

Lecture 8: SGD with Variance Reduction

1 Review of Lecture 7: Introduction to stochastic optimization

We begin by reviewing the Stochastic Gradient Descent (SGD).

1.1 Stochastic Optimization

Consider $\min_{x \in \mathbb{R}^d} F(x)$, where $F(x) := \mathbb{E}_z[f(x; z)]$.

Algorithm: Stochastic Gradient Descent (SGD)

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- 1: **for** $k = 1, 2, \dots$ **do**
 - 2: Compute a stochastic gradient g_k that satisfies $\mathbb{E}_z[g_k] = \nabla F(x_k)$
 - 3: $x_{k+1} = x_k - \eta g_k$.
 - 4: **end for**
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1.2 SGD v.s. GD

	Method	
	SGD	GD
convex (and smooth)	$O\left(\frac{1}{\sqrt{k}}\right)$	$O\left(\frac{1}{k}\right)$
strongly convex and smooth	$O\left(\frac{1}{k}\right)$	$O(\exp(-k))$

Table 1: Convergence rates for different optimization scenarios. [Rakhlin (2012)]

1.3 Iteration complexity of SGD

Denote $i_{1:K}$ all the randomness from iteration 1 to K , i.e., i_1, i_2, \dots, i_K .

Theorem 1. Let $F(x) = \mathbb{E}_z[f(x; z)] : \mathbb{R}^d \rightarrow \mathbb{R}$ be a convex function. Consider the update

$$x_{k+1} = x_k - \eta g_k,$$

where $\mathbb{E}_z[g_k] = \nabla F(x_k)$. Suppose $x_* = \arg \min F(x)$ exists and the initial distance is bounded, i.e., $\|x_1 - x_*\|_2 \leq D$. Then,

$$\frac{1}{K} \sum_{k=1}^K \mathbb{E}_{i_{1:K}} [F(x_k) - F(x_*)] \leq \frac{\eta}{2K} \left(\sum_{k=1}^K \mathbb{E}_{i_{1:K}} [\|g_k\|_2^2] \right) + \frac{\|x_1 - x_*\|_2^2}{2\eta K},$$

where $\bar{x}_K := \frac{1}{K} \sum_{k=1}^K x_k$.

Caution!!! To be rigorous, we need to identify conditions such that the stochastic gradient norm is bounded.

Lemma 1. $\mathbb{E}_{i_k} [\|g_k\|_2^2]$ is an upper bound of the variance of the stochastic gradient.

Proof.

$$\begin{aligned} \text{Var}(g_k) &\triangleq \mathbb{E}_{i_k} [(g_k - \mathbb{E}_{i_k} [g_k])^2] \\ &\quad (\text{since } \mathbb{E}_{i_k} [g_k] = \nabla F(x_k)) \\ &= \mathbb{E}_{i_k} [\|g_k\|_2^2] - 2\mathbb{E}_{i_k} [\langle g_k, \mathbb{E}_{i_k} [g_k] \rangle] + \|\nabla F(x_k)\|_2^2 \\ &= \mathbb{E}_{i_k} [\|g_k\|_2^2] - 2\|\nabla F(x_k)\|_2^2 + \|\nabla F(x_k)\|_2^2 \\ &\leq \mathbb{E}_{i_k} [\|g_k\|_2^2]. \end{aligned}$$

□

1.4 SGD for non-convex problems

Theorem 2. Assume that the variance of the stochastic gradient $\nabla f(x; z)$ is at most σ^2 for all x , i.e., $\mathbb{E}_z [\|\nabla f(x; z) - \nabla F(x)\|_2^2] \leq \sigma^2$. Suppose $F(\cdot)$ is L -smooth. Then, SGD with the step size $\eta \leq \frac{1}{L}$ has

$$\sum_{k=1}^K \mathbb{E}_{i_{1:K}} [\|\nabla F(x_k)\|_2^2] \leq \frac{2(F(x_1) - F_*)}{\eta} + \eta L \sigma^2 K.$$

Proof. (Proof of the theorem) Starting from the smoothness, we have, given x_k ,

$$F(x_{k+1}) \leq F(x_k) + \langle \nabla F(x_k), x_{k+1} - x_k \rangle + \frac{L}{2} \|x_{k+1} - x_k\|^2 \quad (1)$$

$$= F(x_k) - \eta \langle \nabla F(x_k), g_k \rangle + \frac{\eta^2 L}{2} \|g_k\|^2 \quad (2)$$

Take expectation over the randomness from 1 to k on both sides, we have

$$\mathbb{E}_{i_{1:k}}[F(x_{k+1})] \leq \mathbb{E}_{i_{1:k}}[F(x_k)] - \eta \mathbb{E}_{i_{1:k}}[\langle \nabla F(x_k), g_k \rangle] + \frac{\eta^2 L}{2} \mathbb{E}_{i_{1:k}}[\|g_k\|^2] \quad (3)$$

$$= \mathbb{E}_{i_{1:k}}[F(x_k)] - \eta \mathbb{E}_{i_{1:k-1}}[\|\nabla F(x_k)\|^2] + \frac{\eta^2 L}{2} \mathbb{E}_{i_{1:k}}[\|g_k\|^2] \quad (4)$$

$$\leq \mathbb{E}_{i_{1:k}}[F(x_k)] - \eta \mathbb{E}_{i_{1:k-1}}[\|\nabla F(x_k)\|^2] + \frac{\eta^2 L}{2} (\mathbb{E}_{i_{1:k-1}}[\|\nabla F(x_k)\|^2] + \sigma^2) \quad (5)$$

$$\leq \mathbb{E}_{i_{1:k}}[F(x_k)] - \frac{\eta}{2} \mathbb{E}_{i_{1:k-1}}[\|\nabla F(x_k)\|^2] + \frac{\eta^2 L}{2} \sigma^2. \quad (6)$$

$$\leq \mathbb{E}_{i_{1:k}}[F(x_k)] - \frac{\eta}{2} \mathbb{E}_{i_{1:k}}[\|\nabla F(x_k)\|^2] + \frac{\eta^2 L}{2} \sigma^2. \quad (7)$$

It is noted that for (5), we used

$$\mathbb{E}_{i_{1:k}}[\|g_k\|^2] = \mathbb{E}_{i_{1:k-1}}[\mathbb{E}_{i_k}[\|g_k\|^2 | i_{1:k-1}]] \quad (8)$$

$$= \mathbb{E}_{i_{1:k-1}}[\mathbb{E}_{i_k}[\|g_k\|^2 | x_k]] \quad (9)$$

$$\leq \mathbb{E}_{i_{1:k-1}}[\|\nabla F(x_k)\|^2 + \sigma^2], \quad (10)$$

where the last inequality is by the assumption that the variance is bounded by σ^2 .

For (6), we used $\eta \leq \frac{1}{L}$. For (7), we used that i_k is independent from x_k .

Now take expectation over all the randomness on both sides of (7) and sum over $k = 1$ to K ,

$$\mathbb{E}_{i_{1:K}}[F(x_{k+1}) - F(x_1)] \leq - \sum_{k=1}^K \frac{\eta}{2} \mathbb{E}_{i_{1:K}}[\|\nabla F(x_k)\|^2] + \frac{L\eta^2\sigma^2}{2}.$$

□

Corollary 2.1. *If \hat{x} is selected uniformly at random from x_1, \dots, x_K , then we have*

$$\mathbb{E}_{i_{1:K}}[\|\nabla F(\hat{x})\|] \leq \frac{\sqrt{2(F(x_1) - F_*)L}}{\sqrt{K}} + \frac{\sqrt{3\sigma\sqrt{(F(x_1) - F_*)L}}}{K^{1/4}}. \quad (11)$$

2 SGD with variance reduction (SVRG)

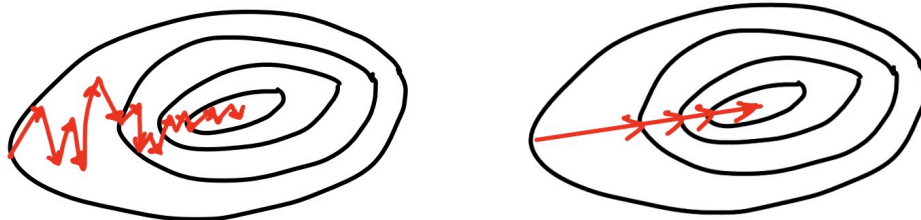


Figure 1: Progress of SGD (left) and GD (right) in practice

The variance of the stochastic gradient can be large. Thus, the question is **how to reduce the variance?**

2.1 SGD with variance reduction (SVRG) Algorithm

$$\min_{x \in \mathbb{R}^d} F(x), \text{ where } F(x) := \frac{1}{n} \sum_{i=1}^n f_i(x)$$

Algorithm: SGD with variance reduction (SVRG)

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- 1: Set $s = 1$. Init $v_1 = x_1$. Learning rate η .
 - 2: **for stage** $s = 1, 2, \dots, S$ **do**
 - 3: **for iteration** $k = 1, 2, \dots, K$ **do**
 - 4: Randomly pick a sample $i_k \in [n]$.
 - 5: Set $g_k = \nabla f_{i_k}(x_k) - \nabla f_{i_k}(v_s) + \nabla F(v_s)$. (variance reduction)
 - 6: Update $x_{k+1} = x_k - \eta g_k$.
 - 7: **end for**
 - 8: Update the snapshot $v_{s+1} = \frac{1}{K} \sum_{k=1}^K x_k$.
 - 9: Set $x_1 = v_{s+1}$
 - 10: **end for**
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2.2 Valid Stochastic Gradient

Let's show that it is a valid stochastic gradient.

Lemma 2. (Unbiased Estimate)

$$\mathbb{E}_{i_k} [\nabla f_{i_k}(x_k) - \nabla f_{i_k}(v_s) + \nabla F(v_s)] = \nabla F(x_k). \quad (12)$$

Proof.

$$\mathbb{E}_{i_k} [\nabla f_{i_k}(x_k) - \nabla f_{i_k}(v_s) + \nabla F(v_s)] = \nabla F(x_k) - \nabla F(v_s) + \nabla F(v_s) = \nabla F(x_k).$$

□

Recall that $\mathbb{E}_{i_k} [\|g_k\|_2^2]$ is an upper bound of the variance of $g_k \in \mathbb{R}^d$. Let us analyze the squared gradient norm $\mathbb{E}_{i_k} [\|g_k\|_2^2]$.

Lemma 3. (Variance bound)

$$\mathbb{E}_{i_k} [\|g_k\|_2^2] \leq 4L (F(x_k) - F(x_*)) + 4L (F(v_s) - F(x_*)). \quad (13)$$

Before we begin the proof of Lemma 3, we need to introduce two additional lemmas as below:

Lemma 4. For any random variable $Y \in \mathbb{R}^d$,

$$\mathbb{E} [\|Y - \mathbb{E}[Y]\|_2^2] = \mathbb{E}[\|Y\|_2^2] - (\mathbb{E}[\|Y\|_2])^2 \leq \mathbb{E}[\|Y\|_2^2]. \quad (14)$$

Lemma 5. If each $f_i(\cdot)$ is L -smooth convex, then

$$\mathbb{E}_{i_k} [\|\nabla f_{i_k}(x) - \nabla f_{i_k}(x_*)\|^2] \leq 2L (F(x) - F(x_*)). \quad (15)$$

Proof. We will proof Lemma 5 in Homework 3. □

Proof. (Proof of Lemma 3)

$$\begin{aligned} \mathbb{E}_{i_k} [\|g_k\|_2^2] &= \mathbb{E}_{i_k} [\|\nabla f_{i_k}(x_k) - \nabla f_{i_k}(v_s) + \nabla F(v_s)\|_2^2] \\ &= \mathbb{E}_{i_k} [\|\nabla f_{i_k}(x_k) - \nabla f_{i_k}(x_*) + \nabla f_{i_k}(x_*) - \nabla f_{i_k}(v_s) + \nabla F(v_s)\|_2^2] \\ &\leq 2\mathbb{E}_{i_k} [\|\nabla f_{i_k}(x_k) - \nabla f_{i_k}(x_*)\|_2^2] \\ &\quad + 2\mathbb{E}_{i_k} [\|\nabla f_{i_k}(x_*) - \nabla f_{i_k}(v_s) + \nabla F(v_s)\|_2^2], \end{aligned}$$

where the last inequality follows from $\|a + b\|_2^2 \leq 2\|a\|_2^2 + 2\|b\|_2^2$. Based on Lemma 4, we can further rewrite the second term in above inequality as

$$\begin{aligned} &2\mathbb{E}_{i_k} [\|\nabla f_{i_k}(x_*) - \nabla f_{i_k}(v_s) + \nabla F(v_s)\|_2^2] \\ &= 2\mathbb{E}_{i_k} \left[\underbrace{\|\nabla f_{i_k}(x_*) - \nabla f_{i_k}(v_s) - (\nabla F(x_*) - \nabla F(v_s))\|_2^2}_{:=Y} \right] \\ &\leq 2\mathbb{E}_{i_k} \left[\underbrace{\|\nabla f_{i_k}(x_*) - \nabla f_{i_k}(v_s)\|_2^2}_{:=\|Y\|_2^2} \right]. \end{aligned}$$

Therefore,

$$\mathbb{E}_{i_k} [\|g_k\|_2^2] \leq 2\mathbb{E}_{i_k} [\|\nabla f_{i_k}(x_k) - \nabla f_{i_k}(x_*)\|_2^2] + 2\mathbb{E}_{i_k} [\|\nabla f_{i_k}(v_s) - \nabla f_{i_k}(x_*)\|_2^2].$$

By using Lemma 5, above equation could be further lead to

$$\mathbb{E}_{i_k} [\|g_k\|_2^2] \leq 4L (F(x_k) - F(x_*)) + 4L (F(v_s) - F(x_*)).$$

□

2.3 Convergence for each stage

Recall $s \in [S]$ is the index of a stage. Denote z_s all the randomness (in the inner iterations) at stage s .

Theorem 3. *Suppose each $f_i(\cdot)$ is L -smooth and μ -strongly convex. Setting $\eta = \frac{1}{8L}$ and $K = 64\frac{L}{\mu}$. Then, at each stage s ,*

$$\mathbb{E}_{z_s} [F(v_{s+1}) - F(x_*)] \leq \frac{3}{4} (F(v_s) - F(x_*)), \quad (16)$$

where $x_* \in \arg \min_x F(x)$.

Proof. By Theorem 1, we have

$$\frac{1}{K} \sum_{k=1}^K \mathbb{E}_{z_s} [F(x_k) - F(x_*)] \leq \frac{\eta}{2K} \left(\sum_{k=1}^K \mathbb{E}_{z_s} [\|g_k\|_2^2] \right) + \frac{F(x_1) - F(x_*)}{\eta\mu K}. \quad (17)$$

Recall the lemma of the variance bound, i.e., Lemma 3, we have, given x_k and v_s ,

$$\mathbb{E}_{i_k} [\|g_k\|_2^2] \leq 4L (F(x_k) - F(x_*)) + 4L (F(v_s) - F(x_*)). \quad (18)$$

Taking expectation over all the randomness at stage s on both sides of (18) further, we have

$$\mathbb{E}_{z_s} [\|g_k\|_2^2] \leq \mathbb{E}_{z_s} \left[4L (F(x_k) - F(x_*)) + 4L (F(v_s) - F(x_*)) \right]. \quad (19)$$

Summing (19) over all the inner iterations at stage s , we get

$$\frac{\eta}{2K} \sum_{k=1}^K \mathbb{E}_{z_s} [\|g_k\|_2^2] \leq \frac{\eta}{2K} \sum_{k=1}^K \mathbb{E}_{z_s} \left[4L (F(x_k) - F(x_*)) + 4L (F(v_s) - F(x_*)) \right]. \quad (20)$$

Combining (17) and (20), we have

$$(1 - 2\eta L) \frac{1}{K} \sum_{k=1}^K \mathbb{E}_{z_s} [F(x_k) - F(x_*)] \leq \left(2\eta L + \frac{1}{\eta\mu K} \right) (F(x_1) - F(x_*)). \quad (21)$$

Setting $\eta = \frac{1}{8L}$ and $K = 64\frac{L}{\mu}$, we have

$$\mathbb{E}_{z_s} [F(\bar{x}_K) - F(x_*)] \leq \frac{1}{K} \sum_{k=1}^K \mathbb{E}_{z_s} [F(x_k) - F(x_*)] \leq \frac{3}{4} (F(x_1) - F(x_*)), \quad (22)$$

where the first inequality follows from Jensen's inequality.

By the algorithm design, we have that x_1 is equal to the snapshot v_s at each stage s . Therefore, $\frac{3}{4} (F(x_1) - F(x_*)) = \frac{3}{4} (F(v_s) - F(x_*))$. Additionally, \bar{x}_k is used to initialize x_1 and the snapshot v_{s+1} in the next stage. Thus, $\mathbb{E}_{z_s} [F(\bar{x}_K) - F(x_*)] = \mathbb{E}_{z_s} [F(v_{s+1}) - F(x_*)]$. We can hence re-write (22) as

$$\mathbb{E}_{z_s} [F(v_{s+1}) - F(x_*)] \leq \frac{3}{4} (F(v_s) - F(x_*)).$$

Thus, the above means that the expected gap is shrinking within a constant factor in each stage. □

3 Complexity Analysis

3.1 Iteration complexity of SVRG

To get an expected ϵ -gap, the total number of stages is:

$$\begin{aligned} & \mathbb{E}_{z_{1:s}} [F(v_{s+1}) - F(x_*)] \\ &= \sum \Pr(z_{1:s-1} = \cdot) \mathbb{E}_{z_s} [F(v_{s+1}) - F(x_*) | z_{1:s-1} = \cdot] \\ &= \mathbb{E}_{z_{1:s-1}} \left[\mathbb{E}_{z_s} [F(v_{s+1}) - F(x_*) | z_{1:s-1}] \right]. \end{aligned} \quad (23)$$

According to Theorem 3, we have

$$\begin{aligned} \mathbb{E}_{z_{1:s}} [F(v_{s+1}) - F(x_*)] &\leq \frac{3}{4} \mathbb{E}_{z_{1:s}} [F(v_s) - F(x_*)] \\ &\leq \left(\frac{3}{4} \right)^s (F(v_1) - F(x_*)) \\ &\leq \epsilon \end{aligned}$$

$$\Leftrightarrow S \geq 4 \log \left(\frac{F(v_1) - F(x_*)}{\epsilon} \right) = \mathcal{O} \left(\log \left(\frac{1}{\epsilon} \right) \right)$$

. According to the above calculations, the total number of stochastic gradient computations could be represented by

$$2 \times K \times S = \mathcal{O} \left(\frac{L}{\mu} \log \left(\frac{1}{\epsilon} \right) \right). \quad (24)$$

Total number of Full gradient computations is

$$S = \mathcal{O} \left(n \log \left(\frac{1}{\epsilon} \right) \right). \quad (25)$$

Here, the cost of the full gradient computation = cost of n stochastic gradient computation. Total number of (equivalent) stochastic gradient computations is

$$\mathcal{O} \left(\frac{L}{\mu} \log \left(\frac{1}{\epsilon} \right) \right) + \mathcal{O} \left(n \log \left(\frac{1}{\epsilon} \right) \right). \quad (26)$$

3.2 SVRG v.s. GD

Therefore, we could obtain

$$\begin{aligned} & \frac{\text{runtime of SVRG}}{\text{runtime of GD}} \\ &= \frac{\# \text{ (equivalent) stochastic gradient computs. of SVRG}}{\# \text{ (equivalent) stochastic gradient computs. of GD}} \\ &= \frac{\left(\frac{L}{\mu} + n \right) \log \left(\frac{1}{\epsilon} \right)}{\frac{L}{\mu} \log \left(\frac{1}{\epsilon} \right) \times n}. \end{aligned} \quad (27)$$

Lets prove that the runtime of SVRG is generally smaller than runtime of GD, i.e.

$$\begin{aligned} \frac{\text{runtime of SVRG}}{\text{runtime of GD}} \leq 1 &\Leftrightarrow \frac{\left(\frac{L}{\mu} + n \right) \log \left(\frac{1}{\epsilon} \right)}{\frac{L}{\mu} \log \left(\frac{1}{\epsilon} \right) \times n} \leq 1 \\ &\Leftrightarrow n \leq (n-1) \frac{L}{\mu} \\ &\Leftrightarrow \mu \leq L, \text{ as } n \rightarrow \infty \end{aligned}$$

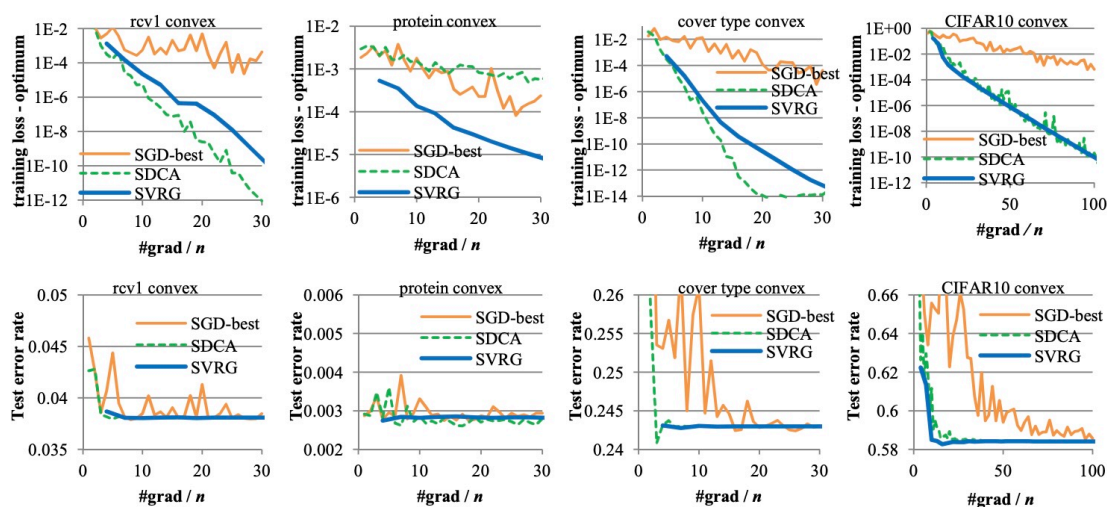
which is always true. The proof is completed.

3.3 SVRG v.s. SGD

$$\frac{\text{runtime of SVRG}}{\text{runtime of SGD}} = \frac{\left(\frac{L}{\mu} + n\right) \log\left(\frac{1}{\epsilon}\right)}{\frac{1}{\epsilon} \times 1}.$$

The condition for SVRG to be faster than SGD is when

$$\left(\frac{L}{\mu} + n\right) \log\left(\frac{1}{\epsilon}\right) \ll \frac{1}{\epsilon} \Leftrightarrow \left(\frac{L}{\mu} + n\right) \ll \frac{1}{\log\left(\frac{1}{\epsilon}\right)}.$$



ℓ_2 -regularized logistic regression on CIFAR-10

Figure 2: ℓ_2 - regularized logistic regression on CIFAR-10. [Johnson (2013)]

Bibliographic notes

More information can be found in [Drusvyatskiy (2020)], [Vishnoi (2021)], [Rakhlin (2012)], and [Johnson (2013)].

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