

Improved Optimization of Finite Sums with Minibatch Stochastic Variance Reduced Proximal Iterations

Jialei Wang
University of Chicago
Tong Zhang
Tencent AI Lab

jialei@uchicago.edu

tongzhang@tongzhang-ml.org

Abstract

We present a novel minibatch stochastic optimization method for empirical risk minimization problems. The method efficiently leverages variance reduced first-order and sub-sampled higher-order information to accelerate the convergence. We prove improved iteration complexity over state-of-the-art methods under suitable conditions.

1 Introduction

We consider the following optimization problem of finite-sums:

$$\min_w f(w) := \frac{1}{n} \sum_{i=1}^n f_i(w), \quad (1)$$

which arises in many machine learning problems. In the context of regularized loss minimization of linear predictors, we have $f_i(w) = \ell(w^\top x_i; b_i) + \frac{\lambda}{2} \|w\|^2$. Let $x_1, x_2, \dots, x_n \in \mathbb{R}^d$ be feature vectors of n data samples, and $b_1, \dots, b_n \in \mathbb{R}$ or $\{-1, 1\}$ be the corresponding target variables of interest. We note that (1) covers many popular models used in machine learning: for example when $\ell(w^\top x_i; b_i) = \log(1 + \exp(-b_i \langle w, x_i \rangle))$ we obtain ℓ_2 regularized logistic regression. The ubiquitousness of such finite-sum optimization problems and the massive scale of modern datasets motivate significant research effort on efficient optimization algorithms to solve (1). Throughout the paper, we assume each component function is L -smooth and λ -strongly convex.

In recent years there have been significant advances in developing fast optimization algorithms for (1), and we refer the readers to Bottou2016optimization for a comprehensive survey of these developments. For large-scale problems in the form of (1), randomized methods are particularly efficient because of their low per iteration computation. Below we briefly review two lines of research: i) randomized variance reduced first-order methods; ii) randomized methods leveraging second-order information.

Variance Reduced First-order Methods The key technique for developing fast stochastic first-order methods is variance reduction, which makes the variance of the randomized update direction approaching zero when the iterate gets closer to the optimum. Representative methods of this category include SAG roux2012stochastic, SVRG johnson2013accelerating, SDCA shalev2013stochastic and SAGA defazio2014saga, etc. In order to find a solution that reaches ϵ -suboptimality, these methods requires $\mathcal{O}\left(\left(n + \frac{L}{\lambda}\right) \log\left(\frac{1}{\epsilon}\right)\right)$ calls to the first-order oracle to compute the gradient of an individual function. In the large condition number regime (e.g. $\frac{L}{\lambda} > n$), by using an acceleration technique (such as Catalyst shalev2016accelerated, frostig2015regularizing, lin2015universal, APCG lin2015accelerated, SPDC zhang2015stochastic, Katyusha allen2016katyusha, etc), one can further improve the iteration complexity to $\mathcal{O}\left(\left(n + \sqrt{n \cdot \frac{L}{\lambda}}\right) \log\left(\frac{1}{\epsilon}\right)\right)$.

Leveraging Second-order Information Second-order information is often useful in improving the convergence of optimization algorithms. However for large-scale problems, obtaining and inverting the exact Hessian matrix is often computational expensive, making vanilla Newton methods not well suited in solving (1). Therefore, there have been emerging studies in designing randomized algorithms that effectively utilize the *approximated* Hessian information. One line of such research is the sub-sampled Newton method which approximates the Hessian matrix based on a sub-sampled minibatch of data. Several work, such as byrd2011use, am2015sub, roosta2016sub, roosta2016sub2, bollapragada2016exact, established local linear

Algorithm 1 MB-SVRP: Minibatch Stochastic Variance Reduced Proximal Iterations.

Parameters $\eta, b, \tilde{\lambda}, \nu, \varepsilon$.

Initialize $\tilde{w}_0 = 0$.

Sampling Sampling b items from $[n]$ to form a minibatch \bar{B} .

for $s = 1, 2, \dots$ **do**

Calculate $\tilde{v} = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\tilde{w}_{s-1})$.

Initialize $y_0 = w_0 = \tilde{w}_s$.

for $t = 1, 2, \dots, m$ **do**

Sampling b items from $[n]$ to form a minibatch B_t .

Find w_t that approximately solve (2) such that $\tilde{f}_t(w_t) - \min_w \tilde{f}_t(w) \leq \varepsilon$.

$$\begin{aligned} \tilde{f}_t(w) := & \frac{1}{2} (w - w_{t-1})^\top \left(\frac{1}{b} \sum_{i \in \bar{B}} \nabla^2 f_i(w_{t-1}) \right) (w - w_{t-1}) \\ & + \left\langle \frac{\eta}{b} \sum_{i \in B_t} \nabla f_i(y_{t-1}) + \eta \tilde{v} - \frac{\eta}{b} \sum_{i \in B_t} \nabla f_i(\tilde{w}_{s-1}), w \right\rangle + \frac{\tilde{\lambda}}{2} \|w - y_{t-1}\|^2. \end{aligned} \quad (2)$$

Update:

$$y_t = w_t + \nu(w_t - w_{t-1}).$$

end for

Update $\tilde{w}_s = w_m$.

end for

Return \tilde{w}_s

convergence rates for different variants of sub-sampled Newton methods, when the size of the sub-sampled data is large enough. All of the aforementioned methods employ the full first-order gradient, and require calling the second-order oracle to compute the Hessian and solving a resulting linear system at every iteration. Therefore the computational complexity (as compared in Table 2 of xu2016sub) are often worse than stochastic algorithms such as SVRG. Another line of research is to consider randomness in both first and second-order information to design lower per-iteration cost algorithms. In particular, byrd2016stochastic considered combining minibatch SGD with Limited-memory BFGS (L-BFGS) liu1989limited type update. Inspired by this, moritz2016linearly,gower2016stochastic,wang2017stochastic proposed to combine variance reduced stochastic gradient with L-BFGS, and proved linear convergence for strongly convex and smooth objectives. However, theoretically it is hard to guarantee the quality of approximated Hessian using L-BFGS update, and thus the iteration complexity obtained by moritz2016linearly,gower2016stochastic,wang2017stochastic can be pessimistic, and can be much worse than vanilla SVRG.

In this paper, we make effort in this direction and make the following contributions: i) we propose a novel approach that combines the advantages of variance-reduced first-order methods and sub-sampled Newton methods, in a efficient way that does not require expensive Hessian matrix computation and inversion. The method can be naturally extended to solve composite optimization problems with non-smooth regularization; ii) we theoretically show under certain conditions the proposed approach can improve state-of-the-art iteration complexity, and empirically demonstrate it can substantially improve the convergence of existing methods.

2 Minibatch Stochastic Variance Reduced Proximal Iterations

In this section we present the proposed approach for minimizing (1). The high-level description is given in Algorithm 1, which consists of two main innovations: i) simultaneous incorporation of first-order and higher-order information via sub-sampling; ii) allowing larger minibatch sizes through acceleration with inexact minimization. We explain these features below.

Sampling both First-order and Higher-order Information

We first discuss the main building block of the algorithm. Suppose at iteration t , given the previous iterate w_{t-1} , we consider the following update rule:

$$w_t \approx \arg \min_w \frac{1}{2} (w - w_{t-1})^\top \left(\frac{1}{b} \sum_{i \in \bar{B}} \nabla^2 f_i(w_{t-1}) \right) (w - w_{t-1}) + \frac{\tilde{\lambda}}{2} \|w - w_{t-1}\|^2 + \left\langle \frac{\eta}{b} \sum_{i \in B_t} \nabla f_i(w_{t-1}) + \eta \nabla f(\tilde{w}) - \frac{\eta}{b} \sum_{i \in B_t} \nabla f_i(\tilde{w}), w \right\rangle \quad (3)$$

$$= w_{t-1} - \eta \left(\frac{1}{b} \sum_{i \in \bar{B}} \nabla^2 f_i(w_{t-1}) + \tilde{\lambda} I \right)^{-1} \left(\frac{1}{b} \sum_{i \in B_t} \nabla f_i(w_{t-1}) + \nabla f(\tilde{w}) - \frac{1}{b} \sum_{i \in B_t} \nabla f_i(\tilde{w}) \right), \quad (4)$$

where \bar{B}, B_t are some randomly sampled minibatch from $1, \dots, n$, both with minibatch size b ; η and $\tilde{\lambda}$ are stepsize parameters, and \tilde{w} is a ‘‘reference’’ predictor used for reducing variance. The main feature of updating rule (3) is it considered both noisy first-order and higher-order information via minibatch sampling. The term $\frac{1}{b} \sum_{i \in \bar{B}} f_i(w) - \langle \frac{1}{b} \sum_{i \in \bar{B}} \nabla f_i(w_{t-1}), w \rangle$ in (3) incorporates noisy higher-order information of the objective function. It which can be treated as a variant of sub-sampled Newton method, combined with the minibatch stochastic gradient with variance reduction. And the update rule (3) can be treated as a preconditioned minibatch SVRG update rule, with $\left(\frac{1}{b} \sum_{i \in \bar{B}} \nabla^2 f_i(w_{t-1}) + \tilde{\lambda} I \right)^{-1}$ as a precondition matrix.

Large Minibatch Size via Acceleration with Inexact Minimization

Using (3) as the building block, we propose the MB-SVRP (minibatch stochastic variance reduced proximal iterations) method, which is detailed in Algorithm 1. At the beginning of the algorithm, we form a minibatch \bar{B} by sampling from $1, \dots, n$ and fix it for the whole optimization process. Then following the SVRG method johnson2013accelerating, the algorithm is divided to multiple stages, indexed by s . At each stage, we iteratively solve a minimization problem of the form (2) based on the randomly sampled minibatch B_t .

Compared with the simple update rule in (3), the major difference in Algorithm 1 is that we consider a momentum scheme by maintaining two sequences $\{w_t, y_t\}$, which is inspired by Nesterov’s acceleration technique nesterov2003introductory and its recent SVRG variant nitanda2014stochastic. The main theoretical advantage over minibatch SVRG without momentum konevny2016mini is that such an acceleration allows us to use a much larger minibatch size (up to a size of $O(\sqrt{n})$) without slowing down the convergence.

Since it is often expensive to find the exact minimizer of (2), we consider an approximate minimizer with objective suboptimality ε . When we choose the appropriate $\tilde{\lambda}$ for $\tilde{f}_t(w)$ to obtain enough strong convexity, the subproblems can be efficiently solved to high accuracy efficiently. For example, using SVRG-type algorithms johnson2013accelerating to solve (2) allows us to find an approximate solution with a small suboptimality ε with a constant number of passes over the data in the minibatch $\bar{B} \cup B_t$, if $\tilde{\lambda}$ is set appropriately.

3 Theoretical Results

Besides the strong convexity and smoothness, we also need the following Hessian Lipschitz condition, and the notion of effective dimension and statistical leverage.

Condition 1. For each component function $f_i(w), \forall i \in [n]$, its Hessian matrix is M -Lipschitz, i.e.

$$\|\nabla^2 f_i(w) - \nabla^2 f_i(w')\| \leq M \|w - w'\|, \forall w, w' \in \mathbb{R}^d, \forall i \in [n].$$

Definition 1. (Effective dimension) Let the $\lambda_1, \dots, \lambda_d$ be the top- d eigenvalues of $H_0(w^*) = (1/n) \sum_{i=1}^n \ell''(w^{*\top} x_i; b_i) x_i x_i^\top$, define the effective dimension $d_{\tilde{\lambda}}$ (for some $\tilde{\lambda} \geq 0$) of $H_0(w^*)$ being $d_{\tilde{\lambda}} = \sum_{j=1}^d \frac{\lambda_j}{\lambda_j + \tilde{\lambda}}$.

Table 1: Comparison of iteration complexity of various finite-sum quadratic optimization algorithms when effective dimension and statistical leverage are bounded, where we compare the different relative scale of condition number $\kappa = L/\lambda$ and sample size n , ignoring logarithmic factors.

	$\kappa \leq n$	$\kappa = n^{4/3}$	$\kappa = n^{3/2}$	$\kappa = n^2$	$\kappa = n^3$
SVRG	n	$n^{4/3}$	$n^{3/2}$	n^2	n^3
MB-SVRP	n	$\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} \cdot n$	$\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} \cdot n$	$\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} \cdot n^{3/2}$	$\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} \cdot n^{5/2}$
Acc-SVRG	n	$n^{7/6}$	$n^{5/4}$	$n^{3/2}$	n^2
Acc-MB-SVRP	n	$\left(\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}}\right)^{1/2} \cdot n$	$\left(\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}}\right)^{1/2} \cdot n$	$\left(\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}}\right)^{1/2} \cdot n^{5/4}$	$\left(\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}}\right)^{1/2} \cdot n^{7/4}$

Definition 2. (*Statistical leverage at $\tilde{\lambda}$*) Let $H_{\tilde{\lambda}}(w^*) = \frac{1}{n} \sum_{i=1}^n \ell''(w^{*\top} x_i; b_i) x_i x_i^\top + \tilde{\lambda} I$, we say the statistical leverage of data matrix X is bounded by $\rho_{\tilde{\lambda}}$ at $\tilde{\lambda}$ if

$$\max_{i \in [n]} \frac{\|H_{\tilde{\lambda}}^{-1/2}(w^*) \ell''(w^{*\top} x_i; b_i)^{1/2} x_i\|}{\sqrt{(1/n) \sum_{j=1}^n \|H_{\tilde{\lambda}}^{-1/2}(w^*) \ell''(w^{*\top} x_j; b_j)^{1/2} x_j\|^2}} \leq \rho_{\tilde{\lambda}}.$$

Theorem 3. Consider Algorithm 1 on problems with L -smooth and λ -strongly convex functions that satisfied Condition 1 with Hessian Lipschitz parameter M . Suppose we sample minibatch \bar{B} uniformly from $1, \dots, n$, and set the tuning parameters as

$$\tilde{\lambda} = \max \left\{ \lambda, \frac{L}{b} \right\}, \quad b \asymp \min \left\{ n, \rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} \left(\frac{L}{\lambda} \right)^{1/3} \right\}, \quad \eta \asymp \min \left\{ \frac{b^3 \lambda}{(\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}})^2 L}, \frac{1}{\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}}} \right\},$$

and suppose we start from the initialization point that is sufficiently close to the optimum: $\|w_0 - w^*\| \leq R = \mathcal{O}\left(\frac{\lambda^4}{L^2 M}\right)$. Given $\epsilon > 0$, and let $\varepsilon \leq \frac{1}{10^5} \cdot \left(\frac{\lambda}{L}\right)^7 \epsilon$. Then for the MP-SVRP algorithm to find the approximate solution \tilde{w}_s of (1) that reaches the expected ϵ -objective suboptimality $\mathbb{E}f(\tilde{w}_s) - \min_w f(w) \leq \epsilon$, the total number of oracle calls to solve (2) is no more than

$$\mathcal{O} \left(\max \left\{ \left(\frac{L}{\lambda} \right)^{1/3}, \frac{\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} L}{\lambda n^2} \right\} \cdot \log \left(\frac{1}{\epsilon} \right) \right).$$

Note that in Algorithm 1, we can use SVRG to solve each subproblem in (2). This leads to the following result.

Corollary 4. Assume that the conditions of Theorem 3 hold. Moreover, if we use SVRG to solve each subproblem in (2) up to the suboptimality ε , then the total number of gradient evaluations used in the whole MP-SVRP algorithm can be upper bounded by

$$\mathcal{O} \left(\max \left\{ \rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} \left(\frac{L}{\lambda} \right)^{2/3}, \frac{\rho_{\tilde{\lambda}}^2 d_{\tilde{\lambda}} L}{\lambda n} \right\} \cdot \log \left(\frac{L}{\lambda} \right) \cdot \log^2 \left(\frac{1}{\epsilon} \right) + n \cdot \log \left(\frac{1}{\epsilon} \right) \right).$$

Acceleration Corollary 4 stated that if the condition number is not too large: $\frac{L}{\lambda} \leq n^{5/4}$, then MB-SVRP only requires logarithmic passes over data to find a solution with high accuracy. When the condition number is large, MP-SVRP can still be slow. By using the accelerated proximal point framework proposed in shalev2016accelerated, frostig2015regularizing, lin2015universal, it is possible to obtain an accelerated convergence rate which has milder dependence on condition number, Table 1 summarized the main results.

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