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Lecture 7: Introduction to Stochastic Optimization

# 1 Review: Projected Gradient Descent and Frank-Wolfe Method

We begin by reviewing some results concerning Projected Gradient Descent and Frank-Wolfe method. Below is a formal statement of the Frank-Wolfe method algorithm.

Algorithm 1 Frank-Wolfe method

1: Initialize  $\mathbf{x}_1 \in C$ . 2: for k = 1, 2, ... do 3:  $\mathbf{v}_k = \arg\min_{\mathbf{v}\in C} \langle \mathbf{v}, \nabla f(\mathbf{x}_k) \rangle$  (linear optimization) 4:  $\mathbf{x}_{k+1} = (1 - \eta_k)\mathbf{x}_k + \eta_k \mathbf{v}_k$ , where  $\eta_k \in [0, 1]$ . 5: end for

**Theorem 1.** Assume  $f(\cdot)$  is a L-smooth convex function. Denote  $D := \max_{\mathbf{x}, \mathbf{y} \in C} \|\mathbf{x} - \mathbf{y}\|_2$ ,  $\forall \mathbf{x}, \mathbf{y} \in C$  as the diameter of the set C. Let  $\eta_k = \min\{1, \frac{2}{k}\} \in [0, 1]$ . Then, Frank-Wolfe has:

$$f(x_K) - f(x_*) \le \frac{2LD^2}{K}.$$

Recall that PGD and GD share the same convergence rate. Specifically, if PGD is to achieve an  $\epsilon$ -optimality gap in a constrained optimization problem:  $f(\mathbf{x}_k) - \min_{\mathbf{x}\in C} f(\mathbf{x}) \leq \epsilon$ , or if GD is to achieve an  $\epsilon$ -optimality gap in an unconstrained optimization problem:  $f(\mathbf{x}_k) - \min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x}) \leq \epsilon$ , then the table below illustrates the convergence rates for both PGD and GD.

Convergence Rate	PGD	GD
L-smooth convex	$O\left(\frac{L}{k}\right)$	$O\left(\frac{L}{k}\right)$
L-smooth and $\mu$ -strongly convex	$O\left(\exp\left(-\frac{\mu}{L}k\right)\right)$	$O\left(\exp\left(-\frac{\mu}{L}k\right)\right)$

A natural question is: Can we achieve a faster convergence rate than  $O\left(\frac{1}{K}\right)$  using Frank-Wolfe method when f is assumed to be smooth and strongly convex? The answer to this crucially relies on the regularity of the constrained set. We present two examples (see [1] and [2]) in the following.

**Example 1** (A negative result). If C is a probability simplex, i.e.,  $C := \{x \in \mathbb{R}^d : \sum_{i=1}^d x[i] \le 1, x[i] \ge 0\}$ , then  $K = \Omega\left(\max\left(\frac{L}{\epsilon}, \frac{d}{2}\right)\right)$ .

**Example 2** (A positive result). Frank-Wolfe method gives a faster convergence rate when C is a  $\mu$ -strongly convex set w.r.t. a norm  $\|\cdot\|$ , i.e.,  $x, z \in C$  implies that a ball centered at  $\alpha x + (1 - \alpha)z$  with a radius in  $\alpha(1 - \alpha)\frac{\mu}{2}\|x - z\|^2$  is in C, where  $\alpha \in [0, 1]$ . In particular, any  $l_p$  norm with  $p \in (1, 2]$  satisfies the requirement.

We refer to [3] and [4] for further details.

## 2 Introduction to Stochastic Optimization

Consider the following problem:

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

Here z denotes the randomness of this problem. Below is a formal statement of the SGD algorithm.

Algorithm 2 Stochastic Gradient Descent (SGD)

1: for k = 1, 2, ... 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

**Example 3** (Finite-sum problem). Let  $F(x) := \frac{1}{n} \sum_{i=1}^{n} f_i(x) = \mathbb{E}_i[f_i(x)]$ . Then the SGD algorithm for finite-sum problem can be explicitly stated as follows:

Algorithm 3 Stochastic Gradient Descent (SGD) for finite-sum problem				
1: <b>f</b>	for $k = 1, 2, \ldots$ do			
2:	Randomly sample $i_k \in [n]$			
3:	Compute $g_k = \nabla f_{i_k}(x_k)$			
4:	$x_{k+1} = x_k - \eta g_k.$			

5: end for

Notice that,

$$\mathbb{E}[g_k] = \sum_{i=1}^n P(i_k = i) \ \nabla f_i(x_k) = \sum_{i=1}^n \frac{1}{n} \nabla f_i(x_k) = \nabla F(x_k)$$

Convergence Rate	SGD	GD
L-smooth convex	$O\left(\frac{1}{\sqrt{K}}\right)$	$O\left(\frac{1}{K}\right)$
<b>L-smooth and</b> $\mu$ -strongly convex	$O\left(\frac{1}{K}\right)$	$O\left(\exp(-K)\right)$

The convergence rates for SGD and GD are presented in the following table.

For SGD, we compute

$$\epsilon = \frac{1}{\sqrt{K}} \Leftrightarrow K = \frac{1}{\epsilon^2},$$

so we asymptotically need  $\frac{1}{\epsilon^2}$  iterations to reach an  $\epsilon\text{-optimality}$  gap. For GD, we compute

$$\epsilon = \frac{1}{K} \Leftrightarrow K = \frac{1}{\epsilon},$$

so we asymptotically need  $\frac{1}{\epsilon}$  iterations to reach an  $\epsilon$ -optimality gap. Therefore, considering the practical scenario where  $0 < \epsilon << 1$ , SGD generally requires more iterations than GD to reach the given optimality gap. However, in terms of running time, formally we have

$$\frac{\text{running time of SGD}}{\text{running time of GD}} = \frac{\# \text{ iterations of SGD}}{\# \text{ iterations of GD}} \times \frac{\text{cost per step SGD}}{\text{cost per step GD}}$$

Comparing the convergence rate of SGD and GD, we have (see [5])  $\frac{\# \text{ iterations of SGD}}{\# \text{ iterations of GD}} = \frac{1}{\epsilon^2}/\frac{1}{\epsilon}$ . In each iteration of SGD, we only need to compute the gradient for one random case among *n* possibilities, so  $\frac{\text{cost per step SGD}}{\text{cost per step GD}} = \frac{1}{n}$ . Therefore,

$$\frac{\text{running time of SGD}}{\text{running time of GD}} = \frac{1}{\epsilon n}$$

In order for SGD to have a better performance than GD, i.e.,  $\frac{\text{running time of SGD}}{\text{running time of GD}} << 1$ , we need to ensure  $\frac{1}{\epsilon} << n$ . This condition is usually fulfilled when we have a very large sample size/data set. For example, consider the empirical risk minimization problem. Let  $\{(y_i, z_i), i \in [n]\}$  be the data set and the function  $F(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x)$ , where  $f_i(x) = \frac{1}{2}(y_i - z_i^T x)^2$ . Since, in practical applications, we may have a very large n and expect a relatively large  $\epsilon$  considering the possible overshooting effect, it is reasonable to assume that  $\frac{1}{\epsilon} << n$ .

# **3** Iteration Complexity of SGD:

We now present a theorem that provides an upper-bound for the optimality gap obtained through SGD.

**Theorem 2.** Let  $F(x) = \mathbb{E}_{z}[f(x;z)] : \mathbb{R}^{d} \to \mathbb{R}$  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.,  $||x_{1} - x_{*}|| \leq D$ . Then,

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

*Proof.* One way to gauge the progress of an iterative optimization algorithm is through the distance metric  $d_k$ , which calculates the Euclidean distance between the updated point in the k-th iteration, denoted as  $x_{k+1}$ , and the global minima point  $x_*$ . This can be expressed as  $d_k = ||x_{k+1} - x_*||_2$ .

Now, when we apply Stochastic Gradient Descent (SGD) to the convex function  $F(x) = \mathbb{E}_z[f(x; z)] : \mathbb{R}^d \to \mathbb{R}$ , it is clear from the nature of the SGD algorithm (refer to Algorithm 2) that the distance metric  $d_k = ||x_{k+1} - x_*||_2$ , will be a random variable since  $x_{k+1}$  is a random variable. Therefore, our first step in this proof will be to consider the expected value of the squared distance metric  $d_k$ , that is  $\mathbb{E}[||x_{k+1} - x_*||_2^2]$ .

We have the following,

$$\mathbb{E}[||x_{k+1} - x_*||_2^2] = \mathbb{E}[||x_k - \eta g_k - x_*||_2^2] \quad (\text{SGD's update, see Algorithm 2})$$

$$= \mathbb{E}[||x_k - x_*||_2^2 - 2\eta \langle g_k, x_k - x_* \rangle + \eta^2 ||g_k||_2^2]$$

Rearranging the above equation we get,

$$2\eta \cdot \mathbb{E}[\langle g_k, x_k - x_* \rangle] = \mathbb{E}[||x_k - x_*||_2^2 - ||x_{k+1} - x_*||_2^2] + \eta^2 \mathbb{E}[||g_k||_2^2]$$

$$\Leftrightarrow \mathbb{E}[\langle g_k, x_k - x_* \rangle] = \frac{\mathbb{E}[||x_k - x_*||_2^2 - ||x_{k+1} - x_*||_2^2]}{2\eta} + \frac{\eta}{2} \mathbb{E}[||g_k||_2^2]$$
(2)

Now, notice the term inside the expectation operator on the L.H.S of the equation

(2), i.e.  $\langle g_k, x_k - x_* \rangle$ . In this term, it is evident that  $g_k$  and  $x_k$  are random variables. Let us understand how.

In line 2 of the SGD Algorithm (refer to 2), it states: "Compute a stochastic gradient  $g_k$  such that  $\mathbb{E}_z[g_k] = \nabla F(x_k)$ ". This definition of the stochastic gradient  $g_k$ indicates that  $g_k$  is influenced by both the current point  $x_k$  and the randomness associated with the k-th iteration, denoted as  $z_k$  (which corresponds to the sampled index number in the finite-sum problem). Consequently, considering the update expression of SGD as  $x_{k+1} = x_k - \eta g_k$ , it follows that the next update  $x_{k+1}$  also depends on the current point  $x_k$  and the randomness of the k-th iteration  $z_k$ .

Let's begin by assuming that the initial point  $x_1$  is known. Consequently, the randomness affecting  $g_1$  (and therefore  $x_2$ ) is entirely based on  $z_1$ . In other words, if  $z_1$ is known, then  $g_1$  (and thus  $x_2$ ) can be computed deterministically.

Now, let's delve into the second iteration step. We understand that the randomness influencing  $g_2$  (and hence  $x_3$ ) relies on both  $z_2$  and the current point  $x_2$ , whose randomness, in turn, depends on  $z_1$ . This implies that if both  $z_1$  and  $z_2$  are known, then  $g_2$  (and hence  $x_3$ ) can be determined with certainty. Consequently, through this analysis and the application of mathematical induction, we can infer that  $g_k$  is influenced by  $z_1, z_2, \ldots, z_k$ , while  $x_k$  depends on  $z_1, z_2, \ldots, z_{k-1}$ .

So, with the analysis that we performed above, and denoting  $z_{1:k} = z_1, z_2, \ldots, z_k$ , we can write that,

$$\mathbb{E}[\langle g_k, x_k - x_* \rangle] = \mathbb{E}_{z_{1:k}}[\langle g_k, x_k - x_* \rangle]$$

$$= \sum_{\circ} \Pr(z_{1:k-1} = \circ) \mathbb{E}_{z_k}[\langle g_k, x_k - x_* \rangle \mid z_{1:k-1} = \circ] \quad \text{(Law of Total Expectation)}$$

$$= \mathbb{E}_{z_{1:k-1}} \left[ \mathbb{E}_{z_k}[\langle g_k, x_k - x_* \rangle \mid z_{1:k-1}] \right]$$

$$= \mathbb{E}_{z_{1:k-1}} \left[ \mathbb{E}_{z_k}[\langle g_k, x_k - x_* \rangle \mid x_k] \right] \quad \text{(Since, } x_k \text{ is determined by } z_{1:k-1} \right]$$

$$(3)$$

Now, let us suppose that we are dealing with the finite-sum problem, where we attempt to minimize  $F(x) := \frac{1}{n} \sum_{i=1}^{n} f_i(x) = \mathbb{E}_i[f_i(x)]$ . From Algorithm 3, it is evident that when SGD is applied for solving this problem, the index  $i_k$  is the source of randomness associated with each iteration. Furthermore, after randomly sampling

 $i_k$ , the stochastic gradient is computed as:  $g_k = \nabla f_{i_k}(x_k)$ . So, the inner expectation term  $\mathbb{E}_{z_k}[\langle g_k, x_k - x_* \rangle | x_k]$  in Equation (3) can be written as follows,

$$\mathbb{E}_{z_k}[\langle g_k, x_k - x_* \rangle | x_k] = \mathbb{E}_{i_k}[\langle \nabla f_{i_k}(x_k), x_k - x_* \rangle | x_k]$$

$$= \sum_{i=1}^n \Pr(i_k = i) \langle \nabla f_i(x_k), x_k - x_* \rangle$$

$$= \sum_{i=1}^n \frac{1}{n} \langle \nabla f_i(x_k), x_k - x_* \rangle$$

$$= \langle \sum_{i=1}^n \frac{1}{n} \nabla f_i(x_k), x_k - x_* \rangle$$

$$= \langle \nabla F(x_k), x_k - x_* \rangle$$
(4)

The final equation follows from the fact that

$$F(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x) \implies \nabla F(x_k) = \sum_{i=1}^{n} \frac{1}{n} \nabla f_i(x_k).$$

Using the above expression for  $\mathbb{E}_{z_k}[\langle g_k, x_k - x_* \rangle | x_k]$  in the R.H.S of Equation (3), we can write the following,

$$\mathbb{E}[\langle g_k, x_k - x_* \rangle] = \mathbb{E}_{z_{1:k-1}} [\langle \nabla F(x_k), x_k - x_* \rangle]$$
$$= \mathbb{E}_{z_{1:k}} [\langle \nabla F(x_k), x_k - x_* \rangle] \quad (\text{Since, } x_k \text{ is independent of } z_k)$$
(5)

Since it is given that  $F(x) = \mathbb{E}_{z}[f(x; z)] : \mathbb{R}^{d} \to \mathbb{R}$  is a convex function, therefore from the first-order characterization of convexity, we can say that the following will be true,

$$F(x_*) \geq F(x_k) + \langle \nabla F(x_k), x_* - x_k \rangle$$
  

$$\Leftrightarrow F(x_k) - F(x_*) \leq \langle \nabla F(x_k), x_k - x_* \rangle$$
  

$$\Rightarrow \mathbb{E}_{z_{1:k}}[F(x_k) - F(x_*)] \leq \mathbb{E}_{z_{1:k}}[\langle \nabla F(x_k), x_k - x_* \rangle].$$
(6)

Using the above inequality in the last line of Equation (5) we get the following,

$$\mathbb{E}_{z_{1:k}}[F(x_k) - F(x_*)] \leq \mathbb{E}[\langle g_k, x_k - x_* \rangle].$$
(7)

Now, if we further combine the inequality result that we obtained above with the final equation of 2 we get that,

$$\mathbb{E}[F(x_k) - F(x_*)] \leq \frac{\mathbb{E}[||x_k - x_*||_2^2 - ||x_{k+1} - x_*||_2^2]}{2\eta} + \frac{\eta}{2} \mathbb{E}[||g_k||_2^2].$$
(8)

Summing up the inequality of (8) from k = 1 to K we get the following,

$$\sum_{k=1}^{K} \mathbb{E}[F(x_k) - F(x_*)] \leq \frac{\mathbb{E}[||x_1 - x_*||_2^2]}{2\eta} - \frac{\mathbb{E}[||x_{K+1} - x_*||_2^2]}{2\eta} + \frac{\eta}{2} \left( \sum_{k=1}^{K} \mathbb{E}[||g_k||_2^2] \right)$$
$$= \frac{||x_1 - x_*||_2^2}{2\eta} - \frac{\mathbb{E}[||x_{K+1} - x_*||_2^2]}{2\eta} + \frac{\eta}{2} \left( \sum_{k=1}^{K} \mathbb{E}[||g_k||_2^2] \right) \quad (x_1 \text{ is known})$$
$$\leq \frac{||x_1 - x_*||_2^2}{2\eta} + \frac{\eta}{2} \left( \sum_{k=1}^{K} \mathbb{E}[||g_k||_2^2] \right) \quad \left( \text{Since, } \frac{\mathbb{E}[||x_{K+1} - x_*||_2^2]}{2\eta} \geq 0 \right).$$
(9)

Using the Linearity of Expectation on the LHS of the inequality (9) we get the

following,

$$\mathbb{E}\left[\sum_{k=1}^{K} (F(x_k) - F(x_*))\right] \leq \frac{||x_1 - x_*||_2^2}{2\eta} + \frac{\eta}{2} \left(\sum_{k=1}^{K} \mathbb{E}\left[||g_k||_2^2\right]\right).$$
(10)

Now, if we divide both sides of the above inequality by K, we finally obtain the following guarantee inequation for the application of SGD to convex functions of the form  $F(x) = \mathbb{E}_z[f(x; z)] : \mathbb{R}^d \to \mathbb{R}$ ,

$$\frac{1}{K}\mathbb{E}\left[\sum_{k=1}^{K} (F(x_k) - F(x_*))\right] \le \frac{\eta}{2K} \left(\sum_{k=1}^{K} \mathbb{E}\left[\|g_k\|_2^2\right]\right) + \frac{\|x_1 - x_*\|_2^2}{2\eta K}.$$
 (11)

**Corollary 1.** Let us denote  $\bar{x}_K := \frac{1}{K} \sum_{k=1}^K x_k$ . Then,

$$\mathbb{E}\left[F(\bar{x}_K) - F(x_*)\right] \leq \frac{1}{K} \mathbb{E}\left[\sum_{k=1}^K (F(x_k) - F(x_*))\right].$$
(12)

*Proof.* Jensen's Inequality states the following: If  $g(\cdot) : \mathbb{R}^d \to \mathbb{R}$  is a convex function, and D is any discrete distribution over  $x_1, x_2, \dots, x_n \in \mathbb{R}^d$ . Then the following inequality holds,

$$g\left(\sum_{i=1}^{n} p_i x_i\right) \leq \sum_{i=1}^{n} p_i \cdot g(x_i), \tag{13}$$

where  $p_i \ge 0, \forall i \in [n]$ , and  $\sum_{i \in [n]} p_i = 1$ .

Therefore, knowing that  $F(x) = \mathbb{E}_{z}[f(x;z)] : \mathbb{R}^{d} \to \mathbb{R}$  is a convex function, and considering D to be the uniform discrete distribution over  $x_{1}, x_{2}, x_{3}, \dots, x_{K}$  (i.e.  $p_{k} = \frac{1}{K}, \forall k \in [K]$ ), we can write the following

$$F\left(\frac{1}{K}\sum_{k=1}^{K}x_{k}\right) \leq \frac{1}{K}\sum_{k=1}^{K}F(x_{k})$$

$$\Leftrightarrow F\left(\frac{1}{K}\sum_{k=1}^{K}x_{k}\right) - F(x_{*}) \leq \left(\frac{1}{K}\sum_{k=1}^{K}F(x_{k})\right) - F(x_{*})$$

$$\Leftrightarrow F(\bar{x}_{K}) - F(x_{*}) \leq \frac{1}{K}\sum_{k=1}^{K}(F(x_{k}) - F(x_{*})) \qquad \left(\text{Denoting } \bar{x}_{K} \coloneqq \frac{1}{K}\sum_{k=1}^{K}x_{k}\right)$$

$$\Rightarrow \mathbb{E}\left[F(\bar{x}_{K}) - F(x_{*})\right] \leq \frac{1}{K}\mathbb{E}\left[\sum_{k=1}^{K}(F(x_{k}) - F(x_{*}))\right].$$
(14)

**Lemma 1.** In addition, let us make another assumption, that the expectation of the squared  $\ell_2$ -norm of stochastic gradient is bounded, i.e.  $\mathbb{E}\left[ ||g_k||_2^2 \right] \leq G^2$ . Then we shall have,

$$\mathbb{E}\left[F(\bar{x}_K) - F(x_*)\right] \leq \frac{\eta}{2}G^2 + \frac{D^2}{2\eta K}.$$
(15)

(For a concrete understanding of the conditions under which this assumption shall hold, refer to Lemma 2.6 in [7])

*Proof.* By taking into account the guarantee of the SGD algorithm (as provided by **Theorem 2** in (1)), and the inequality identity that is provided by **Corollary 1** in (12), we can write the following,

$$\mathbb{E}\left[F(\bar{x}_{K}) - F(x_{*})\right] \leq \frac{\eta}{2K} \left(\sum_{k=1}^{K} \mathbb{E}\left[\|g_{k}\|_{2}^{2}\right]\right) + \frac{\|x_{1} - x_{*}\|^{2}}{2\eta K}.$$
 (16)

Under the assumption that  $\mathbb{E}\left[||g_k||_2^2\right] \leq G^2$ , and using the fact that the initial distance is bounded, i.e.,  $||x_1-x_*|| \leq D$ , we can re-write the final inequality expression

of (16) as follows,

$$\mathbb{E}\left[F(\bar{x}_{K}) - F(x_{*})\right] \leq \frac{\eta}{2K} \left(\sum_{k=1}^{K} \mathbb{E}\left[\|g_{k}\|_{2}^{2}\right]\right) + \frac{\|x_{1} - x_{*}\|^{2}}{2\eta K}$$

$$\leq \frac{\eta}{2}G^{2} + \frac{D^{2}}{2\eta K}.$$

$$(17)$$

**Remark 1:** The inequality of (17), thus gives an upper-bound for the expectation of the optimality gap, when the function  $F(\cdot)$  is evaluated at the point formed by average of the updates  $\left(\bar{x}_{K} = \frac{1}{K} \sum_{k=1}^{K} x_{k}\right)$ .

**Remark 2:** Knowing that the step-size  $\eta$  is always positive, the upper-bound expression can be thought of as a convex function,  $g(\eta) = \left(\frac{\eta}{2}G^2 + \frac{D^2}{2\eta K}\right)$ :  $\mathbb{R} \to \mathbb{R}$ , since the second-order derivative  $g''(\eta) = \frac{D^2}{\eta^3 K}$  is always positive. Furthermore, it can be analytically determined that the minimum value of the upper-bound  $g(\cdot)$  is  $\frac{DG}{\sqrt{K}}$ , which is obtained at  $\eta^* = \frac{D}{G\sqrt{K}}$ .

## 4 SGD for Non-Convex Functions:

**Theorem 3.** Assume that the variance of the stochastic gradient  $\nabla f(x; z)$  is at most  $\sigma^2$  for all x, i.e.,  $\mathbb{E}_z \left[ \|\nabla f(x; z) - \nabla F(x)\|_2^2 \right] \leq \sigma^2$ . Suppose  $F(\cdot)$  is L-smooth. Then, SGD with the step size  $\eta \leq \frac{1}{L}$  has the following guarantee,

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

**Remark 1:** If  $\eta = \min\left(\frac{1}{L}, \frac{\sqrt{F(x_1) - F_*}}{\sigma \sqrt{LK}}\right)$ , then

$$\sum_{k=1}^{K} \mathbb{E}\left[ \|\nabla F(x_k)\|_2^2 \right] \le 2 \left( F(x_1) - F_* \right) L + 3\sigma \sqrt{\left( F(x_1) - F_* \right) LK}.$$
(18)

**Remark 2:** Furthermore, with  $\eta = \min\left(\frac{1}{L}, \frac{\sqrt{F(x_1)-F_*}}{\sigma\sqrt{LK}}\right)$ , if  $\hat{x}$  is selected uniformly at random from  $x_1, \ldots, x_K$ , then we have,

$$\mathbb{E}\left[\|\nabla F(\hat{x})\|\right] \le \frac{\sqrt{2\left(F(x_1) - F_*\right)L}}{\sqrt{K}} + \frac{\sqrt{3\sigma}\sqrt{\left(F(x_1) - F_*\right)L}}{K^{1/4}}.$$
(19)

# 5 Mini-batch SGD for Non-Convex Functions:

**Objective:**  $\min_x F(x)$ , where  $F(x) := \mathbb{E}[f(x; z)]$ 

Below is a formal statement of the Mini-Batch SGD algorithm.

### Algorithm 4 MINI-BATCH STOCHASTIC GRADIENT DESCENT(MINI-BATCH SGD) 1: for k = 1 to K do 2: for i = 1 to B do 3: $g_{k,i} = \nabla f(x_k; z_{(k-1)B+i})$ 4: end for 5: $g_k = \frac{1}{B} \sum_{i=1}^{B} g_{k,i}$ 6: $x_{k+1} = x_k - \eta g_k$ 7: end for

**Remark:** The parameter B is called the *batch size*. When B=1, we have vanilla SGD.

# 5.1 The variance is $\frac{\sigma^2}{B}$

**Lemma 2.** Assume that the variance of the stochastic gradient  $\nabla f(x; z)$  is at most  $\sigma^2$  for all x, i.e.,  $\mathbb{E}_z \left[ \|\nabla f(x; z) - \nabla F(x)\|_2^2 \right] \leq \sigma^2$ . Then,

$$\mathbb{E}_{z}\left[\|g_{k} - \nabla F(x_{k})\|_{2}^{2}\right] \leq \frac{\sigma^{2}}{B}$$

$$\tag{20}$$

*Proof.* Given that  $\mathbb{E}_{z}\left[\|\nabla f(x;z) - \nabla F(x)\|_{2}^{2}\right] \leq \sigma^{2}$ . From the mini-batch SGD algorithm, as shown in 4, we know that,

$$g_k = \frac{1}{B} \sum_{i=1}^{B} g_{k,i} = \frac{1}{B} \sum_{i=1}^{B} \nabla f(x_k; z_{(k-1)B+i})$$
(21)

The above formulation shows that, in order to compute  $g_k$  at each iteration step, the random variable z is sampled B times.

Let us denote,  $z_{k,i} := z_{(k-1)B+i}$ . We can make the generic assumption that in an iteration step k, each random variable  $z_{k,1}, z_{k,2}, \dots, z_{k,B}$  are independent of each other.

So, we have the following,

Consider the second term on the right-hand side of inequality (22). The term  $\|\nabla f(x_k; z_{k,i}) - \nabla F(x_k))\|_2$ depends on  $z_{k,i}$ , while the term  $\|\nabla f(x_k; z_{k,j}) - \nabla F(x_k))\|_2$  depends on  $z_{k,j}$ . When  $i \neq j$ , since  $z_{k,i}$  is independent of  $z_{k,j}$ , it implies that  $\|\nabla f(x_k; z_{k,i}) - \nabla F(x_k))\|_2$  is independent of  $\|\nabla f(x_k; z_{k,j}) - \nabla F(x_k))\|_2$ . Since covariance of independent terms is 0, therefore  $\forall i, j$  with  $i \neq j$ , we can write that,

$$\mathbb{E}_{z_{k,i}, z_{k,j}} \left[ \left\| \nabla f(x_k; z_{k,i}) - \nabla F(x_k) \right) \right\|_2 \left\| \nabla f(x_k; z_{k,j}) - \nabla F(x_k) \right) \right\|_2 \right] = 0.$$

Therefore, the final inequality expression of (22) becomes as follows,

$$\mathbb{E}_{z}\left[\|g_{k} - \nabla F(x_{k})\|_{2}^{2}\right] \leq \frac{1}{B^{2}} \sum_{i=1}^{B} \mathbb{E}_{z_{k,i}}\left[\left\|\nabla f(x_{k}; z_{k,i}) - \nabla F(x_{k})\right)\right\|_{2}^{2}\right].$$
(23)

Now, incorporating our initial assumption that  $\mathbb{E}_{z}\left[\|\nabla f(x;z) - \nabla F(x)\|_{2}^{2}\right] \leq \sigma^{2}$  in the above inequality we get,

$$\mathbb{E}_{z}\left[\|g_{k} - \nabla F(x_{k})\|_{2}^{2}\right] \leq \frac{1}{B^{2}} \sum_{i=1}^{B} \mathbb{E}_{z_{k,i}}\left[\left\|\nabla f(x_{k}; z_{k,i}) - \nabla F(x_{k})\right)\right\|_{2}^{2}\right] \leq \frac{1}{B^{2}} \sigma^{2} B = \frac{\sigma^{2}}{B}.$$
(24)

Thus, we have shown that:  $\mathbb{E}_{z}\left[\|g_{k}-\nabla F(x_{k})\|_{2}^{2}\right] \leq \frac{\sigma^{2}}{B}$ .

#### 

#### 5.2 Iteration complexity of Mini-Batch SGD

Recall **Remark 2** of when SGD is applied to non-convex smooth functions (see 19): with  $\eta = \min\left(\frac{1}{L}, \frac{\sqrt{F(x_1)-F_*}}{\sigma\sqrt{LK}}\right)$ , if  $\hat{x}$  is selected uniformly at random from  $x_1, \ldots, x_K$ , then we have,

$$\mathbb{E}\left[\|\nabla F(\hat{x})\|\right] \le \frac{\sqrt{2(F(x_1) - F_*)L}}{\sqrt{K}} + \frac{\sqrt{3\sigma(\sqrt{F(x_1) - F_*})L}}{K^{1/4}}$$
(25)

So, if we assume that the variance of the stochastic gradient  $\nabla f(x; z)$  is at most  $\sigma^2$ and set  $\eta = \min\left(\frac{1}{L}, \sqrt{\frac{F(x_1) - F^*}{\left(\frac{\sigma}{\sqrt{B}}\right)\sqrt{LK}}}\right)$ , then we could obtain the following guarantee for Mini-batch SGD by substituting  $\sigma \leftarrow \frac{\sigma}{\sqrt{B}}$  in 25,

$$\mathbb{E}\left[\|\nabla F(\hat{x})\|\right] \le \frac{\sqrt{2(F(x_1) - F_*)L}}{\sqrt{K}} + \frac{\sqrt{3\sigma\sqrt{(F(x_1) - F_*)L}}}{(BK)^{1/4}}$$
(26)

## 5.3 Comparison between SGD and Mini-Batch SGD

	Vanilla SGD	Mini-batch SGD
Convergence Rate	$\frac{1}{K^{1/4}}$	$\frac{1}{(BK)^{1/4}}$
number of Stochastic Gradients per Iteration	1	В
total number of stochastic gradients over K	K	BK
Convergence Rate	$\frac{1}{(total \ \# \ of \ sg)^{1/4}}$	$\frac{1}{(total \ \# \ of \ sg)^{1/4}}$

# **Bibliographic notes**

More information on Stochastic Optimization can be found in [6] and [5].

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