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# A Unified Theory of SGD: Variance Reduction, Sampling, Quantization and Coordinate Descent

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## Abstract

In this paper we introduce a unified analysis of a large family of variants of proximal stochastic gradient descent (SGD) which so far have required different intuitions, convergence analyses, have different applications, and which have been developed separately in various communities. We show that our framework includes methods with and without the following tricks, and their combinations: variance reduction, importance sampling, mini-batch sampling, quantization, and coordinate sub-sampling. As a by-product, we obtain the first unified theory of SGD and randomized coordinate descent (RCD) methods, the first unified theory of variance reduced and non-variance-reduced SGD methods, and the first unified theory of quantized and non-quantized methods. A key to our approach is a parametric assumption on the iterates and stochastic gradients. In a single theorem we establish a linear convergence result under this assumption and strong-quasi convexity of the loss function. Whenever we recover an existing method as a special case, our theorem gives the best known complexity result. Our approach can be used to motivate the development of new useful methods, and offers pre-proved convergence guarantees. To illustrate the strength of our approach, we develop five new variants of SGD, and through numerical experiments demonstrate some of their properties.

## 1 Introduction

In this paper we are interested in the optimization problem

$$\min_{x \in \mathbb{R}^d} f(x) + R(x), \quad (1)$$

where  $f$  is convex, differentiable with Lipschitz gradient, and  $R : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$  is a proximable (proper closed convex) regularizer. In particular, we focus on situations when it is prohibitively expensive to compute the gradient of  $f$ , while an unbiased estimator of the gradient can be computed efficiently. This is typically the case for stochastic optimization problems, i.e., when

$$f(x) = \mathbf{E}_{\xi \sim \mathcal{D}} [f_{\xi}(x)], \quad (2)$$

where  $\xi$  is a random variable, and  $f_{\xi} : \mathbb{R}^d \rightarrow \mathbb{R}$  is smooth for all  $\xi$ . Stochastic optimization problems are of key importance in statistical supervised learning theory. In this setup,  $x$  represents a machine learning model described by  $d$  parameters (e.g., logistic regression or a deep neural network),  $\mathcal{D}$  is an unknown distribution of labelled examples,  $f_{\xi}(x)$  represents the loss of model  $x$  on datapoint  $\xi$ , and  $f$  is the generalization error. Problem (1) seeks to find the model  $x$  minimizing the generalization error. In statistical learning theory one assumes that while  $\mathcal{D}$  is not known, samples  $\xi \sim \mathcal{D}$  are available. In such a case,  $\nabla f(x)$  is not computable, while  $\nabla f_{\xi}(x)$ , which is an unbiased estimator of the gradient of  $f$  at  $x$ , is easily computable.

Another prominent example, one of special interest in this paper, are functions  $f$  which arise as averages of a very large number of smooth functions:

$$f(x) = \frac{1}{n} \sum_{i=1}^n f_i(x). \quad (3)$$

This problem often arises by approximation of the stochastic optimization loss function (2) via Monte Carlo integration, and is in this context known as the empirical risk minimization (ERM) problem. ERM is currently the dominant paradigm for solving supervised learning problems (Shalev-Shwartz and Ben-David, 2014). If index  $i$  is chosen uniformly at random

from  $[n] := \{1, 2, \dots, n\}$ ,  $\nabla f_i(x)$  is an unbiased estimator of  $\nabla f(x)$ . Typically,  $\nabla f(x)$  is about  $n$  times more expensive to compute than  $\nabla f_i(x)$ .

Lastly, in some applications, especially in distributed training of supervised models, one considers problem (3), with  $n$  being the number of machines, and each  $f_i$  also having a finite sum structure, i.e.,

$$f_i(x) = \frac{1}{m} \sum_{j=1}^m f_{ij}(x), \quad (4)$$

where  $m$  corresponds to the number of training examples stored on machine  $i$ .

## 2 The Many Faces of Stochastic Gradient Descent

Stochastic gradient descent (SGD) (Robbins and Monro, 1951; Nemirovski et al., 2009; Vaswani et al., 2019) is a state-of-the-art algorithmic paradigm for solving optimization problems (1) in situations when  $f$  is either of structure (2) or (3). In its generic form, (proximal) SGD defines the new iterate by subtracting a multiple of a stochastic gradient from the current iterate, and subsequently applying the proximal operator of  $R$ :

$$x^{k+1} = \text{prox}_{\gamma R}(x^k - \gamma g^k). \quad (5)$$

Here,  $g^k$  is an unbiased estimator of the gradient (i.e., a stochastic gradient),

$$\mathbf{E}[g^k | x^k] = \nabla f(x^k), \quad (6)$$

and  $\text{prox}_{\gamma R}(x) := \text{argmin}_u \{\gamma R(x) + \frac{1}{2} \|u - x\|^2\}$ . However, and this is the starting point of our journey in this paper, there are *infinitely many* ways of obtaining a random vector  $g^k$  satisfying (6). On the one hand, this gives algorithm designers the flexibility to *construct* stochastic gradients in various ways in order to target desirable properties such as convergence speed, iteration cost, parallelizability and generalization. On the other hand, this poses considerable challenges in terms of convergence analysis. Indeed, if one aims to, as one should, obtain the sharpest bounds possible, dedicated analyses are needed to handle each of the particular variants of SGD.

**Vanilla<sup>1</sup> SGD.** The flexibility in the design of efficient strategies for constructing  $g^k$  has led to a creative renaissance in the optimization and machine learning communities, yielding a large number of immensely powerful new variants of SGD, such as those employing

<sup>1</sup>In this paper, by *vanilla* SGD we refer to SGD variants with or without importance sampling and mini-batching, but *excluding* variance-reduced variants, such as SAGA (Defazio et al., 2014) and SVRG (Johnson and Zhang, 2013).

*importance sampling* (Zhao and Zhang, 2015; Needell et al., 2015), and *mini-batching* (Konečný et al., 2016). These efforts are subsumed by the recently developed and remarkably sharp analysis of SGD under *arbitrary sampling* paradigm (Gower et al., 2019), first introduced in the study of randomized coordinate descent methods by (Richtárik and Takáč, 2016). The arbitrary sampling paradigm covers virtually all stationary mini-batch and importance sampling strategies in a unified way, thus making headway towards theoretical unification of two separate strategies for constructing stochastic gradients. For strongly convex  $f$ , the SGD methods analyzed in (Gower et al., 2019) converge linearly to a neighbourhood of the solution  $x^* = \text{arg min}_x f(x)$  for a fixed stepsize  $\gamma^k = \gamma$ . The size of the neighbourhood is proportional to the second moment of the stochastic gradient at the optimum ( $\sigma^2 := \frac{1}{n} \sum_{i=1}^n \|\nabla f_i(x^*)\|^2$ ), to the stepsize ( $\gamma$ ), and inversely proportional to the modulus of strong convexity. The effect of various sampling strategies, such as importance sampling and mini-batching, is twofold: i) improvement of the linear convergence rate by enabling larger stepsizes, and ii) modification of  $\sigma^2$ . However, none of these strategies<sup>2</sup> is able to completely eliminate the adverse effect of  $\sigma^2$ . That is, SGD with a fixed stepsize does not reach the optimum, unless one happens to be in the overparameterized case characterized by the identity  $\sigma^2 = 0$ .

**Variance reduced SGD.** While sampling strategies such as importance sampling and mini-batching reduce the variance of the stochastic gradient, in the finite-sum case (3) a new type of *variance reduction* strategies has been developed over the last few years (Roux et al., 2012; Defazio et al., 2014; Johnson and Zhang, 2013; Shalev-Shwartz and Zhang, 2013; Qu et al., 2015; Nguyen et al., 2017; Kovalev et al., 2019). These variance-reduced SGD methods differ from the sampling strategies discussed before in a significant way: they can iteratively *learn* the stochastic gradients at the optimum, and in so doing are able to eliminate the adverse effect of the gradient noise  $\sigma^2 > 0$  which, as mentioned above, prevents the iterates of vanilla SGD from converging to the optimum. As a result, for strongly convex  $f$ , these new variance-reduced SGD methods converge linearly to  $x^*$ , with a fixed stepsize. At the moment, these variance-reduced variants require a markedly different convergence theory from the vanilla variants of SGD. An exception to this is the situation when  $\sigma^2 = 0$  as then variance reduction is not needed; indeed, vanilla SGD already converges to the optimum, and with a fixed stepsize. We end the discussion here by remarking that this *hints* at a possible existence of a more unified theory, one that would include both vanilla and variance-reduced SGD.

<sup>2</sup>Except for the full batch strategy, which is prohibitively expensive.

**Distributed SGD, quantization and variance reduction.** When SGD is implemented in a distributed fashion, the problem is often expressed in the form (3), where  $n$  is the number of workers/nodes, and  $f_i$  corresponds to the loss based on data stored on node  $i$ . Depending on the number of data points stored on each node, it may or may not be efficient to compute the gradient of  $f_i$  in each iteration. In general, SGD is implemented in this way: each node  $i$  first computes a stochastic gradient  $g_i^k$  of  $f_i$  at the current point  $x^k$  (maintained individually by each node). These gradients are then aggregated by a master node (Shamir et al., 2014; Konečný and Richtárik, 2018), in-network by a switch (Sapio et al., 2019), or a different technique best suited to the architecture used. To alleviate the communication bottleneck, various lossy update compression strategies such as quantization (Seide et al., 2014; Gupta et al., 2015; Zhang et al., 2017), sparsification (Konečný and Richtárik, 2018; Alistarh et al., 2018; Wangni et al., 2018) and dithering (Alistarh et al., 2017) were proposed. The basic idea is for each worker to apply a randomized transformation  $Q : \mathbb{R}^d \rightarrow \mathbb{R}^d$  to  $g_i^k$ , resulting in a vector which is still an unbiased estimator of the gradient, but one that can be communicated with fewer bits. Mathematically, this amounts to injecting additional noise into the already noisy stochastic gradient  $g_i^k$ . The field of quantized SGD is still young, and even some basic questions remained open until recently. For instance, there was no distributed quantized SGD capable of provably solving (1) until the DIANA algorithm (Mishchenko et al., 2019a) was introduced. DIANA applies quantization to *gradient differences*, and in so doing is able to learn the gradients at the optimum, which makes it able to work for any regularizer  $R$ . DIANA has some structural similarities with SEGA (Hanzely et al., 2018)—the first coordinate descent type method which works for non-separable regularizers—but a more precise relationship remains elusive. When the functions of  $f_i$  are of a finite-sum structure as in (4), one can apply variance reduction to reduce the variance of the stochastic gradients  $g_i^k$  together with quantization, resulting in the VR-DIANA method (Horváth et al., 2019). This is the first distributed quantized SGD method which provably converges to the solution of (1)+(4) with a fixed stepsize.

**Randomized coordinate descent (RCD).** Lastly, in a distinctly separate strain, there are SGD methods for the coordinate/subspace descent variety (Nesterov, 2012). While it is possible to see *some* RCD methods as special cases of (5)+(6), most of them do not follow this algorithmic template. First, standard RCD methods use different stepsizes for updating different coordinates (Qu and Richtárik, 2016), and this seems to be crucial to their success. Second, until the recent discovery of the SEGA method, RCD methods were

not able to converge with non-separable regularizers. Third, RCD methods are naturally variance-reduced in the  $R = 0$  case as partial derivatives at the optimum are all zero. As a consequence, attempts at creating variance-reduced RCD methods seem to be futile. Lastly, RCD methods are typically analyzed using different techniques. While there are deep links between standard SGD and RCD methods, these are often indirect and rely on duality (Shalev-Shwartz and Zhang, 2013; Csiba and Richtárik, 2018; Gower and Richtárik, 2015).

### 3 Contributions

As outlined in the previous section, the world of SGD is vast and beautiful. It is formed by many largely disconnected islands populated by elegant and efficient methods, with their own applications, intuitions, and convergence analysis techniques. While some links already exist (e.g., the unification of importance sampling and mini-batching variants under the arbitrary sampling umbrella), there is no comprehensive general theory. It is becoming increasingly difficult for the community to understand the relationships between these variants, both in theory and practice. New variants are yet to be discovered, but it is not clear what tangible principles one should adopt beyond intuition to aid the discovery. This situation is exacerbated by the fact that a number of different assumptions on the stochastic gradient, of various levels of strength, is being used in the literature.

The main contributions of this work include:

- **Unified analysis.** In this work we propose a *unifying theoretical framework* which covers all of the variants of SGD outlined in Section 2. As a by-product, we obtain the *first unified analysis* of vanilla and variance-reduced SGD methods. For instance, our analysis covers as special cases vanilla SGD methods from (Nguyen et al., 2018) and (Gower et al., 2019), variance-reduced SGD methods such as SAGA (Defazio et al., 2014), L-SVRG (Hofmann et al., 2015; Kovalev et al., 2019) and JacSketch (Gower et al., 2018). Another by-product is the *unified analysis of SGD methods which include RCD*. For instance, our theory covers the subspace descent method SEGA (Hanzely et al., 2018) as a special case. Lastly, our framework is general enough to capture the phenomenon of *quantization*. For instance, we obtain the DIANA and VR-DIANA methods in special cases.

- **Generalization of existing methods.** An important yet *relatively* minor contribution of our work is that it enables *generalization* of known methods. For instance, some particular methods we consider, such as L-SVRG (Alg 10) (Kovalev et al., 2019), were not analyzed in the proximal ( $R \neq 0$ ) case before. To illustrate how this can be done within our framework, we

do it here for L-SVRG. Further, most<sup>3</sup> of the methods we analyze can be extended to the *arbitrary sampling* paradigm.

- **Sharp rates.** In all known special cases, the rates obtained from our general theorem (Theorem 4.1) are the *best known rates* for these methods.

- **New methods.** Our general analysis provides estimates for a possibly infinite array of new and yet-to-be-developed variants of SGD. One only needs to verify that Assumption 4.1 holds, and a complexity estimate is readily furnished by Theorem 4.1. Selected existing and new methods that fit our framework are summarized in Table 1. This list is for illustration only, we believe that future work by us and others will lead to its rapid expansion.

- **Experiments.** We show through extensive experimentation that some of the *new* and *generalized* methods proposed here and analyzed via our framework have some intriguing practical properties when compared against appropriately selected existing methods.

## 4 Main Result

We first introduce the key assumption on the stochastic gradients  $g^k$  enabling our general analysis (Assumption 4.1), then state our assumptions on  $f$  (Assumption 4.2), and finally state and comment on our unified convergence result (Theorem 4.1).

**Notation.** We use the following notation.  $\langle x, y \rangle := \sum_i x_i y_i$  is the standard Euclidean inner product, and  $\|x\| := \langle x, x \rangle^{1/2}$  is the induced  $\ell_2$  norm. For simplicity we assume that (1) has a unique minimizer, which we denote  $x^*$ . Let  $D_f(x, y)$  denote the *Bregman divergence* associated with  $f$ :  $D_f(x, y) := f(x) - f(y) - \langle \nabla f(y), x - y \rangle$ . We often write  $[n] := \{1, 2, \dots, n\}$ .

### 4.1 Key assumption

Our first assumption is of key importance. It is mainly an assumption on the sequence of stochastic gradients  $\{g^k\}$  generated by an arbitrary randomized algorithm. Besides unbiasedness (see (7)), we require two recursions to hold for the iterates  $x^k$  and the stochastic gradients  $g^k$  of a randomized method. We allow for flexibility by casting these inequalities in a parametric

<sup>3</sup>Our analysis allows for arbitrary sampling of all methods except of those using partial derivatives such as SEGA or N-SEGA. We shall note that arbitrary sampling for SEGA was developed concurrently in (Hanzely and Richtárik, 2019b). Note that (Hanzely and Richtárik, 2019b) proposes many novel variance reduced algorithms, for some of which we can obtain best rates. A detailed discussion and comparison to (Hanzely and Richtárik, 2019b) is provided in Remark A.4 in the Appendix

manner.

**Assumption 4.1.** Let  $\{x^k\}$  be the random iterates produced by proximal SGD (Algorithm in Eq (5)). We first assume that the stochastic gradients  $g^k$  are unbiased

$$\mathbf{E} [g^k | x^k] = \nabla f(x^k), \quad (7)$$

for all  $k \geq 0$ . Further, we assume that there exist non-negative constants  $A, B, C, D_1, D_2, \rho$  and a (possibly) random sequence  $\{\sigma_k^2\}_{k \geq 0}$  such that the following two relations hold<sup>4</sup>

$$\mathbf{E} \left[ \|g^k - \nabla f(x^*)\|^2 | x^k \right] \leq 2AD_f(x^k, x^*) + B\sigma_k^2 + D_1, \quad (8)$$

$$\mathbf{E} [\sigma_{k+1}^2 | \sigma_k^2] \leq (1 - \rho)\sigma_k^2 + 2CD_f(x^k, x^*) + D_2, \quad (9)$$

The expectation above is with respect to the randomness of the algorithm.

The unbiasedness assumption (7) is standard. The key innovation we bring is inequality (8) coupled with (9). We argue, and justify this statement by furnishing many examples in Section 5, that these inequalities capture the essence of a wide array of existing and some new SGD methods, including vanilla, variance reduced, arbitrary sampling, quantized and coordinate descent variants. Note that in the case when  $\nabla f(x^*) = 0$  (e.g., when  $R = 0$ ), the inequalities in Assumption 4.1 reduce to

$$\mathbf{E} \left[ \|g^k\|^2 | x^k \right] \leq 2A(f(x^k) - f(x^*)) + B\sigma_k^2 + D_1, \quad (10)$$

$$\mathbf{E} [\sigma_{k+1}^2 | \sigma_k^2] \leq (1 - \rho)\sigma_k^2 + 2C(f(x^k) - f(x^*)) + D_2. \quad (11)$$

Similar inequalities can be found in the analysis of stochastic first-order methods. However, this is the first time that such inequalities are generalized, equipped with parameters, and elevated to the status of an assumption that can be used on its own, independently from any other details defining the underlying method that generated them.

To give a further intuition about inequalities (8) and (9), we shall note that sequence  $\sigma_k$  usually represents the portion of noise that can gradually decrease over the course of optimization while constants  $D_1, D_2$  represent a static noise. On the other hand, constants  $A, C$  are usually related to some measure of smoothness of the objective. For instance, the parameters for (deterministic) gradient descent can be chosen as  $A = L, B = C = D_1 = D_2 = \sigma_k^2 = \rho = 0$ . For an overview of parameter choices for specific instances of (5), see Table 2. Note also that the choice of parameters of (8) and (9) is not unique, however this has no impact on convergence rates we provide.

<sup>4</sup>For convex and  $L$ -smooth  $f$ , one can show that  $\|\nabla f(x) - \nabla f(y)\|^2 \leq 2LD_f(x, y)$ . Hence,  $D_f$  can be used as a measure of proximity for the gradients.

## 4.2 Main theorem

For simplicity, we shall assume throughout that  $f$  is  $(\mu, x^*)$ -strongly quasi-convex, which is a generalization of  $\mu$ -strong convexity. We leave an analysis under different assumptions on  $f$  to future work.

**Assumption 4.2** ( $(\mu, x^*)$ -strong quasi-convexity). There exists  $\mu > 0$  such that  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  satisfies the following inequality for all  $x \in \mathbb{R}^d$ :

$$f(x^*) \geq f(x) + \langle \nabla f(x), x^* - x \rangle + \frac{\mu}{2} \|x^* - x\|^2. \quad (12)$$

We are now ready to present the key lemma of this paper which states per iteration recurrence to analyze (5). Due to space limitations, we present the proof in Section 4 of the Appendix.

**Lemma 4.1.** Let Assumptions 4.1 and 4.2 be satisfied. Then the following inequality holds for all  $k \geq 0$ :

$$\begin{aligned} & \mathbf{E} \left[ \|x^{k+1} - x^*\|^2 \right] + M\gamma^2 \mathbf{E} [\sigma_{k+1}^2] \\ & + 2\gamma(1 - \gamma(A + CM)) \mathbf{E} [D_f(x^k, x^*)] \\ & \leq (1 - \gamma\mu) \mathbf{E} \left[ \|x^k - x^*\|^2 \right] + (1 - \rho) M\gamma^2 \mathbf{E} [\sigma_k^2] \\ & + B\gamma^2 \mathbf{E} [\sigma_k^2] + (D_1 + MD_2)\gamma^2. \end{aligned}$$

Using recursively Lemma 4.1, we obtain the convergence rate of proximal SGD, which we state as Theorem 4.1.

**Theorem 4.1.** Let Assumptions 4.1 and 4.2 be satisfied. Choose constant  $M$  such that  $M > \frac{B}{\rho}$ . Choose a stepsize satisfying

$$0 < \gamma \leq \min \left\{ \frac{1}{\mu}, \frac{1}{A + CM} \right\}. \quad (13)$$

Then the iterates  $\{x^k\}_{k \geq 0}$  of proximal SGD (Algorithm (5)) satisfy

$$\begin{aligned} \mathbf{E} [V^k] \leq \max & \left\{ (1 - \gamma\mu)^k, \left( 1 + \frac{B}{M} - \rho \right)^k \right\} V^0 \\ & + \frac{(D_1 + MD_2)\gamma^2}{\min \left\{ \gamma\mu, \rho - \frac{B}{M} \right\}}, \end{aligned} \quad (14)$$

where the Lyapunov function  $V^k$  is defined by  $V^k := \|x^k - x^*\|^2 + M\gamma^2\sigma_k^2$ .

This theorem establishes a linear rate for a wide range of proximal SGD methods up to a certain oscillation radius, controlled by the additive term in (14), and namely, by parameters  $D_1$  and  $D_2$ . As we shall see in Section A (refer to Table 2), the main difference between the vanilla and variance-reduced SGD methods is that while the former satisfy inequality (9) with

$D_1 > 0$  or  $D_2 > 0$ , which in view of (14) prevents them from reaching the optimum  $x^*$  (using a fixed stepsize), the latter methods satisfy inequality (9) with  $D_1 = D_2 = 0$ , which in view of (14) enables them to reach the optimum.

## 5 The Classic, The Recent and The Brand New

In this section we deliver on the promise from the introduction and show how many existing and some new variants of SGD fit our general framework (see Table 1).

**An overview.** As claimed, our framework is powerful enough to include vanilla methods (✗ in the “VR” column) as well as variance-reduced methods (✓ in the “VR” column), methods which generalize to arbitrary sampling (✓ in the “AS” column), methods supporting gradient quantization (✓ in the “Quant” column) and finally, also RCD type methods (✓ in the “RCD” column).

For existing methods we provide a citation; new methods developed in this paper are marked accordingly. Due to space restrictions, all algorithms are described (in detail) in the Appendix; we provide a link to the appropriate section for easy navigation. While these details are important, the main message of this paper, i.e., the generality of our approach, is captured by Table 1. The “Result” column of Table 1 points to a corollary of Theorem 4.1; these corollaries state in detail the convergence statements for the various methods. In all cases where known methods are recovered, these corollaries of Theorem 4.1 recover the best known rates.

**Parameters.** From the point of view of Assumption 4.1, the methods listed in Table 1 exhibit certain patterns. To shed some light on this, in Table 2 we summarize the values of these parameters.

Note, for example, that for all methods the parameter  $A$  is non-zero. Typically, this is a multiple of an appropriately defined smoothness parameter (e.g.,  $L$  is the Lipschitz constant of the gradient of  $f$ ,  $\mathcal{L}$  and  $\mathcal{L}_1$  in SGD-SR<sup>5</sup>, SGD-star and JacSketch are *expected smoothness* parameters). In the three variants of the DIANA method,  $\omega$  captures the variance of the quantization operator  $Q$ . That is, one assumes that  $\mathbf{E}Q(x) = x$

<sup>5</sup>SGD-SR is first SGD method analyzed in the *arbitrary sampling* paradigm. It was developed using the *stochastic reformulation* approach (whence the “SR”) pioneered in (Richtárik and Takáč, 2017) in a numerical linear algebra setting, and later extended to develop the JacSketch variance-reduction technique for finite-sum optimization (Gower et al., 2018).

Table 1: List of specific existing (in some cases generalized) and new methods which fit our general analysis framework. VR = variance reduced method, AS = arbitrary sampling, Quant = supports gradient quantization, RCD = randomized coordinate descent type method. <sup>a</sup> Special case of SVRG with 1 outer loop only; <sup>b</sup> Special case of DIANA with 1 node and quantization of exact gradient.

Problem	Method	Alg #	Citation	VR?	AS?	Quant?	RCD?	Section	Result
(1)+(2)	SGD	Alg 1	Nguyen et al. (2018)	✗	✗	✗	✗	A.1	Cor A.1
(1)+(3)	SGD-SR	Alg 2	Gower et al. (2019)	✗	✓	✗	✗	A.2	Cor A.2
(1)+(3)	SGD-MB	Alg 3	<b>NEW</b>	✗	✗	✗	✗	A.3	Cor A.3
(1)+(3)	SGD-star	Alg 4	<b>NEW</b>	✓	✓	✗	✗	A.4	Cor A.4
(1)+(3)	SAGA	Alg 5	Defazio et al. (2014)	✓	✗	✗	✗	A.5	Cor A.5
(1)+(3)	N-SAGA	Alg 6	<b>NEW</b>	✗	✗	✗	✗	A.6	Cor A.6
(1)	SEGA	Alg 7	Hanzely et al. (2018)	✓	✗	✗	✓	A.7	Cor A.7
(1)	N-SEGA	Alg 8	<b>NEW</b>	✗	✗	✗	✓	A.8	Cor A.8
(1)+(3)	SVRG <sup>a</sup>	Alg 9	Johnson and Zhang (2013)	✓	✗	✗	✗	A.9	Cor A.9
(1)+(3)	L-SVRG	Alg 10	Hofmann et al. (2015)	✓	✗	✗	✗	A.10	Cor A.10
(1)+(3)	DIANA	Alg 11	Mishchenko et al. (2019a)	✗	✗	✓	✗	A.11	Cor A.11
(1)+(3)	DIANA <sup>b</sup>	Alg 12	Mishchenko et al. (2019a)	✓	✗	✓	✗	A.11	Cor A.12
(1)+(3)	Q-SGD-SR	Alg 13	<b>NEW</b>	✗	✓	✓	✗	A.12	Cor A.13
(1)+(3)+(4)	VR-DIANA	Alg 14	Horváth et al. (2019)	✓	✗	✓	✗	A.13	Cor A.15
(1)+(3)	JacSketch	Alg 15	Gower et al. (2018)	✓	✓✗	✗	✗	A.14	Cor A.16

Table 2: The parameters for which the methods from Table 1 (special cases of (5)) satisfy Assumption 4.1. The meaning of the expressions appearing in the table, as well as their justification is defined in detail in the Appendix (Section A).

Method	$A$	$B$	$\rho$	$C$	$D_1$	$D_2$
SGD	$2L$	0	1	0	$2\sigma^2$	0
SGD-SR	$2\mathcal{L}$	0	1	0	$2\sigma^2$	0
SGD-MB	$\frac{A'+L(\tau-1)}{\tau}$	0	1	0	$\frac{D'}{\tau}$	0
SGD-star	$2\mathcal{L}$	0	1	0	0	0
SAGA	$2L$	2	$1/n$	$L/n$	0	0
N-SAGA	$2L$	2	$1/n$	$L/n$	$2\sigma^2$	$\frac{\sigma^2}{n}$
SEGA	$2dL$	$2d$	$1/d$	$L/d$	0	0
N-SEGA	$2dL$	$2d$	$1/d$	$L/d$	$2d\sigma^2$	$\frac{\sigma^2}{d}$
SVRG <sup>a</sup>	$2L$	2	0	0	0	0
L-SVRG	$2L$	2	$p$	$Lp$	0	0
DIANA	$(1 + \frac{2\omega}{n})L$	$\frac{2\omega}{n}$	$\alpha$	$L\alpha$	$\frac{(1+\omega)\sigma^2}{n}$	$\alpha\sigma^2$
DIANA <sup>b</sup>	$(1 + 2\omega)L$	$2\omega$	$\alpha$	$L\alpha$	0	0
Q-SGD-SR	$2(1 + \omega)\mathcal{L}$	0	1	0	$2(1 + \omega)\sigma^2$	0
VR-DIANA	$(1 + \frac{4\omega+2}{n})L$	$\frac{2(\omega+1)}{n}$	$\alpha$	$(\frac{1}{m} + 4\alpha)L$	0	0
JacSketch	$2\mathcal{L}_1$	$\frac{2\lambda_{\max}}{n}$	$\lambda_{\min}$	$\frac{\mathcal{L}_2}{n}$	0	0

and  $\mathbf{E}\|Q(x) - x\|^2 \leq \omega \|x\|^2$  for all  $x \in \mathbb{R}^d$ . In view of (13), large  $A$  means a smaller stepsize, which slows down the rate. Likewise, the variance  $\omega$  also affects the parameter  $B$ , which in view of (14) also has an adverse effect on the rate. Further, as predicted by Theorem 4.1, whenever either  $D_1 > 0$  or  $D_2 > 0$ , the corresponding method converges to an oscillation region only. These methods are not variance-reduced. All symbols used in Table 2 are defined in the appendix, in the same place where the methods are described and analyzed.

**Five new methods.** To illustrate the usefulness of

our general framework, we develop *5 new variants* of SGD never explicitly considered in the literature before (see Table 1). Here we briefly motivate them; details can be found in the Appendix.

- **SGD-MB** (Algorithm 3). This method is specifically designed for functions of the finite-sum structure (4). As we show through experiments, this is a powerful mini-batch SGD method, with mini-batches formed with replacement as follows: in each iteration, we repeatedly ( $\tau$  times) and independently pick  $i \in [n]$  with probability  $p_i > 0$ . Stochastic gradient  $g^k$  is then formed by averaging the stochastic gradients  $\nabla f_i(x^k)$  for all se-

lected indices  $i$  (including each  $i$  as many times as this index was selected). This allows for a more practical importance mini-batch sampling implementation than what was until now possible (see Remark A.1 in the Appendix for more details and experiment in Figure 1).

- **SGD-star** (Algorithm 4). This new method forms a bridge between vanilla and variance-reduced SGD methods. While not practical, it sheds light on the role of variance reduction. Again, we consider functions of the finite-sum form (4). This method answers the following question: assuming that the gradients  $\nabla f_i(x^*)$ ,  $i \in [n]$  are *known*, can they be used to design a more powerful SGD variant? The answer is *yes*, and **SGD-star** is the method. In its most basic form, **SGD-star** constructs the stochastic gradient via  $g^k = \nabla f_i(x^k) - \nabla f_i(x^*) + \nabla f(x^*)$ , where  $i \in [n]$  is chosen uniformly at random. Inferring from Table 2, where  $D_1 = D_2 = 0$ , this method converges to  $x^*$ , and not merely to some oscillation region. Variance-reduced methods essentially work by iteratively constructing increasingly more accurate *estimates* of  $\nabla f_i(x^*)$ . Typically, the term  $\sigma_k^2$  in the Lyapunov function of variance reduced methods will contain a term of the form  $\sum_i \|h_i^k - \nabla f_i(x^*)\|^2$ , with  $h_i^k$  being the estimators maintained by the method. Remarkably, **SGD-star** was never explicitly considered in the literature before.

- **N-SAGA** (Algorithm 6). This is a novel variant of **SAGA** (Defazio et al., 2014), one in which one does not have access to the gradients of  $f_i$ , but instead only has access to *noisy* stochastic estimators thereof (with noise  $\sigma^2$ ). Like **SAGA**, **N-SAGA** is able to reduce the variance inherent in the finite sum structure (4) of the problem. However, it necessarily pays the price of noisy estimates of  $\nabla f_i$ , and hence, just like vanilla SGD methods, is ultimately unable to converge to  $x^*$ . The oscillation region is governed by the noise level  $\sigma^2$  (refer to  $D_1$  and  $D_2$  in Table 2). This method will be of practical importance for problems where each  $f_i$  is of the form (2), i.e., for problems of the “average of expectations” structure. Batch versions of **N-SAGA** would be well suited for distributed optimization, where each  $f_i$  is owned by a different worker, as in such a case one wants the workers to work in parallel.

- **N-SEGA** (Algorithm 8). This is a *noisy* extension of the RCD-type method **SEGA**, in complete analogy with the relationship between **SAGA** and **N-SAGA**. Here we assume that we only have noisy estimates of partial derivatives (with noise  $\sigma^2$ ). This situation is common in derivative-free optimization, where such a noisy estimate can be obtained by taking (a random) finite difference approximation (Nesterov, 2017). Unlike **SEGA**, **N-SEGA** only converges to an oscillation region the size of which is governed by  $\sigma^2$ .

- **Q-SGD-SR** (Algorithm 13). This is a quantized version of **SGD-SR**, which is the first SGD method analyzed in the arbitrary sampling paradigm. As such, **Q-SGD-SR** is a vast generalization of the celebrated **QSGD** method (Alistarh et al., 2017).

## 6 Experiments

In this section we numerically verify the claims from the paper. We present only a fraction of experiments here, the rest is contained in Appendix B. Besides an extended version of experiment described here, we also provide experiments on **SGD-star**, as well as about **N-SEGA** (recall that both are new methods).

In Section A.3, we describe in detail the **SGD-MB** method already outlined before. The main advantage of **SGD-MB** is that the sampling procedure it employs can be implemented in just  $\mathcal{O}(\tau \log n)$  time. In contrast, even the simplest without-replacement sampling which selects each function into the minibatch with a prescribed probability independently (we will refer to it as independent SGD) requires  $n$  calls of a uniform random generator. We demonstrate numerically that **SGD-MB** has essentially identical iteration complexity to independent SGD in practice. We consider logistic regression with Tikhonov regularization. For a fixed expected sampling size  $\tau$ , consider two options for the probability of sampling the  $i$ -th function:

- (i)  $\frac{\tau}{n}$ , or
- (ii)  $\frac{\|a_i\|^2 + \lambda}{\delta + \|a_i\|^2 + \lambda}$ , where  $\delta$  is such that<sup>6</sup>

$$\sum_{i=1}^n \frac{\|a_i\|^2 + \lambda}{\delta + \|a_i\|^2 + \lambda} = 1.$$

The results can be found in Figure 1, where we also report the choice of stepsize  $\gamma$  and the choice of  $\tau$  in the legend and title of the plot, respectively.

Indeed, iteration complexity of **SGD-MB** and independent SGD is almost identical. Since the cost of each iteration of **SGD-MB** is cheaper<sup>7</sup>, we conclude superiority of **SGD-MB** to independent SGD.

## 7 Limitations and Extensions

Although our approach is rather general, we still see several possible directions for future extensions, includ-

<sup>6</sup>An RCD version of this sampling was proposed in (Hanzely and Richtárik, 2019a); it was shown to be superior to uniform sampling both in theory and practice.

<sup>7</sup>The relative difference between iteration costs of **SGD-MB** and independent SGD can be arbitrary, especially for the case when cost of evaluating  $\nabla f_i(x)$  is cheap,  $n$  is huge and  $n \gg \tau$ . In such case, cost of one iteration of **SGD-MB** is  $\tau \text{Cost}(\nabla f_i) + \tau \log(n)$  while the cost of one iteration of independent SGD is  $\tau \text{Cost}(\nabla f_i) + n$ .

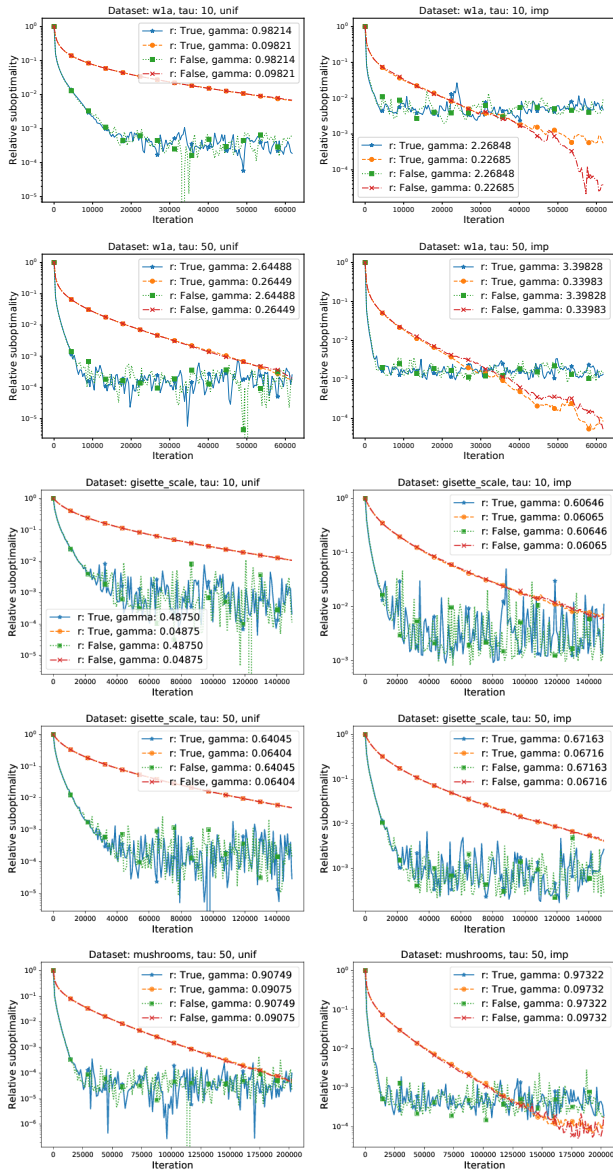


Figure 1: SGD-MB and independent SGD applied on LIBSVM (Chang and Lin, 2011). Title label “unif” corresponds to probabilities chosen by (i) while label “imp” corresponds to probabilities chosen by (ii). Lastly, legend label “r” corresponds to “replacement” with value “True” for SGD-MB and value “False” for independent SGD.

ing:

- We believe our results can be extended to *weakly convex* functions. However, producing a comparable result in the *nonconvex* case remains a major open problem.

- It would be further interesting to unify our theory with *biased* gradient estimators. If this was possible, one could recover methods as SAG (Roux et al., 2012) in special cases, or obtain rates for the zero-order optimization. We have some preliminary results in this direction already.

- Although our theory allows for non-uniform stochasticity, it does not recover the best known rates for RCD type methods with *importance sampling*. It would be thus interesting to provide a more refined analysis capable of capturing importance sampling phenomena more accurately.

- An extension of Assumption 4.1 to *iteration dependent* parameters  $A, B, C, D_1, D_2, \rho$  would enable an array of new methods, such as SGD with decreasing stepsizes. Such an extension is rather very straightforward.

- It would be interesting to provide a unified analysis of stochastic methods with *acceleration* and *momentum*. In fact, (Kulunchakov and Mairal, 2019) provide (separately) a unification of some methods with and without variance reduction. Hence, an attempt to combine our insights with their approach seems to be a promising starting point in these efforts.

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