Speed Maintained SVRG

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***Abstract*—Stochastic gradient desent (SGD) is widely used for large-scale machine learning optimization, but has slow convergence rate due to the highly inherent variance. In recent years, the popular Stochastic Variance Reduced Gradient (SVRG) method mitigates this shortcoming, through computing the full-gradient of the entire dataset occasionally. However, conventional SVRG and its variants usually need a hyper-parameter to identify when to compute such the full gradient, which is essential to the covergene performance. Few previous studies discuss the method to identify such the hyper-parameter, which makes it hard to gain a good convergence performance in parctical machine learning tasks. In our paper, we propose a new stochastic gradient descent with variance reduction technique named SMSVRG which computes the full gradient adaptively. Moreover, we propose an improved method denoted by SMSVRG+, which is comparable to and even better than SVRG with best-tuned epoch sizes for smooth and strongly convex functions.**

I. Introduction

Many machine learning tasks such as logistic regression and linear regression can be formulated to be an optimizaton problem which is described as

$$\min F(\omega), \qquad F(\omega) = \frac{1}{n}\sum_{i=1}^{n} f_i(\omega) + R(\omega). \tag{1}$$

where n is the size of the training data. $F(\omega)$ means the loss function or training loss of a machine model, and ω is its parameter. $R(\omega)$ is the regularizer, which is widely used to avoid overfitting. It is noting that the total number of instances, i.e. n becomes very large with the proliferation of data.

Gradient Descent (GD) is a basic method to solve such the optimization problem. The gradient of $F(\omega)$ is obtained by passing over the entire training data, which is extremely time-consuming when the size of training data, i.e. n becomes large. Besides, GD is an iterative-convergent algorithm, that is, the parameter, i.e. ω, usually needs thousands of iterations to be converged. Since GD needs to compute the gradient of $F(\omega)$ every iteration, when the volume of data is large, the computation cost increases sharply and impairs the convergent performance significantly.

Stochastic Gradient Descent (SGD) mitigates this shortcoming by replacing the calculation of $\nabla F(\omega)$ with a stochastic gradient $\nabla f_i(\omega)$ with $i \in \{1, 2, ..., n\}$. In SGD, i is selected randomly from the entire training data. Thus, SGD outperforms GD on the time efficiency significantly. Take the expectation of i, we obtain $\mathbb{E}[\nabla f_i(\omega)] = \nabla F(\omega)$. The difference between $\nabla f_i(\omega)$ and $\nabla F(\omega)$ represents variance which makes it difficult to achieve the optimum. In order to make the loss function, i.e. $F(\omega)$ converge, a decaying learning rate is usually used to reduce the variance. However, value of the learning rate is decayed to be very small after hundreds of iterations, which impedes the loss function to converge. In a nutshell, SGD with a decaying learning rate incurs a sub-linear convergence rate due to a learning rate.

In recent years, variance reduced variants of SGD such as SVRG [4] is proposed to reduce the variance and gain the linear convergence performance with a constant learning rate. In SVRG, a full gradient is computed occasionally during the inexpensive SGD steps to reduce the variance, dividing the optimization procedure into many epochs. On the basis of SVRG, many variants have been proposed to improve its performance. SVRG-BB [12] uses the Barzilai and Borwein (BB) method proposed by Barzilai and Borwein in [2] to compute the step size before every epoch, which generally achieves the comparable convergence performance to SVRG with the best-tuned step size. CHEAPSVRG [10] and SAMPLEVR aim at reducing the expensive cost of full gradient computation through using a surrogate with a subset of the training dataset. mS2GD [6] uses mini-batch method to obtain a full gradient to reduce the variance, which shows a clear advantage for parallel computation. EMGD [14], SVRGHT [8], Prox-SVRG [13] and **SVRG with second-order information [5]** modify the update rule of stochastic steps, and show advantages to SVRG in some cases. However, there are few studies discussing about how frequently should a full gradient be computed, i.e. how to set the epoch size m.

Most previous researches present that the epoch size, i.e. m should be constant [4, 12, 10] or increased monotonically [6], regardless of the learning rate. It is recommended that $m = 2n$ for convex problems and $m = 5n$ for non-convex problems in SVRG, without theoretical analysis and further experimental verification.

The epoch size, i.e. m has a great impact on the convergence performance of SVRG. More specifically, when m is too small, it wastes too much time to compute the full gradient frequently. When m is rather large, the variance between the stochastic gradient and the full gradient increases sharply, making the convergence of training loss extremely difficult. According

to the analysis of variance in [YaWei], both the epoch size, i.e. m and learning rate, i.e. η have a significant impact on the convergence performance. However, those previous studies do not provide a practical method to set the value of those hyper-parameters. Extensive empirical studies illustrates that the selection of good value for those hyper-parameters costs much time in real machine learning tasks. In this paper, we propose a novel algorithm denoted by SMSVRG which can adjust the epoch size adaptively. Our experiments show that when η is large, the training loss begins to fluctuate after merely a small number of iterations. In the other hands, the algorithm can endure far more than n iterations with a small η. Ideally, if we stop the iterations in one epoch just before the training loss begins to fluctuate, the algorithm will certainly be very efficient and outperform SVRG with constant epoch size. A direct approach is computing the training loss occasionally. However, the training loss computation requires passing over the entire dataset, which is rather time consuming. Intuitively, for strongly convex and smooth problems, the changing amount of parameters, i.e. $\Delta\omega$ is proportional to that of training loss, i.e. ΔF. Hence we can use $\Delta\omega$ instead of ΔF to detect the fluctuation. In spirits of this, SMSVRG computes the changing amounts of parameters at the same interval, if the changing amount of current interval is greater than that of former, it finishes the current epoch and begins the next one. Besides, we analyze and give guidance of how to set the interval size. Since SMSVRG may stop iterations earlier than expectation when η is quite small, we propose an improved algorithm denoted by SMSVRG+. In a nutshell, our contributions are highlighted as follows:

- SMSVRG, an algorithm that can adjust the epoch size dynamically.
- SMSVRG+, an improvement of SMSVRG and outperforming SVRG in any case.
- Extensive empirical studies shows the effectiveness of our proposed algorithms which outperform their countparts on the convergence performance significantly.

This paper is organized as follows: Section II reviews the related work. Section III presents the new variant of SVRG, i.e. SMSVRG. Section IV demonstrates the numerical results of our algorithm. Section V concludes this paper.

II. Related work

Several variants of SVRG focusing on epoch size has been proposed, including SVRG++ [1], S2GD [7], SVRG_Auto_Epoch [1] and so on.

SVRG++ adopts a simple strategy that epoch size m doubles between every consecutive two epochs. This method is absolutely heuristic and sometimes not justified. Our experiments show that when η is big or moderate, the exponential growth of m will incur great variance and impairs convergence.

S2GD designs a probability model of m and shows that a large epoch size is used with a high probability. However it needs to know the lower bound on the strong convexity constant of F, which is hard to estimate in practice. Meanwhile, the maximum of stochastic steps per epoch is also a sensitive parameter.

SVRG_Auto_Epoch is introduced as an additional improvement of SVRG++. It determines the termination of epoch through the quality of the snapshot full gradient. It records $diff_t = \|\nabla f_i(\omega_t^s) - \nabla f_i(\tilde{\omega}^{s-1})\|$ every iteration t and uses it as a tight upper bound on the variance of the gradient estimator. Although this method is reasonable, it has too much parameters to tune. Moreover, it takes much additional computation for every iterations, which impairs performances significantly.

Comparing with the above methods, SMSVRG is apparently reasonable in intuition and does not need to tune extra parameters. Besides, it takes little additional computation cost and outperform the aforementioned three methods.

Algorithm 1 SVRG

Require: learning rate η, epoch size m_0, initial point $\tilde{\omega}$

$\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n}\nabla f_i(\tilde{\omega})$
for $s = 0, 1, ...$ **do**
  $\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n}\nabla f_i(\tilde{\omega}_s)$
  $\omega_0 = \tilde{\omega}_s$
  for $t = 0, 1, 2, ..$ **do**
    Randomly pick $i_t \in \{1, 2, ..., n\}$
    $\omega_t = \omega_{t-1} - \eta(\nabla f_{i_t} - \nabla f_{i_t}(\tilde{\omega}_s) + \tilde{\mu})$
  end for
  Option I: $\tilde{\omega}_{s+1} = \omega_m$
  Option II: $\tilde{\omega}_{s+1} = \omega_t$ for randomly chosen $t \in \{0, ..., m-1\}$
end for

III. Speed Maintained SVRG

In this section we describe two novel algorithms: SMSVRG and SMSVRG+, which can set the appropriate iteration number in each epoch automatically and has superior convergence properties in out experiments. We assume the loss function F and the component functions f_i are convex and L-smooth throughout the paper.

A. smSVRG

When we apply gradient descent to convex problem, as the ω_t will gradually approach the optimal value ω^*, thus the gradient $\nabla F(\omega_t)$ keeps decreasing. Then we have $\|\omega_{t+1} - \omega_t\| < \|\omega_t - \omega_{t-1}\|$. Considering several iterations, we can also have $\|\omega_{t+m_0} - \omega_t\| < \|\omega_t - \omega_{t-m_0}\|$. Inspired by this, algorithm SMSVRG set $\|\omega_{t+m_0} - \omega_t\| > \|\omega_t - \omega_{t-m_0}\|$ as a stop condition in each epoch. Algorithm SMSVRG just requires two parameters: learning rate η, checking interval m_0. Note that the difference between SVRG and SMSVRG is that in the latter we adjust the epoch size dynamically, instead of using a prefixed m as in SVRG. In each epoch, SMSVRG compute the inequality

$$\|\omega_t - \omega_{t-m_0}\| > \|\omega_{t-m_0} - \omega_{t-2m_0}\|$$

every m_0 iterations, if the inequality holds the algorithm will break the inner loop and begin the next epoch.

B. Optimal Choice of checking interval

In SMSVRG, we use the $\Delta\omega$ of several iterations to detect when loss function begin to fluctuate and fail to converge. However, how to choose a suitable value of checking interval i.e. m_0 becomes an important issue. In this section, we analyze the effects of setting different m_0 and provide guidance on setting a optimal value.

First, as the variance incurred by SGD iterations cannot be ignored, when we set m_0 to be small, the variance of $\|\omega_t - \omega_{t-m_0}\|$ is too big thus the confidence of the inequality is low. As a result, the inequality may holds because of variance when the loss function is still decreasing rapid, which wastes much time on computing full gradients. We use $C(m_0)$ to denote the confidence of inequality holds. It is obvious that $C(m_0)$ is a monotonically increasing function of m_0.

When we set m_0 to be relatively big, the variance becomes small and the confidence of inequality holds is high. However, it will be too late to detect the fluctuation of objective function and waste much time to compute iterations which make no process for optimizing the objective function. We use $D_s(m_0)$ to denote the $AbsoluteDelay$ of detecting fluctuation. Furthermore, the $AbsoluteDelay$ makes different effects depending on the epoch size, so it is better to consider the $RelativeDelay$:

$$D_r(m_0) = \frac{D_s(m_0)}{es+n}$$

Note that es denote the number of iterations in a specific epoch and n denotes the size of the dataset. Function $D_r(m_0)$ is also monotonically increasing with respect to m_0.

It is natural that we want to choice a suitable m_0 which can achieve a big $C(m_0)$ and a small $D_r(m_0)$. In order to obtain a trade-off between $C(m_0)$ and $D_r(m_0)$, we convert the parameter choosing problem to the following maximization problem:

$$\begin{aligned} m_0 &= \max_{m_0} C(m_0) - D_r(m_0) \\ &= \max_{m_0} C(m_0) - \frac{D_s(m_0)}{es+n} \\ &\text{s.t.} 0 < m_0 < n \end{aligned} \tag{2}$$

Note that we do not have the exact expression of C and D_s, instead, we only know their monotonicity. Nonetheless, it is enough to guide us to set the parameter m_0. From (2) we can obtain the following conclusions:

1. When epoch size es is small, the D_s tends to be more important than C. Hence we should set m_0 to be relatively small to maximize the objective function. On the contrary, it is recommended to set m_0 to be big. In spirit of this, we can set m_0 to be proportional to the iteration number of previous epoch.

2. According to our experiment on SVRG, when the learning rate η is large, the loss function begin to fluctuate after merely $n/10$ iterations, so we should set the initial m_0 to the same order of magnitude as $10^{-1} \times n$

C. SMSVRG+

On the basis of the analysis of section III-B, we improve our algorithm SMSVRG through dynamically adjusting the checking interval, instead of a constant value. According to the two conclusions, we initialize the m_0 to be $0.1n$ and set it to be $(int(es/n)+1)*(0.1n)$ in each epoch, where es denote the iteration number of previous epoch. With this strategy , when each epoch seems to be capable of enduring more iterations, SMSVRG+ will expand the checking interval to improve the confidence, avoiding stopping the epoch ahead of time due to variance.

Algorithm 2 SMSVRG

Require: learning rate η, checking interval m_0, initial point $\tilde{\omega}$

$\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{\omega})$
for $s = 0, 1, ...$ **do**
  $\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{\omega}_s)$
  $\omega_0 = \tilde{\omega}_s$
  for $t = 0, 1, 2, ..$ **do**
    if $t > m_0$ and $t\%m_0 = 0$ and $\|\omega_t - \omega_{t-m_0}\| > \|\omega_{t-m_0} - \omega_{t-2m_0}\|$ **then**
      break
    end if
    Randomly pick $i_t \in \{1, 2, ..., n\}$
    $\omega_t = \omega_{t-1} - \eta(\nabla f_{i_t} - \nabla f_{i_t}(\tilde{\omega}_s) + \tilde{\mu})$
  end for
  $\tilde{\omega}_{s+1} = \omega_m$
end for
return $\tilde{\omega}_{s+1}$

IV. Numerical Experiments

In this section, we conduct some experiments to demonstrate the efficiency of our proposed algorithm. We evaluate our algorithm on four training datasets, which are public on the LIBSVM website[1]. In our experiments, SMSVRG is applied for two standard machine learning tasks: $l2$-regularized logistic regression and $l2$-regularized ridge regression.

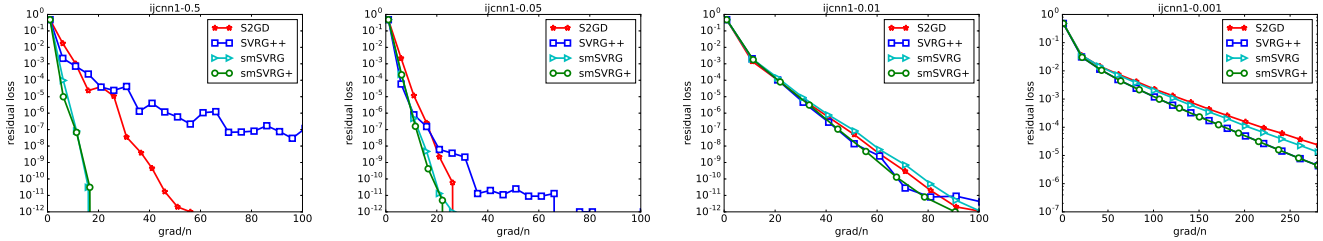
The $l2$-regularized logistic regression task is conducted on the two datasets: ijcnn1, a9a. Since the label of each instance in these datasets is set to be 1 or -1, the loss function of $l2$-regularized logistic regression task is:

$$\min_{\omega} \frac{1}{n}\sum_{i=1}^{n} \log(1 + e^{-y_i \omega^{\mathrm{T}} x_i}) + \lambda \parallel \omega \parallel^2 . \tag{3}$$

The $l2$-regularized ridge regression task is conducted on the four datasets: abalone, cadata, cpusmall, space_ga. The loss function of $l2$-regularized ridge regression task is:

$$\min_{\omega} \frac{1}{n}\sum_{i=1}^{n} \left(\omega^{\mathrm{T}} x_i - y_i\right)^2 + \lambda \parallel \omega \parallel^2 . \tag{4}$$

[1] http://www.csie.ntu.edu.tw/∼cjlin/libsvmtools/datasets/



(a) ijcnn1 $\eta = 0.5$ (b) ijcnn1 $\eta = 0.05$ (c) ijcnn1 $\eta = 0.01$ (d) ijcnn1 $\eta = 0.001$

Fig. 1. Comparison of SMSVRG, SMSVRG+, SVRG++, S2GD

Algorithm 3 SMSVRG+

Require: learning rate η, checking interval m_0, initial point $\tilde{\omega}$

Initialize: $m_0 = 0.1n$

$\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{\omega})$
for $s = 0, 1, ...$ **do**
  $\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\tilde{\omega}_s)$
  $\omega_0 = \tilde{\omega}_s$
  for $t = 0, 1, 2, ..$ **do**
    if $t > m_0$ and $t\%m_0 = 0$ and $\|\omega_t - \omega_{t-m_0}\| > \|\omega_{t-m_0} - \omega_{t-2m_0}\|$ **then**
      break
    end if
    Randomly pick $i_t \in \{1, 2, ..., n\}$
    $\omega_t = \omega_{t-1} - \eta(\nabla f_{i_t} - \nabla f_{i_t}(\tilde{\omega}_s) + \tilde{\mu})$
  end for
  $es = t$
  $m_0 = (int(es/n) + 1) * (0.1n)$
  $\tilde{\omega}_{s+1} = \omega_m$
end for
return $\tilde{\omega}_{s+1}$

TABLE I
DETAIL INFORMATION OF DATASETS AND MODELS

Dataset	size	dimension	model	λ
ijcnn1	49990	22	logistic	10^{-4}
a9a	32561	123	logistic	10^{-4}
YearPredictionMSD	463715	90	linear	10^{-4}
cada	20640	8	linear	10^{-4}

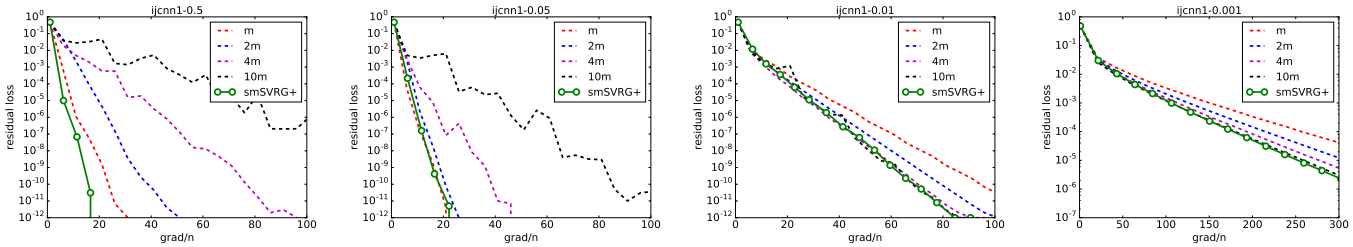
We scale the value of all features to $[-1, 1]$ and set the weighting parameter λ to 10^{-4} for all evaluations. In all figures, the x-axis denotes the computational cost, which is measured by the number of gradient computation divided by the size of training data, i.e. n. The y-axis denotes training loss residual, i.e. $F(\tilde{\omega}_s) - F(\omega^*)$. Note that the optimum ω^* is estimated by running the gradient descent for a long time. Our numerical experiments include two parts: comparing with existing related methods and comparing with SVRG of different epoch sizes. Both experiments show the superior performance of our methods.

A. Comparing with existing related methods

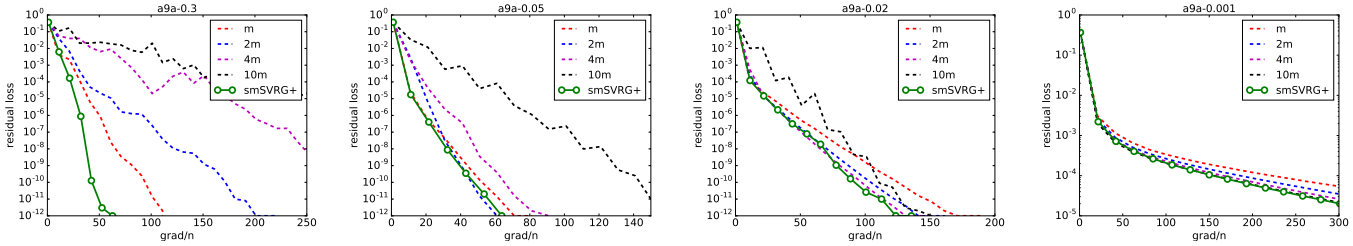
In this section, we compare our SMSVRG(Algorithm 2) and SMSVRG+(Algorithm 3) with two aforementioned existing methods: SVRG++ and S2GD. We do not compare with SVRG_Auto_Epoch in that we find its termination condition of epoch is never satisfied and keeps doing SGD iteration, resulting in nonconvegence. For SVRG++, we initialize $m = n$. For S2GD, we set the maximum of m to be $4n$ and set $gamma$ to be 0. For both SMSVRG and SMSVRG+, we set the checking interval m_0 to be $10/n$. We test these methods by logistic regression on dataset $ijcnn1$. From Figures III-C we can see that at most times SVRG++ fluctuates violently and fails to converge owing to the large variance caused by too excessive epoch size. It only performs well when η is quite small. Figures 1(a), 1(b) show that both SMSVRG and SMSVRG+ converge rapidly with relatively large η for they can constrain m in a small range. However, it can be seen from Figures 1(c), 1(d), when η decreases to small values, the performance of SMSVRG drop gradually and even become inferior to others, while SMSVRG+ always performs the best of all. The main reason is that when η is small, more iterations can be computed in one epoch, thus checking the inequality frequently will resulting algorithm to stop epochs too early because of variance. The strategy of increase checking interval applied by SMSVRG+ can reduce the variance. Hence it always outperform other methods.

B. Comparing with SVRG of different epoch sizes

In order to demonstrate the outstanding adaptability of our algorithm with different learning rate in any case, we conduct sufficient experiments. Since SMSVRG+ performs better than SMSVRG, we only compare the former with SVRG. The experiments are tested by logistic regression and ridge regression on four datasets. For SVRG, we set epoch size m as four different values: $n, 2n, 4n, 10n$. The first three values are chosen for the reason that they are commonly used in many papers. Besides, our experiments show that epoch size bigger that $10n$ perform almost the same. It is easy to comprehend as the full gradient computation becomes less important when epoch size is rather big. In all figures, the dashed lines correspond to SVRG with fixed epoch size given in the legends of the figures, while the green solid lines correspond to SMSVRG

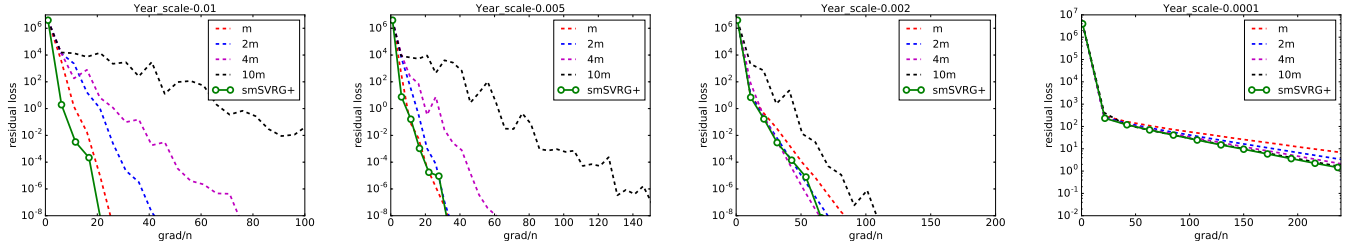


(a) ijcnn1 $\eta = 0.5$ (b) ijcnn1 $\eta = 0.05$ (c) ijcnn1 $\eta = 0.01$ (d) ijcnn1 $\eta = 0.001$

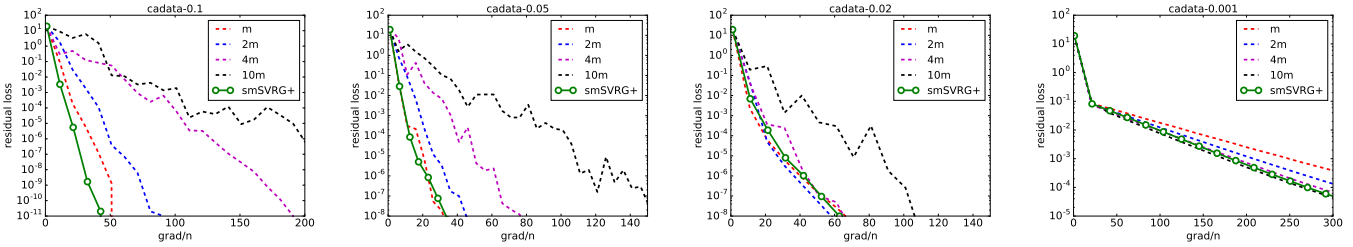


(e) a9a $\eta = 0.3$ (f) a9a $\eta = 0.05$ (g) a9a $\eta = 0.02$ (h) a9a $\eta = 0.001$

Fig. 2. Generally, SMSVRG can automatically set an appropriate m with different learning rates for the $l2$-regularized logistic regression



(a) YearPredictionMSD $\eta = 0.01$ (b) YearPredictionMSD $\eta = 0.005$ (c) YearPredictionMSD $\eta = 0.002$ (d) YearPredictionMSD $\eta = 0.0001$



(e) cadata $\eta = 0.1$ (f) cadata $\eta = 0.05$ (g) cadata $\eta = 0.02$ (h) cadata $\eta = 0.001$

Fig. 3. Generally, SMSVRG can automatically set an appropriate m with different learning rates for the $l2$-regularized linear regression

It can be seen from Figures 2(a) to 3(h) that SMSVRG can always have the similar performance as SVRG with most suitable epoch size. We observe that when η is big, setting m to be a small value, i.e. n, can achieve better performance. The main reason is that when η is big, the variance becomes big simultaneously, so m must be set small to constrain the variance. As η diminishes, the optimal value of m increases, which means that the algorithm can tolerate more variance induced by extra iterations. As illustrated in Figures, our method is comparable to and sometimes even better than SVRG with best-tuned epoch sizes when learning rate is large or medium. However, if η is set to be too small, SMSVRG performs slightly inferior to SVRG with large epoch sizes, but outperforms SVRG with recommended epoch sizes, i.e. n and $2n$. It is noting that setting η to be too small is not a practical approach when using SVRG or its variants, because the convergence rate will be extremely low. Therefore, the sub-optimal performance of SMSVRG with very small η is acceptable.

V. Conclusion

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