Improved SVRG for quadratic functions

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Abstract

We analyse an iterative algorithm to minimize quadratic functions whose Hessian matrix $H$ is the expectation of a random symmetric $d \times d$ matrix. The algorithm is a variant of the stochastic variance reduced gradient (SVRG). In several applications, including least-squares regressions, ridge regressions, linear discriminant analysis and regularized linear discriminant analysis, the running time of each iteration is proportional to $d$. Under smoothness and convexity conditions, the algorithm has linear convergence. When applied to quadratic functions, our analysis improves the state-of-the-art performance of SVRG up to a logarithmic factor. Furthermore, for well-conditioned quadratic problems, our analysis improves the state-of-the-art running times of accelerated SVRG, and is better than the known matching lower bound, by a logarithmic factor. Our theoretical results are backed with numerical experiments.

Keywords: least-squares regression, ridge regression, linear discriminant analysis, stochastic gradient descent, Hessian matrix.

1 Introduction

The recent availability of massive volumes of data fosters the need to design computationally efficient algorithms for optimization in high dimensions. In large-scale machine learning, stochastic gradient descent (SGD) algorithms are among the most effective optimization methods (Bottou, Curtis and Nocedal 2018). For strongly-convex functions, i.e., when the smallest eigenvalue of the Hessian matrix is bounded away from 0, averaged SGD achieves the rate of convergence of $O(1/k)$ after $k$ iterations (Nemirovski, Juditsky, Lan and Shapiro 2009). The stochastic average gradient method (SAG) of Roux, Schmidt and Bach (2012) optimizes the sum of $n$ convex functions with a linear convergence rate (i.e., a rate that decreases exponentially with the number of iterations) in the strongly-convex case. Alternative variance-reduced SGD algorithms include stochastic dual coordinate ascent (SDCA) (Shalev-Shwartz and Zhang 2013) and stochastic variance reduced gradient (SVRG) (Johnson and Zhang 2013). SGD and variance-reduced SGD algorithms typically minimize a real-valued function $f$ of the form

$$f(\theta) = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta),$$  \hspace{1cm} (1.1)

where $\theta$ is a $d$-dimensional column vector and each $f_i$ is convex and $L_i$-smooth. In least-squares regressions, for instance, $f_i(\theta) = (x_i \theta - y_i)^2/2$, where $x_i$ is the $i$-th row of an $n \times d$ matrix $X$, and $y_i$ is the $i$-th coordinate of an $n$-dimensional column vector $Y$. Using similar notation, for ridge regressions, $f_i(\theta) = (x_i \theta - y_i)^2/2 + \lambda \|\theta\|^2/2$, where $\lambda$ is a positive constant. We will concentrate on the case where $f$ is $\mu$-convex. To approximately minimize $f$, SGD uses the recursion

$$\theta_{k+1} := \theta_k - \alpha f'_i(\theta_k),$$  \hspace{1cm} (1.2)

$k \geq 0$, where $\alpha$ is a suitable step-size and $i$ is chosen uniformly at random in $\{1, \ldots, n\}$. Basic variance-reduced SGD algorithms replace $f'_i$ in $\mathbf{12}$ with a variance-reduced stochastic gradient. For instance, the SVRG algorithm uses several epochs. At the beginning of each epoch, a full gradient is calculated and is used to generate variance-reduced stochastic gradients throughout the epoch. Basic variance-reduced algorithms typically achieve precision $\epsilon$ in $O((n + \kappa_{\text{max}}) \log(1/\epsilon))$ stochastic gradient computations, where $\kappa_{\text{max}} := \max_i (L_i/\mu)$. Xiao and Zhang (2014) show that a version of SVRG with non-uniform sampling achieves precision $\epsilon$ in $O((n + \kappa_{\text{avg}}) \log(1/\epsilon))$ stochastic gradient computations, where

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\( \kappa_{\text{avg}} := (1/n) \sum_{i=1}^{n} L_i / \mu. \) Variants of SVRG are analysed in (Hofmann, Lucchi, Lacoste-Julien and McWilliams 2015, Allen-Zhu and Yuan 2016, Lei and Jordan 2017, Sebbouh, Gazagnadou, Jelassi, Bach and Gower 2019, Kulunchakov and Mairal 2020). Recently, Kovalev, Horváth and Richtárik (2020) developed L-SVRG, a loopless version of SVRG that does not require the knowledge of the condition number and achieves precision \( \epsilon \) in \( O((n + \kappa_{\text{max}}) \log(1/\epsilon)) \) stochastic gradient computations. Accelerated variance-reduced SGD methods are analysed in (Shalev-Shwartz and Zhang 2014, Nitanda 2014, Allen-Zhu 2018, Lan and Zhou 2018, Kovalev, Horváth and Richtárik 2020). In particular, Allen-Zhu (2018) provides an accelerated extension of SVRG that achieves precision \( \epsilon \) in \( O((n + \sqrt{n \kappa_{\text{max}}}) \log(1/\epsilon)) \) stochastic gradient computations. This matches the lower bound given by Lan and Zhou (2018). Gower, Schmidt, Bach and Richtarik (2020) provide a recent review on variance-reduced optimization algorithms for machine learning.

Several optimization problems that arise in scientific computing and data analysis involve the minimization of quadratic functions of the form

\[
f(\theta) = \frac{1}{2} \theta^T H \theta - c^T \theta, \tag{1.3}
\]

where \( H \) is a positive definite \( d \times d \) matrix, \( c \) is a \( d \)-dimensional column vector, and \( \theta \) ranges over all \( d \)-dimensional column vectors. This paper assumes that \( f \) is \( \mu \)-convex with \( \mu > 0 \), and that \( H = E(Q) \), where \( Q \) is a random symmetric \( d \times d \) matrix with \( E(\theta^2) \leq LH \), where \( L > 0 \) is a known constant. The latter condition holds if the eigenvalues of \( Q \) are between 0 and \( L \). As shown in Section 3, this framework is suitable to several applications including least-squares regressions, ridge regressions, linear discriminant analysis and regularized linear discriminant analysis. These methods are widely used for inference and prediction, and many of the modern machine learning techniques such as the logistic regression, the lasso method and neural networks can be considered as extensions of these techniques. As \( f'(\theta) = H \theta - c \), a stochastic gradient of \( f \) is \( Q \theta - c \). We introduce Q-SVRG, a variant of the SVRG algorithm adapted to quadratic functions, to minimize \( f \) at an arbitrary precision. The algorithm Q-SVRG does not require the explicit computation of \( H \). It is similar to the variant of SVRG developed by Xiao and Zhang (2014), and consists of \( l \) epochs each comprising \( m \) inner iterations. A full gradient is calculated at the beginning of every epoch, and each inner iteration calculates a stochastic gradient. In the aforementioned applications, the calculation of the full gradient takes \( O(n d) \) time, and the running time of each inner iteration of Q-SVRG is \( O(d) \). Non-uniform sampling is handled by Q-SVRG in a straightforward manner by choosing a non-uniform distribution for \( Q \). The theoretical design and analysis of SVRG in (Xiao and Zhang 2014) and of Q-SVRG is based on the average of iterates, and so do our numerical experiments on Q-SVRG. Xiao and Zhang (2014) use however the last iterate in their numerical experiments on SVRG. Q-SVRG enjoys the following properties:

1. For any fixed \( l \geq 1 \), Q-SVRG achieves a rate of convergence of \( O((\kappa/m)^l) \) with \( l \) epochs comprising \( m \) inner iterations each, where \( \kappa := L/\mu \) is the condition number, and can be simulated without the knowledge of \( \mu \). In contrast, for any fixed number of epochs, the analysis in (Xiao and Zhang 2014) implies a constant optimality gap when the number of inner iterations goes to infinity. For least-squares and ridge regressions with constant \( \kappa \), Q-SVRG achieves precision \( \epsilon = O(n^{-1}) \) in \( O(nd) \) total time. We are not aware of any previous result showing such time-accuracy tradeoff.

2. When \( \mu \) is known and the calculation of a full gradient of \( f \) requires \( n \) stochastic gradients, Q-SVRG has linear convergence and achieves precision \( \epsilon \) in

\[
O(\frac{n + \kappa}{\max(1, \log(n/\kappa))} \log \frac{1}{\epsilon})
\]

stochastic gradient computations. This improves the state-of-the-art performance of SVRG (Xiao and Zhang 2014) up to a logarithmic factor. When \( \kappa \) is constant, the gradient-complexity of Q-SVRG outperforms that of SVRG in (Xiao and Zhang 2014), accelerated SVRG in (Allen-Zhu 2018), and is better than the aforementioned lower bound of Lan and Zhou (2018), by a factor of order \( \log(n) \). This lower bound was established for a quadratic objective function that falls into the framework and a class of randomized gradient methods which sequentially calculate the gradient of a random component function. This class does not include, stricto sensu, Q-SVRG, which acquires the full gradient at the beginning of every epoch. Thus the Lan and Zhou (2018) complexity lower bound does not apply to Q-SVRG.

3. The theoretical analysis of Q-SVRG allows a step-size of length up to \( 1/L \). This is larger by a multiplicative constant than step-sizes given by previous theoretical analysis of variance-reduced methods.
1.1 Other related work

An exact solution to the least-squares regression problem can be found in $O(nd^2)$ time (Golub and Van Loan 2013). Rokhlin and Tygert (2008) describe a randomized algorithm based on a preconditioning matrix that minimizes least-squares regressions with relative precision $\epsilon$ in $O(d^3 + nd\log(d/\epsilon))$ time, for $\epsilon > 0$. For non-strongly-convex linear regressions, Bach and Moulines (2013) show a convergence rate of $O(1/k)$ after $k$ iterations for an averaged SGD algorithm with constant step-size in an on-line setting. Gower and Richtárik (2015) describe a randomized iterative method with a linear rate for solving linear systems, that is also applicable to least squares regressions. However, when applied to least squares, a naive implementation of their iterative step requires $O(nd)$ time. This can be reduced to $O(d)$ time if $X^T X$ is precomputed, which takes $O(nd^2)$ time. Pilanci and Wainwright (2016) provide algorithms for constrained least-squares through a random projection on a lower dimensional space. They show how to minimize least-squares regressions with relative precision $\epsilon$ in $O(nd\log(d) + d^3\log(1/\epsilon))$ time. Dieuleveut, Flammarion and Bach (2017) study an averaged accelerated regularized SGD algorithm for least-squares regressions. Mini-batching and tail-averaging SGD algorithms for least-squares regressions are analyzed by Jain, Kakade, Kidambi, Netrapalli and Sidford (2018). Our updating rule is similar to the recursion used by Kahalé (2019) to approximately simulate high-dimensional Gaussian vectors with a given covariance matrix. Loizou and Richtárik (2020) provide stochastic algorithms with linear rates to minimize the expectation of a random quadratic function. In their framework, however, stochastic gradients vanish at the optimum, which is not the case in our setting. The remainder of the paper is organized as follows. Section 2 describes Q-SVRG and its properties. Section 3 describes applications of Q-SVRG. Section 4 gives numerical experiments. Section 5 contains concluding remarks. Omitted proofs are in the supplementary material. The running time refers to the number of arithmetic operations.

2 The algorithm description and properties

Let $I$ denote the $d \times d$ identity matrix. This section makes the following assumptions.

Assumption 1 (A1). $H \preceq \mu I$, where $\mu$ is a positive constant.

Assumption 2 (A2). There is a random sequence $(Q_k : k \geq 0)$ of independent symmetric $d \times d$ matrices such that $E(Q_k) = H$ and $E(Q_k^2) \leq LH$.

Define the condition number $\kappa := L/\mu$. Let $t_H$ (resp. $t_Q$) be the time needed to calculate $H\theta$ (resp. $Q_k\theta$) for a given $d$-dimensional vector $\theta$. Assumption A1 implies that $H$ is invertible and that $\mu$ is smaller than the smallest eigenvalue of $H$. A2 implies that $H \preceq LI$. Conversely, if A1 holds and $H \preceq LI$, then A2 trivially holds by choosing $Q_k = H$ for $k \geq 0$. Our applications, though, use matrices $Q_k$ such that $t_Q$ is much larger than $t_H$, which is typically of order $d$.

Given an initial $d$-dimensional column vector $\theta_0$ and a real number $\alpha \in (0, 1/L]$, define the sequence of $d$-dimensional column vectors $(\theta_k : k \geq 0)$ via the recursion

$$\theta_{k+1} := \theta_k - \alpha(Q_k(\theta_k - \theta_0) - c + H\theta_0),$$

for $k \geq 0$. As $f'(\theta) = H\theta - c$ and, by A2,

$$E(Q_k(\theta_k - \theta_0) - c + H\theta_0|\theta_k) = H\theta_k - c,$$

(2.1) can be viewed as a variant of SGD. Since $Q_k(\theta_k - \theta_0)$ is equal to the difference between the stochastic gradients $Q_k\theta_k - c$ and $Q_k\theta_0 - c$, (2.1) can be considered as a variance-reduced SGD, and is essentially the same recursion used in the inner iteration of SVRG (Johnson and Zhang 2013). For $k \geq 1$, let

$$\tilde{\theta}_k := \frac{\theta_0 + \cdots + \theta_{k-1}}{k}.$$

Thus, the calculation of $\tilde{\theta}_k$ takes $O(t_H + kd + kt_Q)$ time and involves one full gradient and $k$ stochastic gradient computations (following the literature convention on variance-reduced SGD methods applied to quadratic problems, we consider that calculating $Q_k(\theta_k - \theta_0)$ involves one, rather than two, stochastic gradient computations).
Given $m \geq 1$, let $T_m$ be the random operator that maps any $d$-dimensional column vector $\theta_0$ to $\bar{\theta}_m$. For $l \geq 1$, denote by $T_{lm}$ the random operator on the set of $d$-dimensional column vectors obtained by composing $l$ times the operator $T_m$. Thus, calculating $T_{lm}(\theta)$ from $\theta$ takes $O((lH + md + mtQ))$ time and involves $l$ full gradient and $lm$ stochastic gradient computations. Algorithm 1 gives a pseudo-code that outputs $T_{lm}(0)$.

**Algorithm 1** Procedure Q-SVRG

```
procedure Q-SVRG($\alpha$, $m$, $l$)
    $\theta_0 \leftarrow 0$
    for $h \leftarrow 1, l$
        $\tilde{c} \leftarrow c - H\theta_0$
        for $k \leftarrow 0, m - 1$
            $\theta_{k+1} = \theta_k - \alpha(Q_k(\theta_k - \theta_0) - \tilde{c})$
        end for
        $\theta_0 \leftarrow (\theta_0 + \cdots + \theta_{m-1})/m$
    end for
    return $\theta_0$
end procedure
```

2.1 The worst-case analysis

As $H$ is invertible, there is a unique $d$-dimensional column vector $\theta^*$ such that

$$H\theta^* = c. \quad (2.2)$$

By a standard calculation, for any $d$-dimensional column vector $\theta$,

$$f(\theta) - f(\theta^*) = \frac{1}{2} \left( \| \theta - \theta^* \|_2^2 - \| (\theta - \theta^*)H(\theta - \theta^*) \|_2^2 \right), \quad (2.3)$$

and so $f$ attains its minimum at $\theta^*$. Theorem 2.1 analyses the convergence properties of Q-SVRG.

**Theorem 2.1.** Assume that $A1$ and $A2$ hold. Let $\theta^*$ be the unique $d$-dimensional vector satisfying (2.2). Then, for any $\theta \in \mathbb{R}^d$, $\alpha \in (0, 1/L]$, $l \geq 1$, and $m \geq 1$,

$$E(f(T_{lm}(\theta))) - f(\theta^*) \leq \left( \frac{9}{\alpha \mu m} \right)^l (f(\theta) - f(\theta^*)). \quad (2.4)$$

The proof of Theorem 2.1 follows by induction on $l$ and bounding separately bias and variance terms. As (2.3) implies that

$$\| \theta - \theta^* \|_2^2 \leq \frac{2}{\mu} (f(\theta) - f(\theta^*)), \quad (2.5)$$

it follows from Theorem 2.1 that

$$E(\| T_{lm}(\theta_0) - \theta^* \|_2^2) \leq \frac{2}{\mu} \left( \frac{9}{\alpha \mu m} \right)^l (f(\theta_0) - f(\theta^*)).$$

When $A1$ and $A2$ hold and $\alpha = 1/L$, Theorem 2.1 implies that $E(f(T_{lm}(\theta_0))) - f(\theta^*) = O((\kappa/m)^l)$ as $m$ goes to infinity, for any fixed $l \geq 1$. Observe that $T_{lm}(\theta)$ can be simulated without the explicit knowledge of $\mu$.

Assume now that $\mu$ is known and that one full gradient is a weighted sum of $n$ stochastic gradients, with known weights. The latter condition implies that each epoch with $m$ inner iterations involves $n + m$ stochastic gradient calculations. This condition holds in several applications with $n$ data points (see Section 3). Set $\alpha = 1/L$. By Theorem 2.1, Q-SVRG minimizes $f$ with expected error $\epsilon$ with $l$ epochs, each containing $m$ inner iterations, where $m = 9 \max(e \kappa, n)$ and

$$l = \frac{1}{\max(1, \log(n/\kappa))} \log \frac{f(\theta_0) - f(\theta^*)}{\epsilon}.$$
Thus, the total number of stochastic gradient computations required by Q-SVRG to minimize $f$ with expected error $\epsilon$ is
\[
N_\epsilon \leq l(n + m) = \frac{n + \kappa}{\max(1, \log(n/\kappa))} \log \frac{f(\theta_0) - f(\theta^*)}{\epsilon}.
\]
This improves the $O((n + \kappa)\log(1/\epsilon))$ gradient-complexity of SVRG (Xiao and Zhang 2014) up to a logarithmic factor. In particular, when $\kappa$ is constant,
\[
N_\epsilon = O\left(\frac{n}{\log(n)} \log \frac{1}{\epsilon}\right),
\]
which is better than the gradient-complexity of SVRG in (Xiao and Zhang 2014), accelerated SVRG in (Allen-Zhu 2018), and the aforementioned lower bound of Lan and Zhou (2018), by a factor of order $\log(n)$.

3 Examples

This section gives examples where A1 and A2 hold.

3.1 Least-squares regression

Given an $n \times d$ matrix $X$ with rank $d$ and an $n$-dimensional column vector $Y$, the least-squares regression consists of minimizing the function $g(\theta) := (2n)^{-1}\|X\theta - Y\|^2$, where $\theta$ ranges over all $d$-dimensional column vectors. This problem can be reduced to (3.2) by setting $H := \text{tr}(X^T X)^{-1}X^T X$ and $c := \text{tr}(X^T X)^{-1}X^T Y$, which implies that $g(\theta) = \tilde{L}f(\theta) + g(0)$, where $\tilde{L} := \text{tr}(X^T X)/n$ is the average squared norm of a line of $X$. As $H$ and $X$ have the same rank, $H$ is invertible and A1 holds with $\mu$ being the smallest eigenvalue of $H$. For $1 \leq i \leq n$, let $e_i$ be the $n$-dimensional column vector whose $i$-th component is 1 and remaining components are 0, and let
\[
p_i = \frac{\|X^T e_i\|^2}{\text{tr}(X^T X)}.
\]
Note that the numerator in (3.1) is the sum of the squared entries of the $i$-th line of $X$, while the denominator is the sum of squared entries of $X$. Thus the $p_i$'s sum up to 1. Let $(i(k) : k \geq 0)$ be a sequence of independent integral random variables on $\{1, \ldots, n\}$ such that, for $1 \leq j \leq n$,
\[
\Pr(i(k) = j) = p_j.
\]
For $k \geq 0$, let $u_k := \|X^T e_{i(k)}\|^{-1}(X^T e_{i(k)})$ and $Q_k := u_k u_k^T$. As $u_k$ is a unit vector, the largest eigenvalue of $Q_k$ is equal to 1. Furthermore, by the definition of $u_k$,
\[
E(Q_k) = \sum_{j=1}^{n} p_j\|X^T e_j\|^{-2}(X^T e_j e_j^T X) = \frac{1}{\text{tr}(X^T X)}X^T(\sum_{j=1}^{n} e_j e_j^T)X = H.
\]
The second equation follows from (3.1), and the last one by observing that $\sum_{j=1}^{n} e_j e_j^T$ is the $n \times n$ identity matrix. Thus A2 holds with $L = 1$. The recursion (2.1) becomes
\[
\theta_{k+1} = \theta_k - \alpha((u_k^T \theta_k - \theta_0))u_k - c + H\theta_0,
\]
for $k \geq 0$.

As $X^T e_i$ is the $i$-th column of $X^T$, for $1 \leq i \leq n$, the total time to calculate $c$, $H\theta_0$, and the $p_i$'s is $O(nd)$. After an initial preprocessing cost of $O(n)$, the random variable $i(k)$ can be simulated in constant time using the alias method (Devroye 1986, Section III.4). Thus the cost of each iteration in (2.1) is $O(d)$. Algorithm 2 gives a pseudo-code for the Q-SVRG algorithm applied to least-squares regressions.
Algorithm 2 Procedure Q-SVRG for least squares regression

\begin{algorithm}
\begin{algorithmic}
\Procedure{Q-SVRG}{$\alpha, m, l$}
\For{$i \leftarrow 1, n$}
    \State $p_i \leftarrow ||X^T e_i||^2 / \text{tr}(X^T X)$
\EndFor
\State $\theta_0 \leftarrow 0$
\For{$h \leftarrow 1, l$}
    \State $\tilde{c} \leftarrow \text{tr}(X^T X)^{-1}X^T (y - X \theta_0)$
    \For{$k \leftarrow 0, m - 1$}
        \State Sample $i(k)$ from \{1, \ldots, $n$\} such that $\Pr(i(k) = j) = p_j$ for $1 \leq j \leq n$
        \State $u_k \leftarrow ||X^T e_{i(k)}||^{-1}(X^T e_{i(k)})$
        \State $\theta_{k+1} = \theta_k - \alpha(u_k^T (\theta_k - \theta_0)) - \tilde{c}$
    \EndFor
    \State $\theta_0 \leftarrow (\theta_0 + \cdots + \theta_{m-1})/m$
\EndFor
\State \Return $\theta_0$
\EndProcedure
\end{algorithmic}
\end{algorithm}

As $Q_k \theta = u_k^T (u_k^T \theta)$, we have $t_Q = O(d)$. Moreover, $t_H = O(nd)$. It follows from (3.2) that one full gradient is a weighted sum of $n$ stochastic gradients.

The recursion (3.3) uses a non-uniform sampling scheme with sampling probabilities determined by the squared norm of each row vector. A similar sampling scheme has been applied by Frieze, Kannan and Vempala (2004) in the context of low-rank approximations of a matrix, by Strohmer and Vershynin (2009) to approximately solve linear systems via an iterative algorithm, and by Défossez and Bach (2015) to design an averaged SGD for least-squares regressions. However, while the updating rule of the conventional SGD, of Strohmer and Vershynin (2009) and of Défossez and Bach (2015) uses a single random coordinate of $Y$, (3.3) uses the vector $c$ that depends on the entire vector $Y$. Strohmer and Vershynin (2009) establish a linear convergence rate for their method in the strongly-convex case. Défossez and Bach (2015) give a detailed asymptotic analysis (as the number of iterations goes to infinity) of their algorithm.

3.2 Ridge regression

Given a non-zero $n \times d$ matrix $X$, an $n$-dimensional column vector $Y$, and $\lambda > 0$, the ridge regression consists of minimizing the function

$$g(\theta) := \frac{1}{2n} ||X \theta - Y||^2 + \frac{\lambda}{2} ||\theta||^2,$$

where $\theta$ ranges over all $d$-dimensional column vectors. This problem can be reduced to (1.3) by setting

$$H := (\lambda + \bar{L})^{-1}(\lambda I + n^{-1}X^T X)$$

and $c := (\lambda n + \bar{L}n)^{-1}X^T Y$, where $\bar{L} := \text{tr}(X^T X)/n$, which implies that $g(\theta) = (\lambda + \bar{L}) f(\theta) + g(0)$. As $X^T X$ is symmetric positive semidefinite, A1 holds with $\mu = \lambda/(\lambda + \bar{L})$. Let

$$Q_k := (\lambda + \bar{L})^{-1}(\lambda I + Lu_k u_k^T),$$

where $u_k$ is defined as in Section 3.1. Then $Q_k \leq I$ and $E(Q_k) = H$. Thus A2 holds with $L = 1$. An analysis similar to the one in Section 3.1 shows that, after a total preprocessing cost of $O(nd)$, the cost of each iteration in (2.1) is $O(d)$. Furthermore, $t_Q = O(d)$ and $t_H = O(nd)$, and one full gradient is a weighted sum of $n$ stochastic gradients. Thus the Q-SVRG algorithm with $\alpha = 1$ and $m = 9 \max(c(\lambda + \bar{L})/\lambda, n)$ has a linear convergence rate.

3.3 Linear discriminant analysis

Consider $d$-dimensional column vectors $x_1, \ldots, x_n$, where $x_i$ belongs to class $g(i)$, with $g(i) \in \{1, \ldots, K\}$. For $1 \leq k \leq K$, let $n_k$ be the number of observations in class $k$, and let

$$\bar{\mu}_k := \frac{1}{n_k} \sum_{i : g(i) = k} x_i$$
Table 1: datasets used in the simulations

|         | Variables | Data Points |
|---------|-----------|-------------|
| sonar   | 60        | 208         |
| madelon | 500       | 2000        |
| sido0   | 4932      | 12678       |

be their average. Assume that the $d \times d$ matrix

$$\hat{\Sigma} := \frac{1}{n-K} \sum_{i=1}^{n} (x_i - \hat{\mu}_g(i))(x_i - \hat{\mu}_g(i))^T$$

is invertible. The linear discriminant analysis method (Hastie, Tibshirani and Friedman 2009, Section 4.3) classifies a $d$-dimensional column vector $x$ by calculating the linear discriminant functions

$$\delta_k(x) = (x - \frac{1}{2} \hat{\mu}_k)^T \hat{\Sigma}^{-1} \hat{\mu}_k + \log(n_k/n),$$

$1 \leq k \leq K$. Then $x$ is assigned to $\arg \max_k \delta_k(x)$. Note that

$$\text{tr}(\hat{\Sigma}) = \frac{1}{n-K} \sum_{i=1}^{n} (x_i - \hat{\mu}_g(i))^T (x_i - \hat{\mu}_g(i))$$

can be calculated in $O(nd)$ time. Given $k \in \{1, \ldots, K\}$, let $H := \text{tr}(\hat{\Sigma})^{-1}\hat{\Sigma}$ and $c := \text{tr}(\hat{\Sigma})^{-1}\hat{\mu}_k$. Then

$$\hat{\Sigma}^{-1}\hat{\mu}_k = \arg \min f,$$

where $f$ is given by (1.3). As $\hat{\Sigma} = X^TX$, where $X$ is the $n \times d$ matrix whose $i$-th line is $(n-K)^{-1/2}(x_i - \hat{\mu}_g(i))^T$, the function $f$ can be minimized via (2.1) using the approach outlined in Section 3.1. Here again, $t_Q = O(d)$ and $t_H = O(nd)$, and one full gradient is a weighted sum of $n$ stochastic gradients. Regularized linear discriminant analysis can be treated in a similar way.

4 Numerical experiments

Our numerical experiments were conducted for ridge regressions on the sonar\(^1\), madelon\(^2\) and sido0\(^2\) binary datasets, whose characteristics are summarized in Table 1. The variables were centered, a constant variable was added to each dataset, and all variables were normalized. The codes were written in the C++ programming language, the compiler used was Microsoft Visual C++ 2013, and the experiments were performed on a laptop PC with an Intel processor and 8 GB of RAM running Windows 10 Professional. For each dataset, we have implemented the following methods using the null vector as starting point and the notation in Section 3.2:

- the averaged SGD algorithm with uniform sampling and step-size $1/(4(\lambda + \max_{1\leq i \leq n} ||X^T e_i||^2))$, adapted from (Bach and Moulines 2013).
- the averaged SGD algorithm with non-uniform probabilities adapted from (Défossez and Bach 2015), with step-size $1/(\lambda + \bar{L})$.
- the SAG algorithm with non-uniform probabilities adapted from (Schmidt, Le Roux and Bach 2017), with step-size $1/(\lambda + \bar{L})$, where the lines are sampled according to the $p_i$’s, and the output is the vector among the final iterate and the average of iterates that minimizes $g$.
- the SVRG algorithm with non-uniform probabilities. Following the experimental recommendations of Xiao and Zhang (2014), each epoch comprises $2n$ inner iterations, outputs the final iterate, and the step-size is $0.1/(\lambda + \bar{L})$.
- the L-SVRG method with uniform sampling as described by Kovalev, Horváth and Richtárik (2020), with average epoch-length $n$ and step-size $1/(6(\lambda + \max_{1\leq i \leq n} ||X^T e_i||^2))$.

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1 http://archive.ics.uci.edu

2 http://www.causality.inf.ethz.ch
A limitation of Q-SVRG is that it is applicable only to quadratic problems. SVRG, and is better than the matching lower bound of Lan and Zhou (2018), by a logarithmic factor. Furthermore, when \( \kappa \) convergence rate and improves the previously known running time of SVRG by up a logarithmic factor.

\[
\text{Number of effective passes} = \frac{\bar{m}}{n}, \quad \lambda \frac{\bar{m}}{\bar{m}}(0) \text{ via Algorithm 1, with } m = [N/l], \quad \alpha = 1.
\]

Thus, ignoring integrality constraints, \( m = \min(N/4, \max(n, L/\lambda)) \). The second argument of the min function is within a constant factor from the value of \( m \) suggested in Section 3.2.

The lower bound 4 on \( l \) was chosen after running a few computer simulations.

The results are reported in Figure 1. The running time is measured by the number of effective passes, defined as the total number of stochastic gradients divided by \( n \). Each iteration of the averaged SGD and SAG methods accounts for one stochastic gradient, while each epoch of the SVRG, L-SVRG and Q-SVRG algorithms containing \( m \) inner iterations accounts for \( n + m \) stochastic gradients. In all our computer experiments, when the number of effective passes is sufficiently large, Q-SVRG outperforms the averaged SGD, SVRG, L-SVRG and SAG methods, expect for the sonar dataset, where Q-SVRG is sometimes outperformed by SAG.

**Conclusion**

We have analysed a variant of SVRG to approximately minimize a class of quadratic functions. Our method, Q-SVRG, is applicable to minimization problems involving \( n \) points in dimension \( d \) that arise in several applications such as least-squares regressions, ridge regressions, linear discriminant analysis and regularized linear discriminant analysis. When the Hessian matrix is positive definite, Q-SVRG yields a convergence rate of \( O(\kappa/m^3) \) in \( O(l(n + m)) \) stochastic gradients for arbitrary \( l \geq 1 \), and can be simulated without the knowledge of \( \mu \). In addition, when \( \mu \) is known, Q-SVRG achieves a linear convergence rate and improves the previously known running time of SVRG by up a logarithmic factor. Furthermore, when \( \kappa \) is a constant, our analysis improves the state-of-the-art running times of accelerated SVRG, and is better than the matching lower bound of Lan and Zhou (2018), by a logarithmic factor. A limitation of Q-SVRG is that it is applicable only to quadratic problems.
5 Acknowledgements

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A Proof of Theorem 2.1

We prove the theorem in the case \( l = 1 \). An inductive argument then implies that Theorem 2.1 holds for any \( l \geq 1 \). We first show that it can be assumed without loss of generality that \( \theta_0 = 0 \). Let \( \theta^* := \theta^* - \theta_0 \), \( \hat{\theta}_k := \theta_k - \theta_0 \) for \( k \geq 0 \), and

\[
\hat{f}(\theta) := \frac{1}{2} \theta^T H \theta - \hat{c}^T \theta,
\]

for any \( d \)-dimensional column vector \( \theta \). Then (2.2) holds for the triplet \((H, \hat{\theta}^*, \hat{c})\), and the sequence \((\hat{\theta}_k : k \geq 0)\), satisfies the recursion

\[
\hat{\theta}_{k+1} = \hat{\theta}_k - \alpha(Q_k \hat{\theta}_k - \hat{c}),
\]

which is of the same type as (2.1). For \( k \geq 1 \), let

\[
\hat{\theta}_k := \frac{\theta_0 + \cdots + \hat{\theta}_{k-1}}{k}.
\]

Applying (2.3) to the triplet \((H, \hat{\theta}^*, \hat{c})\) shows that, for any \( d \)-dimensional column vector \( \theta \),

\[
\hat{f}(\theta) - f(\theta^*) = \hat{f}(\theta - \theta_0) - \hat{f}(\hat{\theta}^*).
\]

Consequently, as \( \hat{\theta}_k = \hat{\theta}_k - \theta_0 \),

\[
f(\hat{\theta}_k) - f(\theta^*) = \hat{f}(\hat{\theta}_k) - \hat{f}(\hat{\theta}^*).
\]

Thus, if Theorem 2.1 holds for the triplet \((H, \hat{\theta}^*, \hat{c})\) and the sequence \((\hat{\theta}_k : k \geq 0)\), which satisfies \( \hat{\theta}_0 = 0 \), it also holds for the triplet \((H, \theta^*, c)\) and the sequence \((\theta_k : k \geq 0)\). The rest of the proof assumes that \( \theta_0 = 0 \). We will also assume without loss of generality that \( L = 1 \). This assumption can be justified by a suitable scaling of \( \alpha, H \) and \( (Q_k : k \geq 0) \).

For \( k \geq 0 \), define the \( d \times d \) random matrix \( P_k := I - \alpha Q_k \). Thus (2.1) can be rewritten as

\[
\theta_{k+1} = P_k \theta_k + \alpha c.
\]

By A2, we have

\[
E(P_k) = I - \alpha H.
\]

Define the sequence of \( d \)-dimensional column vectors \((\beta_k : k \geq 0)\) recursively as follows. Let \( \beta_0 = \theta^* \) and, for \( k \geq 0 \), let

\[
\beta_{k+1} = P_k \beta_k + \alpha c.
\]

Thus, \((\beta_k : k \geq 0)\) satisfies the same recursion as \((\theta_k : k \geq 0)\). It follows by induction from (A.2) and (A.4) that, for any \( k \geq 0 \), the vectors \( \theta_k \) and \( \beta_k \) are square-integrable.

A.1 Bounding the bias

Lemma A.1. For \( k \geq 0 \), we have

\[
E(\theta_k) = (I - (I - \alpha H)k)\theta^*
\]

and

\[
E(\beta_k) = \theta^*.
\]

Proof. By (A.2), \( \theta_k \) is a deterministic function of \( P_0, \cdots, P_{k-1} \), and so \( \theta_k \) is independent of \( P_k \). We prove (A.5) by induction on \( k \). Clearly, (A.5) holds for \( k = 0 \). Assume that (A.5) holds for \( k \). Then, \( \theta_{k+1} \)

\[
E(\theta_{k+1}) = E(P_k)E(\theta_k) + \alpha c
\]

\[
= (I - \alpha H)(I - (I - \alpha H)^k)\theta^* + \alpha H\theta^*
\]

\[
= (I - (I - \alpha H)^{k+1})\theta^*,
\]

and so (A.5) holds for \( k + 1 \). A similar inductive proof implies (A.6). \( \square \)
Lemma A.2. For $k \geq 1$, 
\[
E((\hat{\theta}_k - \theta^*)^T H E(\bar{\theta}_k - \theta^*)) \leq \frac{||\theta^*||^2}{\alpha k}.
\]

Proof. By (A.5), for $0 \leq i \leq k - 1$,
\[
E((\theta_i - \theta^*)^T H E(\theta_i - \theta^*)) = \theta^T (I - \alpha H)^{2i} H \theta^*.
\]
As $H$ is symmetric positive semidefinite, the quadratic function $x \mapsto x^T H x$ is convex over $\mathbb{R}^d$, and so
\[
E((\bar{\theta}_k - \theta^*)^T H E(\bar{\theta}_k - \theta^*)) \leq \frac{1}{k} \sum_{i=0}^{k-1} E((\theta_i - \theta^*)^T H E(\theta_i - \theta^*)) \leq \frac{1}{k} \sum_{i=0}^{2k-2} \alpha H^{i+1} H \theta^* \leq \frac{1}{\alpha k} \theta^T (I - \alpha H)^{2k-1} \theta^*.
\]

The third equation follows by observing that $(I - \alpha H)^{2k-1} H$ is positive semidefinite since all eigenvalues of $\alpha H$ are between 0 and 1. The last equation follows from the identity
\[
\sum_{i=0}^j (I - H)^i H' = I - (I - H')^{j+1}, \quad j \geq 0, \tag{A.7}
\]
for any $d \times d$ matrix $H'$. As $(I - \alpha H)^{2k-1}$ is positive semidefinite, this completes the proof. \qed

A.2 Bounding the variance

Lemma A.3. For $k \geq 0$, we have $E(||\beta_k - \theta^*||^2) \leq (\alpha/\mu) \theta^*^T H \theta^*$.

Proof. By (2.2) and (A.4), we have $\beta_k = \beta_{k-1} + \alpha H \theta^*$. Hence
\[
\beta_k - \theta^* = \beta_{k-1} (\beta_{k-1} - \theta^*) + \alpha (H - Q_{k-1}) \theta^*. \tag{A.8}
\]

Since $\beta_{k-1}$ and $Q_{k-1}$ are independent, it follows from (A.6) that
\[
E((\beta_{k-1} - \theta^*)^T P_{k-1} (H - Q_{k-1}) \theta^*) = 0.
\]

As $E(||U + V||^2) = E(||U||^2) + E(||V||^2)$ for any square-integrable random $d$-dimensional column vectors $U$ and $V$ with $E(U^T V) = 0$, (A.8) implies that
\[
E(||\beta_k - \theta^*||^2) = E((\beta_{k-1} - \theta^*)^T P_{k-1} (H - Q_{k-1}) \theta^*) + \alpha^2 \theta^T E((H - Q_{k-1})^2) \theta^*. \tag{A.9}
\]

On the other hand,
\[
E(P_j^2) = E(I - 2\alpha Q_j + \alpha^2 Q_j^2) \leq I - 2\alpha H + \alpha^2 H \leq I - \alpha H \leq (1 - \alpha \mu) I,
\]
and
\[
E((H - Q_j)^2) = E(H^2 - H Q_j - Q_j H + Q_j^2) \leq E(Q_j^2) - H^2 \leq H.
\]

As $P_{k-1}$ and $\beta_{k-1}$ are independent, it follows from (A.10) that
\[
E(||\beta_k - \theta^*||^2) \leq (1 - \alpha \mu) E(||\beta_{k-1} - \theta^*||^2) + \alpha^2 \theta^T H \theta^*. \tag{A.10}
\]

An induction on $k$ completes the proof. \qed
For any square-integrable $d$-dimensional random column vectors $U$ and $V$, let
\[
\text{rCov}(U, V) := E(U^T V) - E(U^T)E(V),
\]
and $\text{Var}(U) := \text{rCov}(U, U)$. For any square-integrable $d$-dimensional random column vectors $U$, $V$ and $V'$, any deterministic symmetric $d \times d$ matrix $A$, and any bounded $d \times d$ random matrix $B$ independent of $(U, V')$, it can be shown that $\text{rCov}(U, V + V') = \text{rCov}(U, V) + \text{rCov}(U, V')$, and $\text{rCov}(A U, V) = \text{rCov}(U, A V)$, with $\text{rCov}(U, B V) = E(B U V)$ and $\text{Var}(U + V) \leq 2(\text{Var}(U) + \text{Var}(V))$. Furthermore, if $A$ is positive semidefinite, then $\text{rCov}(U, A U) \geq 0$.

For $0 \leq j \leq k$, let $M_{j,k} = P_{k-j} P_{k-2} \cdots P_j$, with $M_{k,k} = I$.

**Lemma A.4.** For nonnegative integers $k, j$, we have
\[
\text{rCov}(H \theta_k, \theta_{k+j}) = \text{rCov}(H \theta_k, (I - \alpha H)^j \theta_k).
\]

**Proof.** We show by induction on $j$ that, for $j \geq 0$,
\[
\theta_{k+j} = M_{k,k+j} \theta_k + \alpha \sum_{i=k+1}^{k+j} M_{i,k+j} c.
\]

Clearly, (A.12) holds for $j = 0$. Assume now that (A.12) holds for $j$. Then
\[
\theta_{k+j+1} = P_{k+j} \theta_{k+j} + \alpha c
\]
\[
= P_{k+j}(M_{k,k+j} \theta_k + \alpha \sum_{i=k+1}^{k+j} M_{i,k+j} c) + \alpha c
\]
\[
= M_{k,k+j+1} \theta_k + \alpha \sum_{i=k+1}^{k+j} M_{i,k+j+1} c + c,
\]
and so (A.12) holds for $j + 1$. As $\theta_k$ is independent of $M_{i,k+j}$, for $k \leq i \leq k + j$, it follows from (A.12) that
\[
\text{rCov}(H \theta_k, \theta_{k+j}) = \text{rCov}(H \theta_k, M_{k,k+j} \theta_k)
\]
\[
= \text{rCov}(H \theta_k, E(M_{k,k+j}) \theta_k)
\]
\[
= \text{rCov}(H \theta_k, (I - \alpha H)^j \theta_k).
\]
The last equation follows from (A.3).

**Lemma A.5.** For $0 \leq i \leq k$, we have
\[
\sum_{j=i}^{k} \text{rCov}(H \theta_i, \theta_j) \leq \frac{4}{\alpha \mu} \theta^* H \theta^*.
\]

**Proof.** By Lemma A.4,
\[
\sum_{j=i}^{k} \text{rCov}(H \theta_i, \theta_j) = \sum_{j=i}^{k} \text{rCov}(H \theta_i, (I - \alpha H)^{j-i} \theta_i)
\]
\[
= \sum_{j=i}^{k} \text{rCov}(\theta_i, H(I - \alpha H)^{j-i} \theta_i)
\]
\[
= \alpha^{j-i} \text{rCov}(\theta_i, (I - \alpha H)^{k+1-i} \theta_i)
\]
\[
\leq \alpha^{j-i} \text{Var}(\theta_i).
\]
The third equation follows from (A.7), and the last one from the positive semidefiniteness of $(I - \alpha H)^{k+1-i}$. On the other hand,
\[
\text{Var}(\theta_i) \leq 2(\text{Var}(\beta_i) + \text{Var}(\theta_i - \beta_i))
\]
\[
\leq 2(\text{E}(|\beta_i - \theta^*|^2) + ||\theta^*||^2)
\]
\[
\leq \frac{4}{\mu} \theta^* H \theta^*.
\]
The second equation follows from the inequality $\text{E}(|\theta_i - \beta_i|^2) \leq ||\theta^*||^2$, which can be shown by induction on $i$. The last equation is a consequence of Lemma A.3 and the inequality $\theta^* H \theta^* \geq \mu ||\theta^*||^2$. This concludes the proof.
A.3 Combining bias and variance terms

By (2.3),

\[ E(f(\hat{\theta}_k)) - f(\theta^*) = \frac{1}{2} E((\hat{\theta}_k - \theta^*)^T H (\hat{\theta}_k - \theta^*)). \]

On the other hand, by (A.11),

\[ E((\bar{\theta}_k - \theta^*)^T H (\bar{\theta}_k - \theta^*)) = E((\bar{\theta}_k - \theta^*)^T H E(\bar{\theta}_k - \theta^*) + \text{rCov}(H(\bar{\theta}_k - \theta^*), \bar{\theta}_k - \theta^*)) \]

Because \( H \) is symmetric positive semidefinite,

\[ \text{rCov}(H\theta_k, \bar{\theta}_k) = \frac{1}{k^2} \left( \sum_{i=0}^{k-1} \text{rCov}(H\theta_i, \theta_i) + 2 \sum_{i=0}^{k-1} \sum_{j=i+1}^{k-1} \text{rCov}(H\theta_i, \theta_j) \right) \]

\leq \frac{2}{k^2} \sum_{i=0}^{k-1} \sum_{j=i}^{k-1} \text{rCov}(H\theta_i, \theta_j) \]

\leq \frac{8}{\alpha \mu k} \theta^*^T H \theta^* .

The last equation follows from Lemma [A.5]. Together with Lemma [A.2], this implies that

\[ E((\bar{\theta}_k - \theta^*)^T H (\bar{\theta}_k - \theta^*)) \leq \frac{||\theta^*||^2}{\alpha k} + \frac{8}{\alpha \mu k} \theta^*^T H \theta^* \]

\leq \frac{9}{\alpha \mu k} \theta^*^T H \theta^* ,

where the second equation follows from the inequality \( \theta^*^T H \theta^* \geq \mu ||\theta^*||^2 \). It follows that

\[ E(f(\hat{\theta}_k)) - f(\theta^*) \leq \frac{9 \theta^*^T H \theta^*}{2 \alpha \mu k} \]

\leq \frac{9(f(0) - f(\theta^*))}{\alpha \mu k} .

This concludes the proof.

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