On the line-search gradient methods for stochastic optimization *

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Abstract: We consider several line-search based gradient methods for stochastic optimization: a gradient and accelerated gradient methods for convex optimization and gradient method for non-convex optimization. The methods simultaneously adapt to the unknown Lipschitz constant of the gradient and variance of the stochastic approximation for the gradient. The focus of this paper is to numerically compare such methods with state-of-the-art adaptive methods which are based on a different idea of taking norm of the stochastic gradient to define the stepsize, e.g., AdaGrad and Adam.

Keywords: convex and non-convex optimization, stochastic optimization, first-order method, adaptive method, gradient descent, complexity bounds, mini-batch.

1. INTRODUCTION

In this paper we consider unconstrained minimization problem
\[ \min_{x \in \mathbb{R}^n} f(x), \quad (1) \]
where \( f(x) \) is a smooth, possibly non-convex function with \( L \)-Lipschitz continuous gradient. We say that a function \( f : E \rightarrow \mathbb{R} \) has a \( L \)-Lipschitz continuous gradient if it is continuously differentiable and its gradient satisfies
\[ f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} \| x - y \|^2, \quad \forall \ x, y \in E. \]
We assume that the access to the objective \( f \) is given through stochastic oracle \( \nabla f(x, \xi) \), where \( \xi \) is a random variable. The main assumptions on the stochastic oracle are standard for stochastic approximation literature
\[ \mathbb{E} \nabla f(x, \xi) = \nabla f(x), \quad \mathbb{E} \| \nabla f(x, \xi) - \nabla f(x) \|^2 \leq D. \]

In papers Duchi et al. (2011); Byrd et al. (2012); Friedlander and Schmidt (2012); Kingma and Ba (2015); Isele et al. (2019); Gasnikov (2017); Levy et al. (2018); Deng et al. (2018); Ogaltsov and Tyurin (2019); Ward et al. (2019); Bach and Levy (2019); Kamzolov et al. (2020); Dvurechensky et al. (2020) there proposed different approaches to choose in an adaptive manner \( L \) and \( D \), see Table for details.

In this paper we extend the idea of Armijo-type line search in variants from Gasnikov (2017); Ogaltsov and Tyurin (2019) for the adaptive methods for convex and non-convex stochastic optimization. Surprisingly, the adaptation is needed not to each parameter separately, but to the ratio \( D/L \), which can be considered as signal to noise ratio or an effective Lipschitz constant of the gradient in this case. We propose an accelerated and non-accelerated gradient descent for stochastic convex optimization and a gradient method for stochastic non-convex optimization. Our methods are flexible enough to use optimal choice of mini-batch size without additional information on the problem. Moreover, our procedure allows an increase of the stepsize, which accelerated the methods in the areas where the Lipschitz constant is small. Also, as opposed to the existing methods, our algorithms do not need to know neither the distance to the solution, nor a set of complicated hyperparameters, which are usually fine-tuned...
by multiple repetition of minimization process. Moreover, since our methods are based on inexact oracle model (see e.g. Devolder et al. (2014); Gasnikov and Dvurechensky (2016); Dvurechensky and Gasnikov (2016)), they are adaptive not only for a stochastic error, but also for deterministic, e.g. non-smoothness of the problem. This means that our methods are universal for smooth and non-smooth optimization Nesterov (2015); Yurtsever et al. (2015); Dvurechensky (2017). Our focus in this paper is to demonstrate in the experiments that our methods work faster than state-of-the-art methods Duchi et al. (2011); Kingma and Ba (2015). The rigorous proofs are deferred to a separate paper.

The paper is structured as follows. In Sect. 2 we present adaptive stochastic algorithms based on stochastic gradient method to solve a problem of type (1) with convex objective function. Sect. 3 renews Sect. 2 for non-convex objective function. Finally, in Sect. 4 we show numerical experiments supporting the theory in above sections.

2. STOCHASTIC CONVEX OPTIMIZATION

In this section we solve problem (1) for convex objective by adaptive algorithm which does not need the information about Lipschitz constant. Then we comment on its acceleration and practical implementation.

2.1 Adaptive algorithm

We assume that the constant $L$ may be unknown. If the true variance $D$ is unavailable we use its upper bound $D_0 \ge D$. We provide adaptive algorithm (Alg. 1) which iteratively tunes the Lipschitz constant. Importantly, the approximation of the Lipschitz constant used by the algorithm may decrease as iteration go, leading to larger steps and faster convergence. Further, we comment on its rates of convergence.

From Lipschitz continuity of $\nabla f(x)$ we have

$$f(x^{k+1}) \le f(x^k) + \langle \nabla f(x^k), x^{k+1} - x^k \rangle + \frac{L_{k+1}}{2} \|x^{k+1} - x^k\|^2. \quad (3)$$

We provide adaptive algorithm (Alg. 1) which iteratively tunes the Lipschitz constant. Important, the approximation of the Lipschitz constant used by the algorithm may decrease as iteration go, leading to larger steps and faster convergence. Further, we comment on its rates of convergence.

Algorithm 1 Adaptive Stochastic Gradient Descent

Require: Number of iterations $N$, accuracy $\varepsilon$, $D_0$, initial guess $L_0$.

1: for $k = 0, \ldots, N - 1$ do
2: $L_{k+1} : = L_k/4$
3: repeat
4: $L_{k+1} : = 2L_{k+1}$
5: Calculate batch size $r_{k+1} = \max \left\{ \frac{D_0}{L_{k+1} + \varepsilon}, 1 \right\}$
6: $x^{k+1} = x^k - \frac{1}{2L_{k+1}} \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r), x^{k+1} - x^k)$
7: until $f(x^{k+1}) - f(x^k) - \langle \nabla f(x^k, \{\xi_l^{k+1}\}_{l=1}^r), x^{k+1} - x^k \rangle + L_{k+1} \|x^{k+1} - x^k\|^2 + \varepsilon/2$
8: end for

Ensure: $\tilde{x}_N = \frac{1}{N} \sum_{k=1}^N x^k$.

By Cauchy–Schwarz inequality and since $ab \le \frac{a^2}{2} + \frac{b^2}{2}$ for any $a, b$, we get

$$\langle \nabla f(x^k) - \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r), x^{k+1} - x^k \rangle \le \frac{1}{2L_{k+1}} \| \nabla f(x^k) - \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r) \|^2 + \frac{L_{k+1}}{2} \|x^{k+1} - x^k\|^2. \quad (4)$$

Then add and subtract $\nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r)$ in (3).

Using (4) and (2) we get

$$f(x^{k+1}) - f(x^k) \le -\frac{1}{4L_{k+1}^2} \| \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r) \|^2 + \frac{1}{2L_{k+1}} \| \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r) - \nabla f(x^k) \|^2. \quad (5)$$

From (2) we have for any $x$

$$\| x^{k+1} - x\|^2 \ge \|x^k - x^k - \frac{1}{2L_{k+1}} \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r) \|^2 \equiv \| x^k - x\|^2 + \frac{1}{4L_{k+1}^2} \| \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r) \|^2 - \frac{1}{L_{k+1}} \langle \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r), x^k - x \rangle. \quad (6)$$

From (5) and (6) we get

$$\langle \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r), x^k - x \rangle \le f(x^k) - f(x^{k+1}) + L_{k+1} \|x^{k+1} - x\|^2 + \varepsilon/2, \quad (7)$$

where we used batch size $r_{k+1} = \max \left\{ \frac{D_0}{L_{k+1} + \varepsilon}, 1 \right\}$ to fulfill $E[\| \nabla r_{k+1} f(x^k, \{\xi_l^{k+1}\}_{l=1}^r) - \nabla f(x^k) \|^2] = \varepsilon L_{k+1}$.

Since $L_{k+1}$ is random, $r_{k+1}$ will be random as well and, consequently, the total number of oracle calls $T$ is not precisely determined. Let us choose it according to the number of oracle calls for non-adaptive counterpart of Algorithm 1

$$T = \sum_{k=1}^{N-1} r_{k+1} = O \left( \frac{D_0 R^2}{\varepsilon^2} \right). \quad (8)$$

This number of oracle calls (8) can be provided by choosing the last batch size $R_N$ as a residual of the sum (8) and calculate the last Lipschitz constant $L_N = \frac{D_0}{r_N}$. In practice, we do not need to limit ourselves by fixing the number of oracle calls $T$.  

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From the convexity of $f$ we have
\[ f(x^k) - f(x) \leq \langle \nabla f(x), x^k - x \rangle. \] (9)
Then from (9) we get
\[ \langle \nabla r_{k+1} f(x, \{\xi_{k+1}^{l}\}_{l=1}^{r_{k+1}}) - \nabla f(x^k), x^k - x \rangle. \]
From this and (7) we have
\[ \frac{1}{L_{k+1}} \frac{1}{L_{k+1}} (f(x^k) - f(x)) \]
\[ + \frac{1}{L_{k+1}} (r_{k+1} f(x, \{\xi_{k+1}^{l}\}_{l=1}^{r_{k+1}}) - \nabla f(x^k), x^k - x) \]
\[ \leq \|x^k - x\|^2 - \|x^k - x\|^2 \frac{1}{L_{k+1}} (f(x^k) - f(x^k)) + \frac{\varepsilon}{2L_{k+1}}. \]

We notice that the following sum
\[ \sum_{k=0}^{N-1} \frac{1}{L_{k+1}} (r_{k+1} f(x^k, \{\xi_{k+1}^{l}\}_{l=1}^{r_{k+1}}) - \nabla f(x^k), x^k - x) \]
\[ \leq \frac{\|x^k - x\|^2}{2} - \frac{\|x^k - x\|^2}{2} \frac{1}{L_{k+1}} (f(x^k) - f(x^k)) + \frac{\varepsilon}{2L_{k+1}}. \]

To compare our complexity bounds for adaptive stochastic gradient descent with the bounds for accelerated variant of our algorithm we refer to Goldtsov and Tsyurin (2019). For the reader convenience we provide that accelerated algorithm in a simpler form and complexity bounds presented there without proof.

\section*{Algorithm 2 Adaptive Stochastic Accelerated Gradient Method}

\textbf{Require:} Number of iterations $N$, $D_0$ accuracy $\varepsilon$, $\Omega \geq 1$, $A_0 = 0$, initial guess $L_0$.
1: for $k = 0, \ldots, N - 1$ do
2: $L_{k+1} := L_k / 4$
3: repeat
4: $L_{k+1} := 2L_{k+1}$
5: $\alpha_{k+1} := \frac{1}{\sqrt{2L_{k+1}}} A_{k+1} = A_k + \alpha_{k+1}$
6: Calculate batch size $r_{k+1} = \max \left\{ \frac{D_0 + D_0}{\varepsilon}, 1 \right\}$
7: $y_{k+1} = (a_{k+1} u^k + A_k x^k) / A_{k+1}$
8: $u_{k+1} = u^k - \alpha_{k+1} \nabla r_{k+1} f(y_{k+1}, \{\xi_{k+1}^{l}\}_{l=1}^{r_{k+1}})$
9: $x_{k+1} = (a_{k+1} u_{k+1} + A_k x^k) / A_{k+1}$
10: until $f(x_{k+1}) \leq f(y_{k+1})$
11: for $k = 0, \ldots, N - 1$ do
12: $\hat{x} = \arg \min_{x \in X} \|\nabla f(x^k)\|_2$
13: $\rho = \frac{\varepsilon}{2L_{k+1}}$
14: until $f(x_{k+1}) \leq f(x^k) + \langle \nabla f(x^k), (\xi_{k+1}^{l})_{l=1}^{r_{k+1}} \rangle + \frac{\rho^2}{2} + \frac{\rho^2}{2} + \frac{\rho^2}{2} + \frac{\rho^2}{2}$
15: end for

3. STOCHASTIC NON-CONVEX OPTIMIZATION

In this section we assume that the objective $f$ may be non-convex. We consider adaptive algorithm and provide the complexity bounds for it.

\section*{Algorithm 3 Adaptive Non-Convex Stochastic Gradient Descent}

\textbf{Require:} Number of iterations $N$, $D_0$ accuracy $\varepsilon$, initial guess $L_0$.
1: Calculate batch size $r = \max \left\{ \frac{D_0 + D_0}{\varepsilon}, 1 \right\}$
2: for $k = 0, \ldots, N - 1$ do
3: $L_{k+1} := L_k / 4$
4: repeat
5: $L_{k+1} := 2L_{k+1}$
6: $x_{k+1} = x^k - \frac{1}{2L_{k+1}} \nabla r_{k+1} f(x^k, \{\xi_{k+1}^{l}\}_{l=1}^{r_{k+1}})$
7: until $f(x_{k+1}) \leq f(x^k) + \langle \nabla r_{k+1} f(x^k, \{\xi_{k+1}^{l}\}_{l=1}^{r_{k+1}}), x_{k+1} - x^k \rangle$
8: end for

Theorem 1. Algorithm 3 with expected number of stochastic gradient oracle calls $\hat{T} = \frac{D_0 L(f(x^k) - f(x^N))}{\varepsilon^4}$ and
expected number of iterations $\tilde{N} = O\left(\frac{L(f(x^0) - f(x^\infty))}{\varepsilon^2}\right)$
outputs a point $\hat{x}_{\tilde{N}}$ satisfying
\[E\|\nabla f(\hat{x}_{\tilde{N}})\|^2_2 \leq \varepsilon^2.\]

**Sketch of the Proof.** From (14) using (13) we get
\[f(x^{k+1}) - f(x^k) \leq -\frac{1}{4L} \|\nabla f(x^k)\|^2_2 + \frac{\varepsilon^2}{32L_{k+1}}.\quad (15)\]
Due to $\|a\|^2 \leq 2\|b\|^2 + 2\|a - b\|^2$ for any $a, b \in \mathbb{R}^n$ we get
\[\|\nabla f(x^k)\|^2_2 \geq \frac{1}{2} \|\nabla f(x^k)\|^2_2 - \|\nabla f(x^k) - \nabla f(x^k, \{\xi^k_{l+1}\}_{l=1}^\infty)\|^2_2.\quad (16)\]
From (15) and (16) we have
\[f(x^{k+1}) - f(x^k) \leq -\frac{1}{8L} \|\nabla f(x^k)\|^2_2 + \frac{\varepsilon^2}{32L_{k+1}}.\]
If $\|\nabla f(x^k)\|^2_2 \geq \varepsilon^2$. Then
\[f(x^{k+1}) - f(x^k) \leq \frac{(8\varepsilon^2 + 3\varepsilon^2)}{32L_{k+1}}.\quad (17)\]
Based on iterated procedure (10) we may expect that $L_{k+1} \leq 2L$. The exact proof of this fact in probability of large deviations terminology was provided in Ogaltsov and Tyurin (2019) (numerical coefficient needs to be corrected). In our work, we limit ourselves by assuming this inequality holds ‘in average’.
If $3\varepsilon^2 - 8\varepsilon^2 \geq 0$ we may replace $L_{k+1}$ by $2L$. Therefore, we rewrite (17) with minor changing and after taking the expectation we get
\[E[f(x^{k+1}) - E[f(x^k)] \leq \frac{(8\varepsilon^2 + 3\varepsilon^2)}{64L}.\]
Ensuring $E\varepsilon^2 \geq \frac{\varepsilon^2}{8}$ we obtain
\[E[f(x^{k+1}) - E[f(x^k)] \leq \frac{-\varepsilon^2}{64L}.\]
Summing this over expected number of iteration we get
\[\tilde{N} = 64L(f(x^0) - f(x^\infty))/\varepsilon^2.\quad (18)\]
This $\tilde{N}$ ensures that for some $k$ we get $\|\nabla f(x^k)\|^2_2 \leq \varepsilon^2$. We choose the batch size according to
\[E\varepsilon^2_{k+1} = E[\|\nabla f(x^k, \{\xi^k_{l+1}\}_{l=1}^\infty) - \nabla f(x^k)\|^2_2] = \frac{\varepsilon^2}{8} \leq \frac{D_0}{r}.\]
Consequently, $r = \frac{8D_0}{\varepsilon^2}$. Using the expected number of iterations (18) we get expected number of oracle calls
\[\tilde{T} = \tilde{N}r = 512D_0L(f(x^0) - f(x^\infty))/\varepsilon^4.\]

More accurate proof of Theorem 1 can be done using large deviations technique and sub-Gaussian variance, see Dvurechensky et al. (2018a).

### 4. EXPERIMENTS

We perform experiments using proposed methods with and without acceleration on convex and non-convex problems and compare results with commonly used methods — Adam, Kingma and Ba (2015) and Adagrad, Duchi et al. (2011). Experiments consist of four problems:

(1) Training logistic regression on MNIST dataset (Lecun et al. (1998)) (convex problem). Number of optimized parameters is 7850.
(2) Training fully-connected sigmoid-activated neural network with two hidden layers of size 1000 on MNIST dataset (non-convex problem). Number of optimized parameters is 795010.
(3) Training fully-connected relu-activated neural network with two hidden layers of size 1000 also on MNIST dataset (non-differentiable and non-convex problem). Number of optimized parameters is 795010.
(4) Training small convolutional neural network with three filters and three fully-connected layers on CIFAR10 dataset (Krizhevsky (2009)) (non-convex problem). Number of optimized parameters is 62000.

Objective for all the problems is cross-entropy function between predicted class distribution and ground-truth class labels. Hyper-parameters set for proposed methods varies depending only on convexity of the problem. Hyper-parameters for all our algorithms in convex case were $D_0 = 0.01, \varepsilon = 10^{-5}$, $L_k = 100$, and $D_0 = 0.1, L_0 = 1, \varepsilon = 0.002$ for all non-convex problems. This hyperparameter set is chosen experimentally to obtain universal hyperparameters for broad range of settings. Adam and Adagrad had batch size equal to 128, learning rate = 0.001 and $\beta_1 = 0.9, \beta_2 = 0.999$ — these parameters are frequently used in various machine learning tasks and are used in Kingma and Ba (2015). Training set is 60K samples for MNIST dataset and 50K samples for CIFAR10 dataset. Dynamics of objective function value is depicted on Fig 1. Since batch size is variable we also compare algorithms by epochs (one epoch is one full pass through dataset). We also performed grid search of hyper-parameters for all algorithms to compare best versions of the laters. Result for tuned algorithms by epochs for logistic regression and fully connected neural network are in Fig 2. Although Adam performs better than our methods in case of fully connected network, we show that our algorithms are more robust to hyper-parameter choice. Final experiment series is follows. We pick logistic regression for computational simplicity, choice hyper-parameter set and do 10 epochs of optimization procedure than average results for each epoch. Hyper-parameter set for Adam and Adagrad is all pairs of batch size $(8, 32, 64, 128, 256, 512, 1024)$ and learning rate $(10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1)$. Hyperparameter set for our methods is all combinations of $D_0 (10^{-5}, 10^{-4}, 10^{-3}, L_0 (10^4, 10^3, 10^2), \varepsilon (10^{-6}, 10^{-5}, 10^{-4})$. Median for each epoch (to omit sensitivity to outliers) with one standard deviation are on Fig 3. One can see that underestimate of hyper-parameters for our algorithms does not lead to substantial deviations and that all proposed algorithms outperform Adam and Adagrad in terms of robustness. The code for all algorithms is available, visit http://github.com/alexo256/Adaptive-Gradient-Descent-for-Convex-and-Non-Convex-Stochastic-Optimization

![Image](https://example.com/fig1.png)

![Image](https://example.com/fig2.png)

![Image](https://example.com/fig3.png)

5. CONCLUSION

In this paper we focus on adaptive methods for stochastic convex and non-convex optimization. It would be interesting to combine these ideas with the notion of inexact model
Stonyakin et al. (2019a) to obtain adaptive and universal methods using stochastic inexact model. We leave this for future work.

It seems that the results of this paper can be generalized on gradient-free method for stochastic optimization Dvurechensky et al. (2017). In particular, for sum-type problems. It would be interesting to apply these methods for stochastic optimization in the context of Wasserstein barycenters Dvurechensky et al. (2018b); Dvinskikh et al. (2019); Kroshnin et al. (2019); Uribe et al. (2018).

Note also, that if we replace step 2 in Alg. 1 and Alg. 2 by \( L_{k+1} := L_k/2 \), take \( r_{k+1} \equiv \max\{2D_0/(L_k \varepsilon), 1\} \) and forbid \( L_{k+1} \) to be outside the range \([L_d, L_u]\), where \( L_d \equiv L_0 \equiv L_u \mod 2 \), \( L_0 \in [L_d, L_u] \), then based on union bound inequality and theory of empirical process Giné and Nickl (2016) one can prove the desired estimates up to a logarithmic factors.

See the complete version of this paper at https://arxiv.org/pdf/1911.08380.pdf for details.

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