} \leq \nu^2 \|H_k \nabla F(x_k)\|^2, \quad (32)$$

for some large $\nu > 0$.

Assumptions B.2. *We assume that the eigenvalues of H_k are bounded for all k , i.e.*

$$\Lambda_1 I \preceq H_k \preceq \Lambda_2 I, \quad (33)$$

for $\Lambda_2 \geq \Lambda_1 > 0$. In particular, H_k is positive definite.

Condition (32) ensures that the stochastic quasi-Newton direction is bounded away from orthogonality to $-H_k \nabla F(x_k)$ with high probability. Specifically, it prevents the variance in the individual quasi-Newton directions to be too large relative to the variance in the individual quasi-Newton directions along $-H_k \nabla F(x_k)$. Assumption B.2 is a well-known result for the convex case, and can be established for the nonconvex case by introducing a safeguarding procedure; see Berahas, et al. (2016) for a proof for stochastic L-BFGS matrices.

We begin by establishing a technical lemma.

Lemma B.3. *Suppose that F is twice continuously differentiable and that there exists a constant $L > 0$ such that*

$$\nabla^2 F(x) \preceq LI, \quad \forall x \in \mathbb{R}^d. \quad (34)$$

Let $\{x_k\}$ be generated by iteration (29) for any x_0 , where $|S_k|$ is chosen by the (exact variance) inner product quasi-Newton test (31) for given constant $\theta > 0$ and suppose that the Assumptions B.1 and B.2 hold. Then, for any k ,

$$\mathbb{E} \left[\|H_k g_k^{S_k}\|^2 \right] \leq (1 + \theta^2 + \nu^2) \|H_k \nabla F(x_k)\|^2. \quad (35)$$

Moreover, if α_k satisfies

$$\alpha_k = \alpha \leq \frac{1}{(1 + \theta^2 + \nu^2)L\Lambda_2}, \quad (36)$$

we have that

$$\mathbb{E}[F(x_{k+1})] \leq \mathbb{E}[F(x_k)] - \frac{\alpha}{2} \|H_k^{1/2} \nabla F(x_k)\|^2. \quad (37)$$

Proof. By Assumption (B.1), the orthogonality condition, we have that

$$\begin{aligned} \mathbb{E} \left[\left\| H_k g_k^{S_k} - \frac{(H_k g_k^{S_k})^T (H_k \nabla F(x_k))}{\|H_k \nabla F(x_k)\|^2} H_k \nabla F(x_k) \right\|^2 \right] &\leq \frac{\mathbb{E} \left[\left\| H_k g_k^i - \frac{(H_k g_k^i)^T (H_k \nabla F(x_k))}{\|H_k \nabla F(x_k)\|^2} H_k \nabla F(x_k) \right\|^2 \right]}{|S_k|} \\ &\leq \nu^2 \|H_k \nabla F(x_k)\|^2. \end{aligned} \quad (38)$$

Now, expanding the left hand side of inequality (38), we get

$$\begin{aligned} &\mathbb{E} \left[\left\| H_k g_k^{S_k} - \frac{(H_k g_k^{S_k})^T (H_k \nabla F(x_k))}{\|H_k \nabla F(x_k)\|^2} H_k \nabla F(x_k) \right\|^2 \right] \\ &= \mathbb{E} \left[\|H_k g_k^{S_k}\|^2 \right] - \frac{2\mathbb{E} \left[\left((H_k g_k^{S_k})^T (H_k \nabla F(x_k)) \right)^2 \right]}{\|H_k \nabla F(x_k)\|^2} + \frac{\mathbb{E} \left[\left((H_k g_k^{S_k})^T (H_k \nabla F(x_k)) \right)^2 \right]}{\|H_k \nabla F(x_k)\|^2} \\ &= \mathbb{E} \left[\|H_k g_k^{S_k}\|^2 \right] - \frac{\mathbb{E} \left[\left((H_k g_k^{S_k})^T (H_k \nabla F(x_k)) \right)^2 \right]}{\|H_k \nabla F(x_k)\|^2} \\ &\leq \nu^2 \|H_k \nabla F(x_k)\|^2. \end{aligned}$$

Therefore, rearranging gives the inequality

$$\mathbb{E} \left[\|H_k g_k^{S_k}\|^2 \right] \leq \frac{\mathbb{E} \left[\left((H_k g_k^{S_k})^T (H_k \nabla F(x_k)) \right)^2 \right]}{\|H_k \nabla F(x_k)\|^2} + \nu^2 \|H_k \nabla F(x_k)\|^2. \quad (39)$$

To bound the first term on the right side of this inequality, we use the inner product quasi-Newton test; in particular, $|S_k|$ satisfies

$$\begin{aligned} \mathbb{E} \left[\left((H_k \nabla F(x_k))^T (H_k g_k^{S_k}) - \|H_k \nabla F(x_k)\|^2 \right)^2 \right] &\leq \frac{\mathbb{E} \left[\left((H_k \nabla F(x_k))^T (H_k g_k^i) - \|H_k \nabla F(x_k)\|^2 \right)^2 \right]}{|S_k|} \\ &\leq \theta^2 \|H_k \nabla F(x_k)\|^4, \end{aligned} \quad (40)$$

where the second inequality holds by the IPQN test. Since

$$\mathbb{E} \left[\left((H_k \nabla F(x_k))^T (H_k g_k^{S_k}) - \|H_k \nabla F(x_k)\|^2 \right)^2 \right] = \mathbb{E} \left[\left((H_k \nabla F(x_k))^T (H_k g_k^{S_k}) \right)^2 \right] - \|H_k \nabla F(x_k)\|^4, \quad (41)$$

we have

$$\begin{aligned} \mathbb{E} \left[\left((H_k g_k^{S_k})^T (H_k \nabla F(x_k)) \right)^2 \right] &\leq \|H_k \nabla F(x_k)\|^4 + \theta^2 \|H_k \nabla F(x_k)\|^4 \\ &= (1 + \theta^2) \|H_k \nabla F(x_k)\|^4, \end{aligned} \quad (42)$$

by (40) and (41). Substituting (42) into (39), we get the following bound on the length of the search direction:

$$\mathbb{E} \left[\|H_k g_k^{S_k}\|^2 \right] \leq (1 + \theta^2 + \nu^2) \|H_k \nabla F(x_k)\|^2,$$

which proves (35). Using this inequality, Assumption B.2, and bounds on the Hessian and steplength (34) and (24), we have

$$\begin{aligned} \mathbb{E}[F(x_{k+1})] &\leq \mathbb{E}[F(x_k)] - \mathbb{E} \left[\alpha (H_k g_k^{S_k})^T \nabla F(x_k) \right] + \mathbb{E} \left[\frac{L\alpha^2}{2} \|H_k g_k^{S_k}\|^2 \right] \\ &= \mathbb{E}[F(x_k)] - \alpha \nabla F(x_k)^T H_k \nabla F(x_k) + \frac{L\alpha^2}{2} \mathbb{E}[\|H_k g_k^{S_k}\|^2] \\ &\leq \mathbb{E}[F(x_k)] - \alpha \nabla F(x_k)^T H_k \nabla F(x_k) + \frac{L\alpha^2}{2} (1 + \theta^2 + \nu^2) \|H_k \nabla F(x_k)\|^2 \\ &= \mathbb{E}[F(x_k)] - \alpha (H_k^{1/2} \nabla F(x_k))^T \left(I - \frac{L\alpha(1 + \theta^2 + \nu^2)}{2} H_k \right) H_k^{1/2} \nabla F(x_k) \\ &\leq \mathbb{E}[F(x_k)] - \alpha \left(1 - \frac{L\Lambda_2 \alpha (1 + \theta^2 + \nu^2)}{2} \right) \|H_k^{1/2} \nabla F(x_k)\|^2 \\ &\leq \mathbb{E}[F(x_k)] - \frac{\alpha}{2} \|H_k^{1/2} \nabla F(x_k)\|^2. \end{aligned}$$

□

We now show that the stochastic quasi-Newton iteration (29) with a fixed steplength α is linearly convergent when F is strongly convex. In the following discussion, x^* denotes the minimizer of F .

Theorem B.4. *Suppose that F is twice continuously differentiable and that there exist constants $0 < \mu \leq L$ such that*

$$\mu I \preceq \nabla^2 F(x) \preceq LI, \quad \forall x \in \mathbb{R}^d. \quad (43)$$

Let $\{x_k\}$ be generated by iteration (29), for any x_0 , where $|S_k|$ is chosen by the (exact variance) inner product quasi-Newton test (31) and suppose that the Assumptions B.1 and B.2 hold. Then, if α_k satisfies (36) we have that

$$\mathbb{E}[F(x_k) - F(x^*)] \leq \rho^k (F(x_0) - F(x^*)), \quad (44)$$

where x^* denotes the minimizer of F , and $\rho = 1 - \mu\Lambda_1\alpha$.

Proof. It is well-known (Bertsekas et al., 2003) that for strongly convex functions,

$$\|\nabla F(x_k)\|^2 \geq 2\mu[F(x_k) - F(x^*)].$$

Substituting this into (37) and subtracting $F(x^*)$ from both sides, we obtain

$$\begin{aligned} \mathbb{E}[F(x_{k+1}) - F(x^*)] &\leq \mathbb{E}[F(x_k) - F(x^*)] - \frac{\alpha}{2} \|H_k^{1/2} \nabla F(x_k)\|^2 \\ &\leq \mathbb{E}[F(x_k) - F(x^*)] - \frac{\alpha}{2} \Lambda_1 \|\nabla F(x_k)\|^2 \\ &\leq (1 - \mu\Lambda_1\alpha) \mathbb{E}[F(x_k) - F(x^*)], \end{aligned}$$

from which the theorem follows. □

Note that when $\theta = \nu = 0$, we recover the classical result for the exact gradient method.

We now consider the case when F is nonconvex and bounded below.

Theorem B.5. *Suppose that F is twice continuously differentiable and bounded below, and that there exists a constant $L > 0$ such that*

$$\nabla^2 F(x) \preceq LI, \quad \forall x \in \mathbb{R}^d. \quad (45)$$

Let $\{x_k\}$ be generated by iteration (29), for any x_0 , where $|S_k|$ is chosen by the (exact variance) inner product quasi-Newton test (31) and suppose that the Assumptions B.1 and B.2 hold. Then, if α_k satisfies (36), we have

$$\lim_{k \rightarrow \infty} \mathbb{E}[\|\nabla F(x_k)\|^2] \rightarrow 0. \quad (46)$$

Moreover, for any positive integer T we have that

$$\min_{0 \leq k \leq T-1} \mathbb{E}[\|\nabla F(x_k)\|^2] \leq \frac{2}{\alpha T \Lambda_1} (F(x_0) - F_{min}),$$

where F_{min} is a lower bound on F in \mathbb{R}^d .

Proof. From Lemma B.3, we have

$$\mathbb{E}[F(x_{k+1})] \leq \mathbb{E}[F(x_k)] - \frac{\alpha}{2} \mathbb{E}[\|H_k^{1/2} \nabla F(x_k)\|^2],$$

and hence

$$\mathbb{E}[\|H_k^{1/2} \nabla F(x_k)\|^2] \leq \frac{2}{\alpha} \mathbb{E}[F(x_k) - F(x_{k+1})].$$

Summing both sides of this inequality from $k = 0$ to $T - 1$, and since F is bounded below by F_{min} , we get

$$\sum_{k=0}^{T-1} \mathbb{E}[\|H_k^{1/2} \nabla F(x_k)\|^2] \leq \frac{2}{\alpha} \mathbb{E}[F(x_0) - F(x_T)] \leq \frac{2}{\alpha} [F(x_0) - F_{min}].$$

Using the bound on the eigenvalues of H_k and taking limits, we obtain

$$\Lambda_1 \lim_{T \rightarrow \infty} \sum_{k=0}^{T-1} \mathbb{E}[\|\nabla F(x_k)\|^2] \leq \lim_{T \rightarrow \infty} \sum_{k=0}^{T-1} \mathbb{E}[\|H_k^{1/2} \nabla F(x_k)\|^2] < \infty,$$

which implies (46). We can also conclude that

$$\min_{0 \leq k \leq T-1} \mathbb{E}[\|\nabla F(x_k)\|^2] \leq \frac{1}{T} \sum_{k=0}^{T-1} \mathbb{E}[\|\nabla F(x_k)\|^2] \leq \frac{2}{\alpha T \Lambda_1} (F(x_0) - F_{min}).$$

□

C. Additional Numerical Experiments

C.1. Datasets

Table 2 summarizes the datasets used for the experiments. Some of these datasets divide the data into training and testing sets; for the rest, we randomly divide the data so that the training set constitutes 90% of the total.

Table 2. Characteristics of all datasets used in the experiments.

Dataset	# Data Points (train; test)	# Features	# Classes	Source
gisette	(6,000; 1,000)	5,000	2	(Chang & Lin, 2011)
mushrooms	(7,311; 813)	112	2	(Chang & Lin, 2011)
sido	(11,410; 1,268)	4,932	2	(Guyon et al., 2008)
ijcnn	(35,000; 91701)	22	2	(Chang & Lin, 2011)
spam	(82,970; 9,219)	823,470	2	(Cormack & Lynam, 2005; Carbonetto, 2009)
alpha	(450,000; 50,000)	500	2	synthetic
coverttype	(522,910; 58,102)	54	2	(Chang & Lin, 2011)
url	(2,156,517; 239,613)	3,231,961	2	(Chang & Lin, 2011)
MNIST	(60,000; 10,000)	28×28	10	(LeCun et al., 1998)
CIFAR-10	(50,000; 10,000)	32×32	10	(Krizhevsky, 2009)

The alpha dataset is a synthetic dataset that is available at <ftp://largescale.ml.tu-berlin.de>.

C.2. Logistic Regression Experiments

We report the numerical results on binary classification logistic regression problems on the 8 datasets given in Table 2. We plot the performance measured in terms of training error, test loss and test accuracy against the gradient evaluations. We also report the behavior of the batch sizes and steplengths for both variants of the PBQN method.

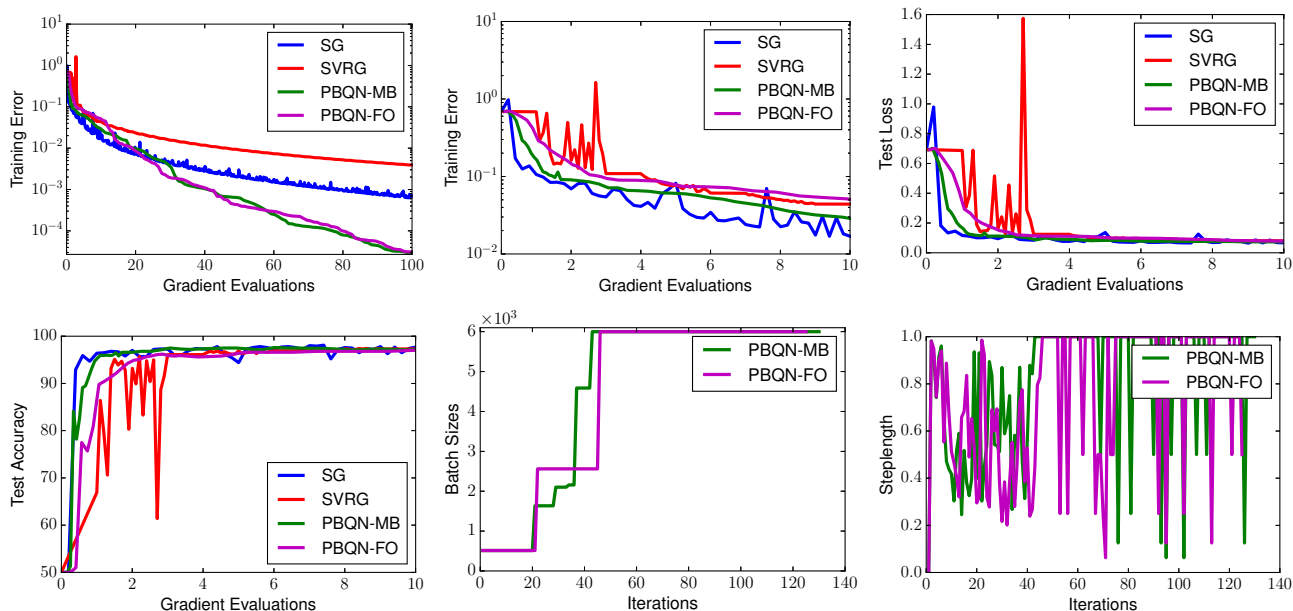


Figure 5. **gisette dataset:** Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

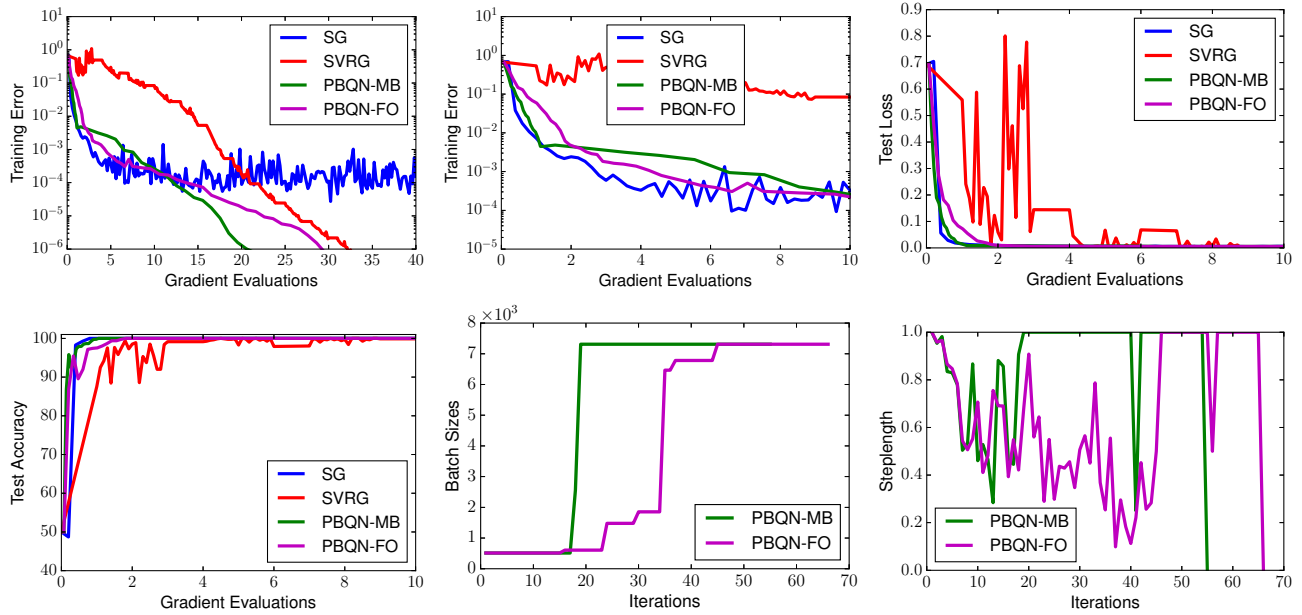


Figure 6. **mushrooms dataset**: Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

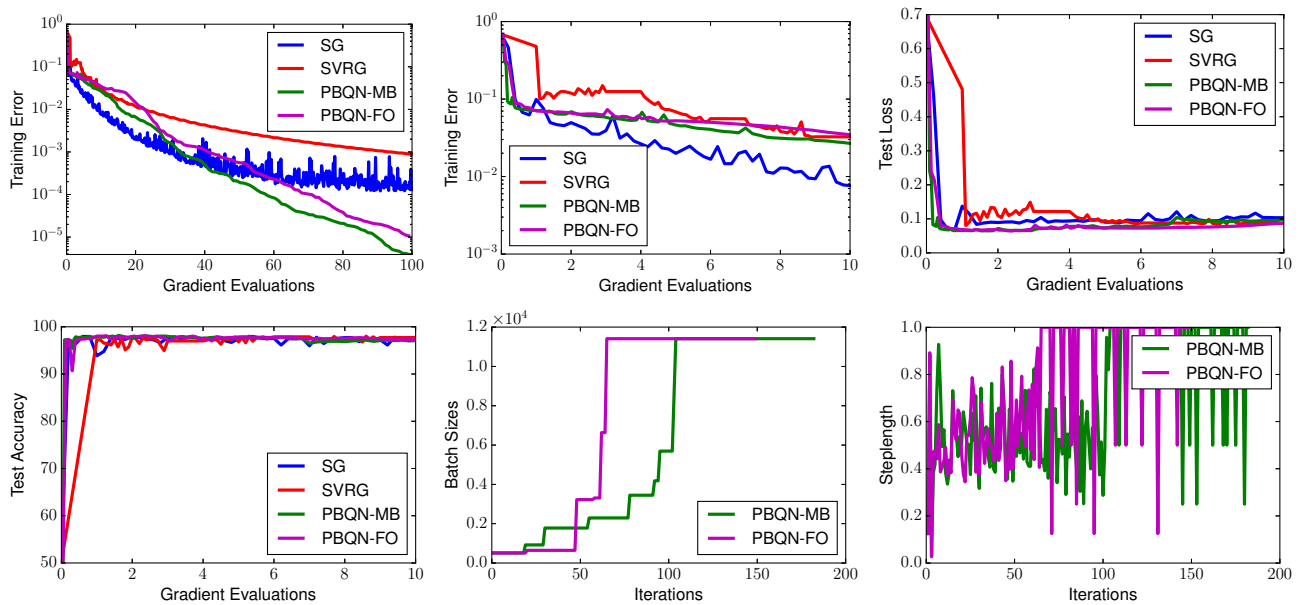


Figure 7. **sido dataset**: Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

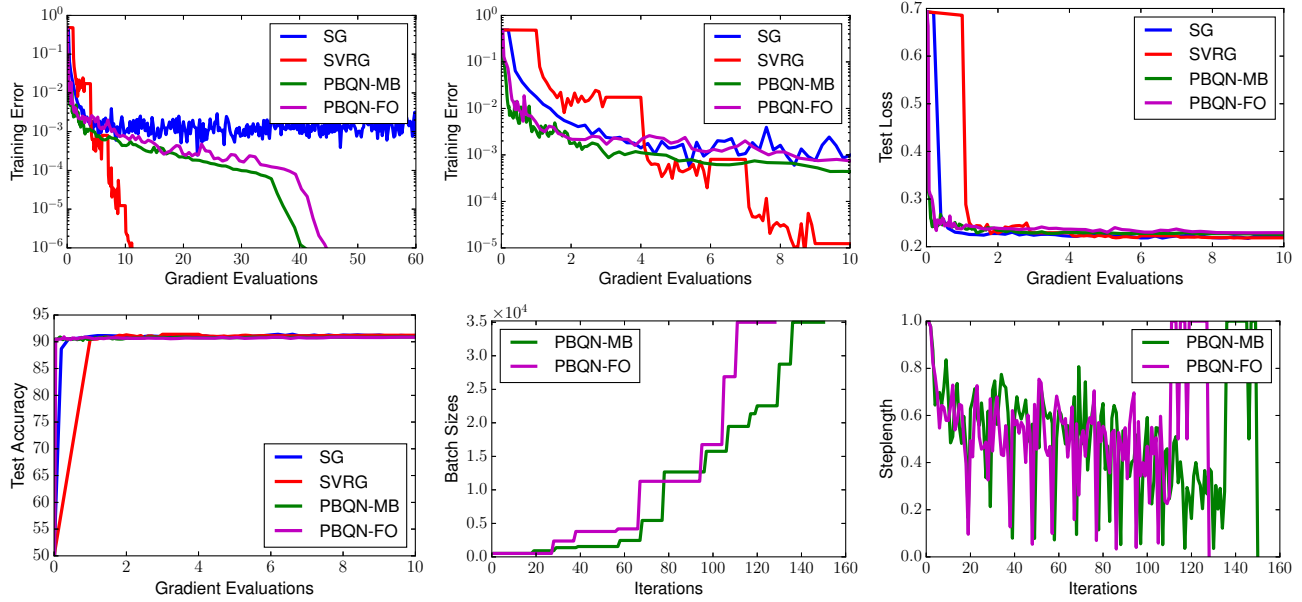


Figure 8. **ijcnn** dataset: Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

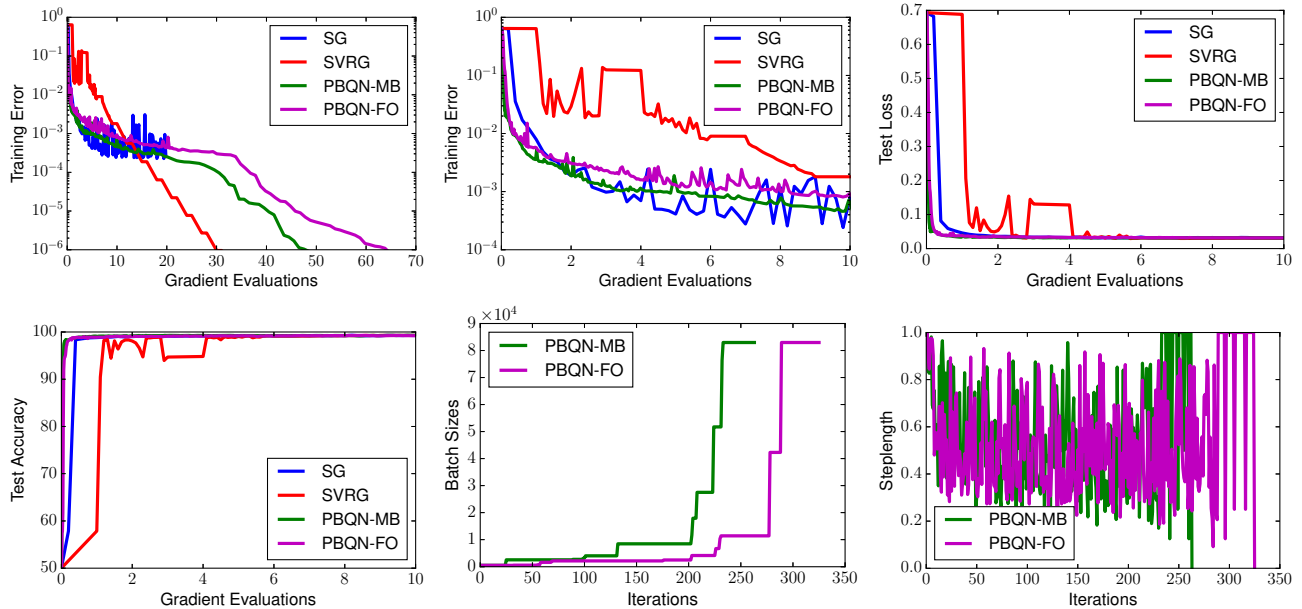


Figure 9. **spam** dataset: Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

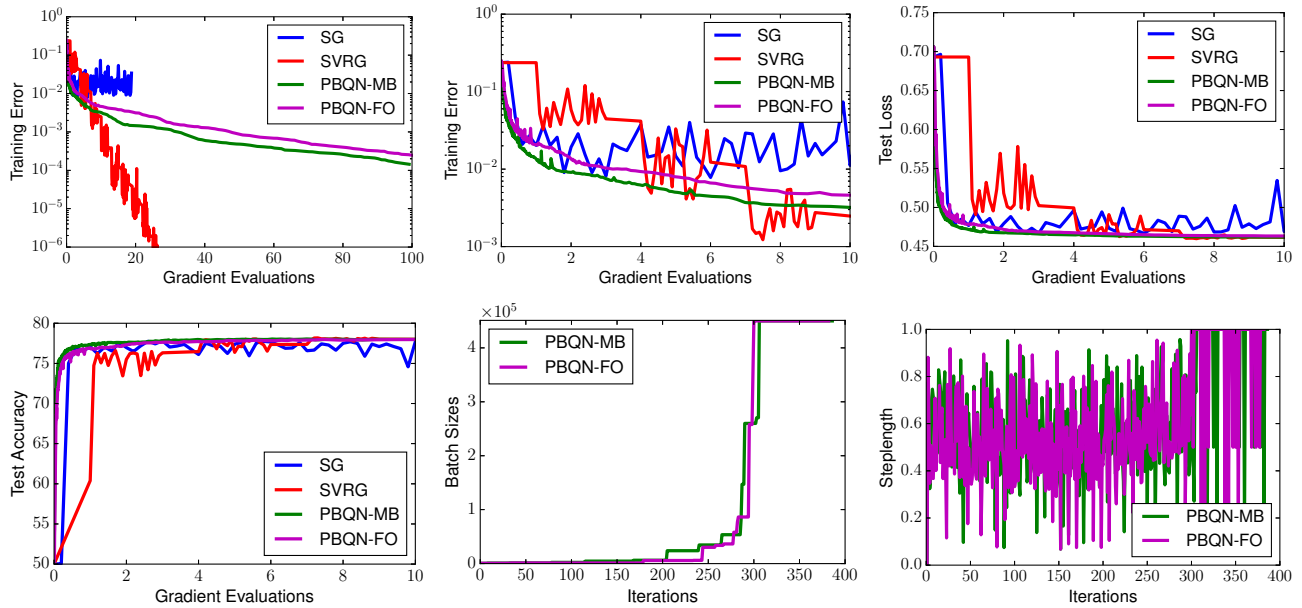


Figure 10. **alpha dataset:** Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

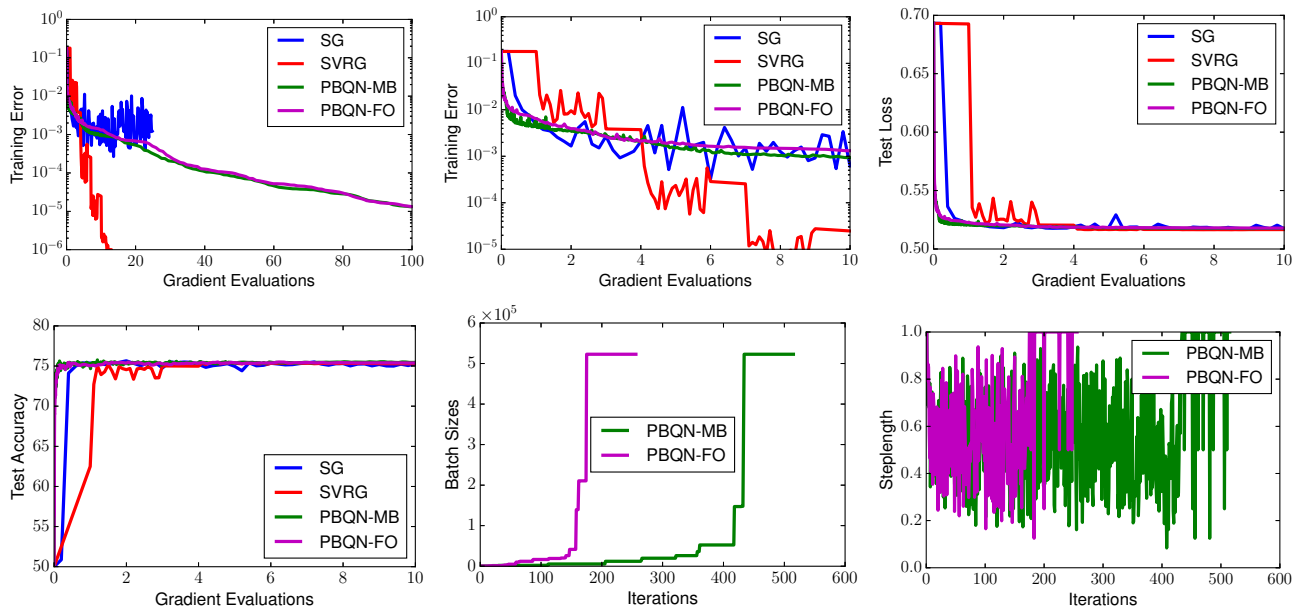


Figure 11. **covtype dataset:** Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods.

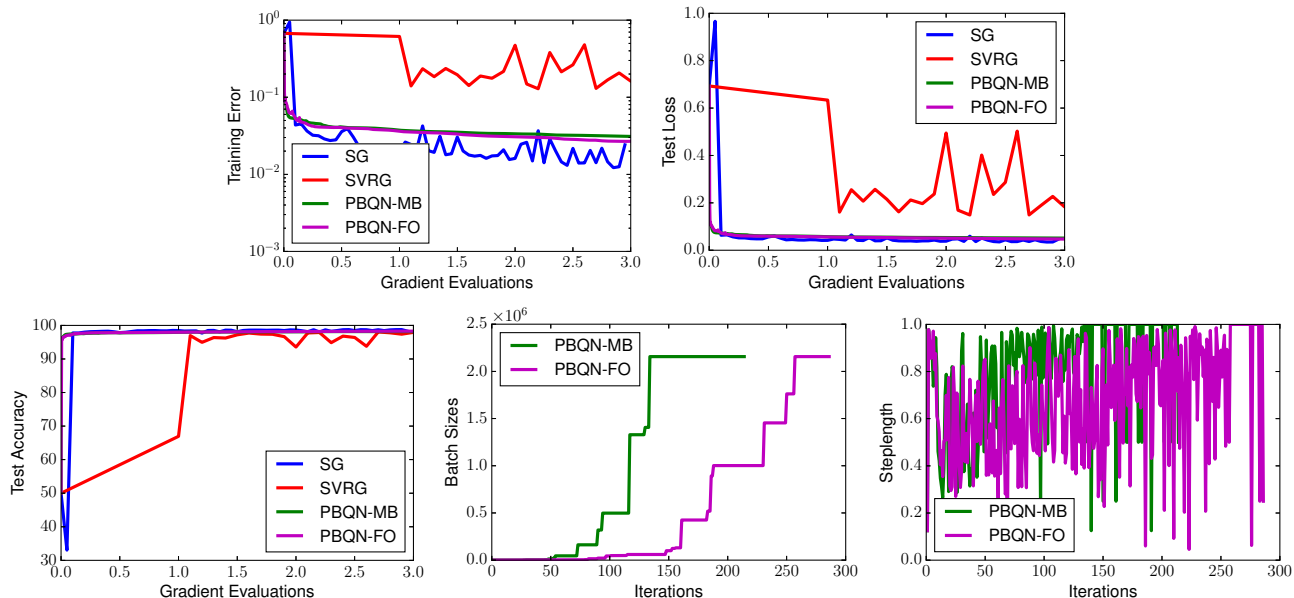


Figure 12. **url dataset:** Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and SVRG methods. Note that we only ran the SG and SVRG algorithms for 3 gradient evaluations since the equivalent number of iterations already reached of order of magnitude 10^7 .

C.3. Neural Network Experiments

We describe each neural network architecture below. We also plot the training loss, test loss and test accuracy against the total number of iterations and gradient evaluations. We also report the behavior of the batch sizes and steplengths for both variants of the PBQN method.

C.3.1. CIFAR-10 CONVOLUTIONAL NETWORK (\mathcal{C}) ARCHITECTURE

The small convolutional neural network (ConvNet) is a 2-layer convolutional network with two alternating stages of 5×5 kernels and 2×2 max pooling followed by a fully connected layer with 1000 ReLU units. The first convolutional layer yields 6 output channels and the second convolutional layer yields 16 output channels.

C.3.2. CIFAR-10 AND MNIST ALEXNET-LIKE NETWORK ($\mathcal{A}_1, \mathcal{A}_2$) ARCHITECTURE

The larger convolutional network (AlexNet) is an adaptation of the AlexNet architecture (Krizhevsky et al., 2012) for CIFAR-10 and MNIST. The CIFAR-10 version consists of three convolutional layers with max pooling followed by two fully-connected layers. The first convolutional layer uses a 5×5 kernel with a stride of 2 and 64 output channels. The second and third convolutional layers use a 3×3 kernel with a stride of 1 and 64 output channels. Following each convolutional layer is a set of ReLU activations and 3×3 max poolings with strides of 2. This is all followed by two fully-connected layers with 384 and 192 neurons with ReLU activations, respectively. The MNIST version of this network modifies this by only using a 2×2 max pooling layer after the last convolutional layer.

C.3.3. CIFAR-10 RESIDUAL NETWORK (\mathcal{R}) ARCHITECTURE

The residual network (ResNet18) is a slight modification of the ImageNet ResNet18 architecture for CIFAR-10 (He et al., 2016). It follows the same architecture as ResNet18 for ImageNet but removes the global average pooling layer before the 1000 neuron fully-connected layer. ReLU activations and max poolings are included appropriately.

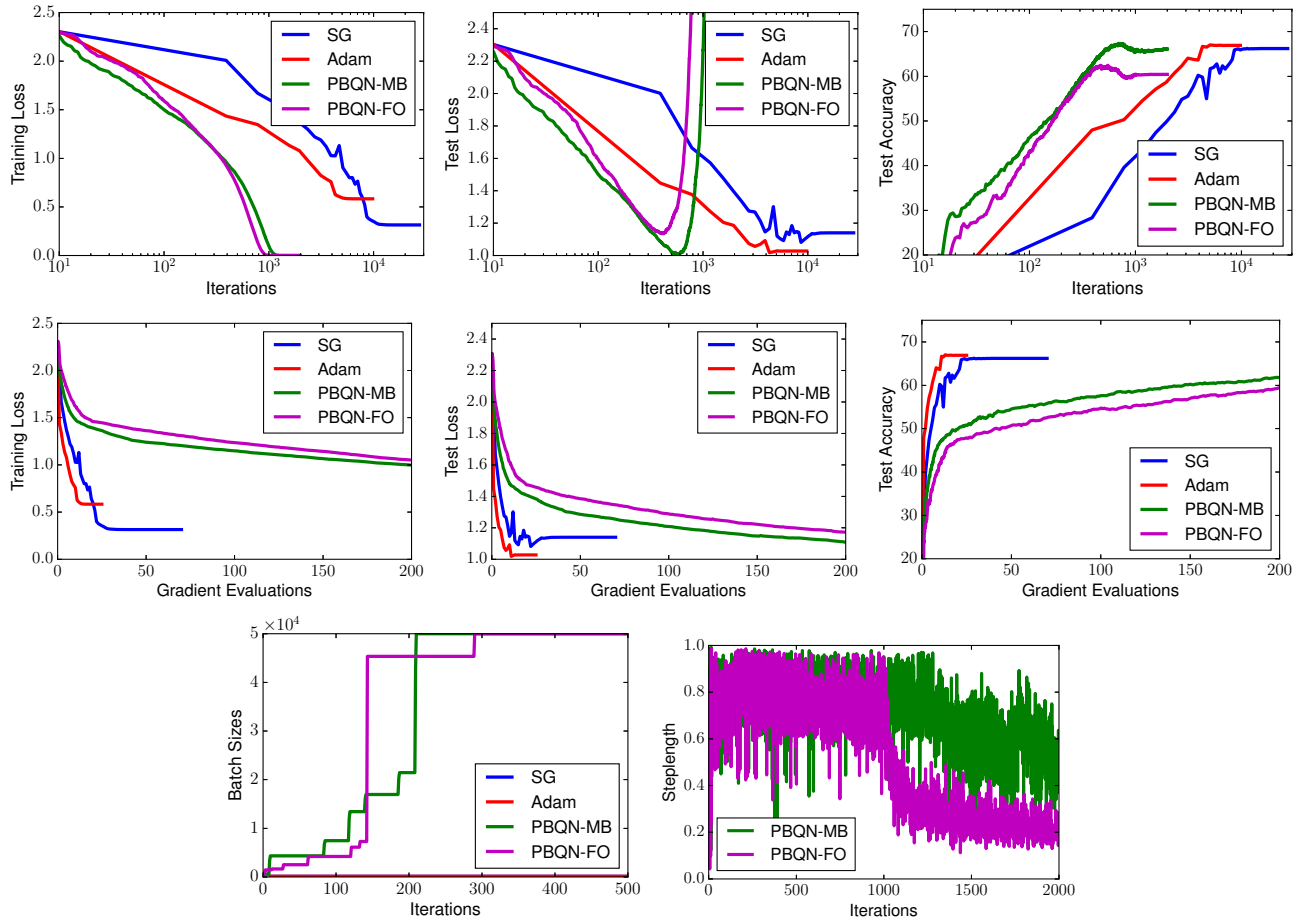


Figure 13. CIFAR-10 ConvNet (C): Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and Adam methods. The best results for L-BFGS are achieved with $\theta = 0.9$.

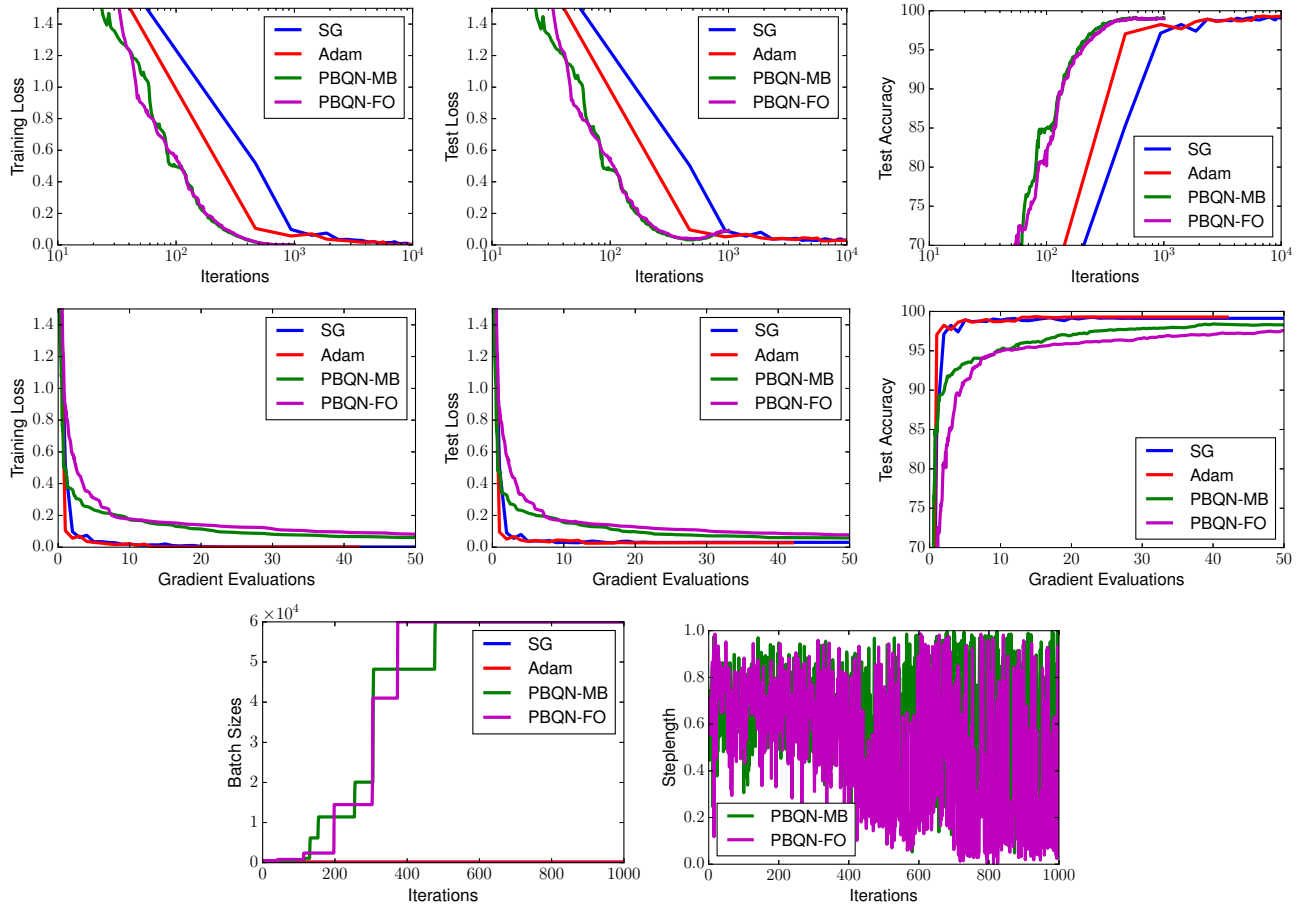


Figure 14. MNIST AlexNet (\mathcal{A}_1): Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and Adam methods. The best results for L-BFGS are achieved with $\theta = 2$.

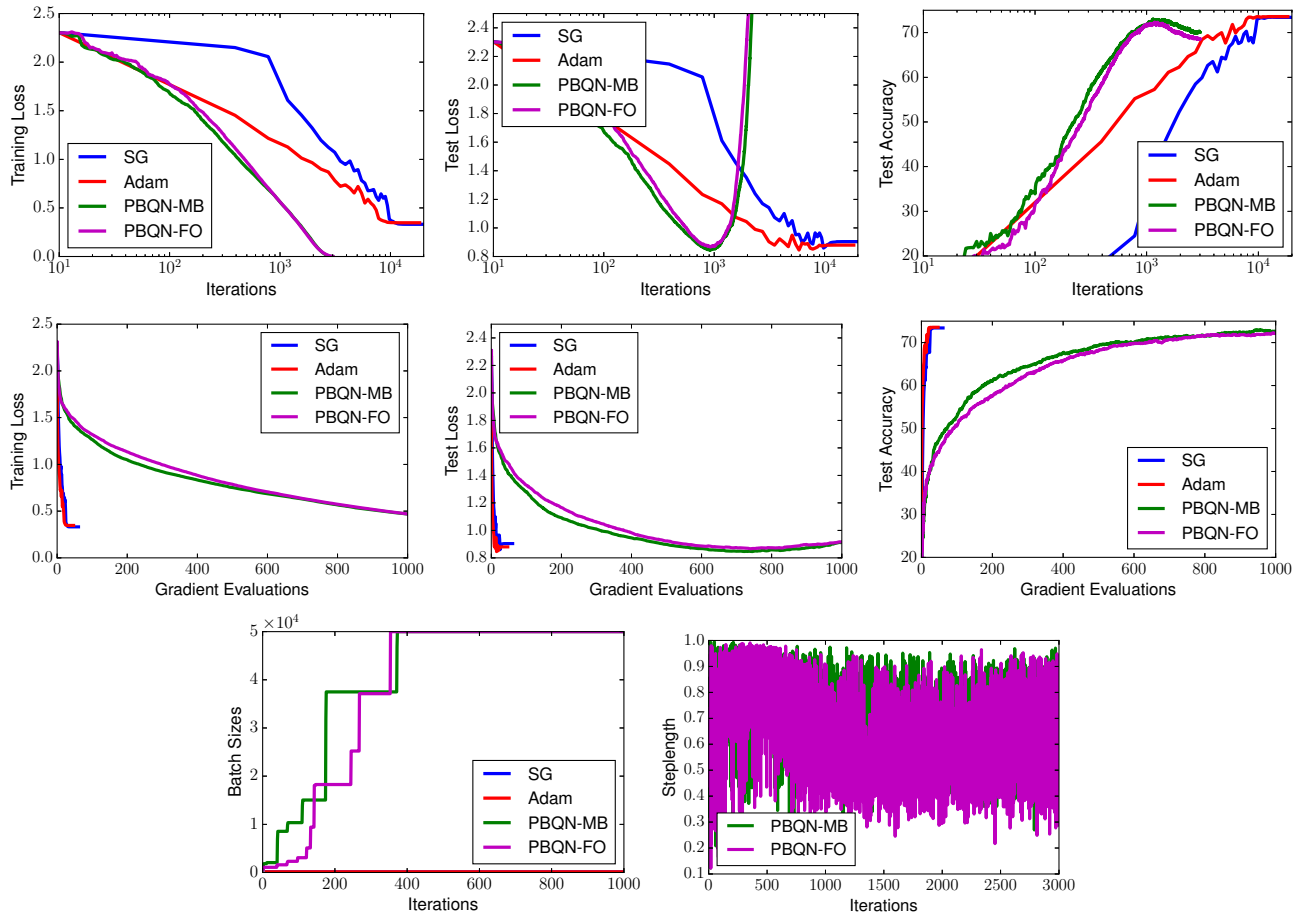


Figure 15. CIFAR-10 AlexNet (\mathcal{A}_2): Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and Adam methods. The best results for L-BFGS are achieved with $\theta = 0.9$.

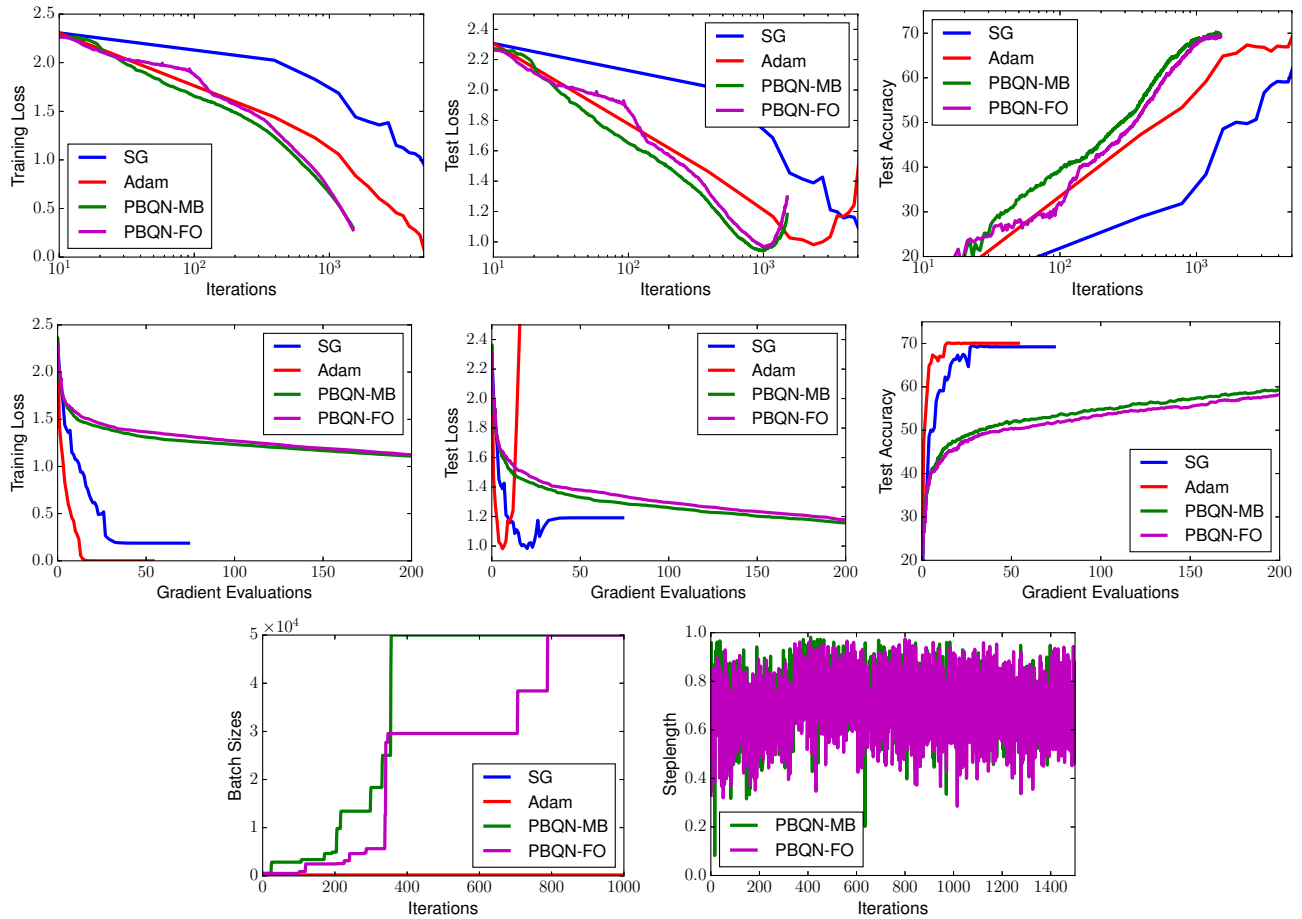


Figure 16. CIFAR-10 ResNet18 (\mathcal{R}): Performance of the progressive batching L-BFGS methods, with multi-batch (25% overlap) and full-overlap approaches, and the SG and Adam methods. The best results for L-BFGS are achieved with $\theta = 2$.

D. Performance Model

The use of increasing sample sizes in the PBQN algorithm results in a larger effective batch size compared to SG, allowing PBQN to scale to a larger number of nodes than currently possible even with large batch SG training (Goyal et al., 2017). With improved scalability and richer gradient information, we expect the training time to reduce as well. To demonstrate the potential to reduce training time, we extend the idealized performance model from (Keskar et al., 2016) to the PBQN algorithm. For PBQN to be competitive, it must achieve the following: (i) the quality of its solution should match or improve SG’s solution (as shown in Table 1); (ii) it should utilize a larger effective batch size; and (iii) it should converge to the solution in a lower number of iterations. We analyze this by establishing the analytic requirements for improved training time.

Let the effective batch size for PBQN be \widehat{B}_L and the conventional SG batch size be B_S . From Algorithm 1, we observe that the PBQN iteration involves extra computation in addition to the gradient computation as in SG. The additional steps are as follows: the L-BFGS two-loop recursion, which includes several model evaluations (Algorithm 1:6); the stochastic line search for identifying the steplength (Algorithm 1:7-16); and curvature pair updating (Algorithm 1:18-21). However, most of these supplemental operations are performed on the weights of the network, which is orders of magnitude lower than computing the gradient. The only exception is the additional model evaluations that are required as part of the L-BFGS two loop recursion, which involves forward propagating several ($O(10)$) times over the model. This amounts to $\frac{1}{3}$ the cost of gradient computation (forward propagation, back propagation with respect to activations and weights). Hence, the ratio of cost-per-iteration for PBQN C_L to SG’s cost-per-iteration C_S is $\frac{4}{3}$. Let I_S and I_L be the number of iterations that it takes SG and PBQN, respectively, to reach similar test accuracy. The target number of nodes to be used for training is N , such that $N < \widehat{B}_L$. For N nodes, the parallel efficiency of SG is assumed to be $P_e(N)$ and we assume that for the target node count, there is no drop in parallel efficiency for PBQN due to the large effective batch size.

For a lower training time with the PBQN method, the following relation should hold:

$$I_L C_L \frac{\widehat{B}_L}{N} < I_S C_S \frac{B_S}{N P_e(N)}. \tag{47}$$

In terms of iterations, we can rewrite this as

$$\frac{I_L}{I_S} < \frac{C_S B_S}{C_L \widehat{B}_L} \frac{1}{P_e(N)}. \tag{48}$$

If $P_e(N) = 0.2$, $\widehat{B}_L/B_S = 10$, and $C_L/C_S = 4/3$, PBQN must converge more than 3 times fewer iterations than SG in order to achieve lower training time. From Section 4, the results show that PBQN converges well within 3 times less iterations than SG, hence establishing the potential for lower training times. We refer the reader to (Das et al., 2016) for a more detailed model and commentary on the effect of batch size on performance.