On the convergence of the Stochastic Heavy Ball Method

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Abstract

We provide a comprehensive analysis of the Stochastic Heavy Ball (SHB) method (otherwise known as the momentum method), including a convergence of the last iterate of SHB, establishing a faster rate of convergence than existing bounds on the last iterate of Stochastic Gradient Descent (SGD) in the convex setting. Our analysis shows that unlike SGD, no final iterate averaging is necessary with the SHB method. We detail new iteration dependent step sizes (learning rates) and momentum parameters for the SHB that result in this fast convergence. Moreover, assuming only smoothness and convexity, we prove that the iterates of SHB converge *almost surely* to a minimizer, and that the convergence of the function values of (S)HB is asymptotically faster than that of (S)GD in the overparametrized and in the deterministic settings. Our analysis is general, in that it includes all forms of mini-batching and non-uniform samplings as a special case, using an arbitrary sampling framework. Furthermore, our analysis does not rely on the bounded gradient assumptions. Instead, it only relies on smoothness, which is an assumption that can be more readily verified. Finally, we present extensive numerical experiments that show that our theoretically motivated parameter settings give a statistically significant faster convergence across a diverse collection of datasets.

1 Introduction

Consider the problem of minimizing an average of loss functions

$$x^* \in \operatorname*{argmin}_{x \in \mathbb{R}^d} f(x) \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n f_i(x),\tag{1}$$

where each f_i is the loss function over the *i*th data point. Let $\mathcal{X}^* \subset \mathbb{R}^d$ be the set of solutions of (1).

The interest in efficiently solving (1) is growing due to the significant growth in data sets. In particular, the number of data points n can be exceedingly large. In this setting, stochastic gradient descent (SGD) [30] type methods have proven to be very effective. In particular, a new strand of SGD type methods based on momentum and adaptive step sizes are quickly becoming the state-of-the-art.

While adaptive methods date back at least to ADAGrad [6], it is the more recent notorious ADAM [17] that has sparked a renewed interest in both momentum techniques and adaptive step sizes. ADAM has shown to work very well in several settings [37, 26, 28], and with this practical success has now come a push to 1) provide theory that shows how to set the parameters so that these adaptive momentum methods work well 2) design better new adaptive methods. On the theoretical side, the initial proof of convergence of ADAM was shown to be incorrect [29], and several new methods with accompanying proofs have now been proposed as a solution, including AMSgrad [29], ADAMX [24] and more [20].

^{*}Part of this work was done while the first author was an intern at RIKEN AIP.

As far as we are aware, there exists no proof that these new adaptive momentum methods converge faster than plain vanilla SGD (despite their clear practical success). This is perhaps not surprising since even the simplest of the momentum-based methods, namely *Stochastic Heavy Ball* (SHB) has not been shown to converge faster than SGD. It is this gap that motivates our paper.

Here we provide a careful and comprehensive convergence theory of the stochastic heavy ball (SHB) method in the convex and strongly convex setting. The iterates of the SHB method are given by

$$x_{k+1} = x_k - \alpha_k \nabla f_{i_k}(x_k) + \beta_k \left(x_k - x_{k-1} \right), \tag{2}$$

where $x_{-1} = x_0$, the index i_k is sampled i.i.d at each iteration, and the *step sizes* $(\alpha_k)_k \ge 0$ and *momentum parameters* $(\beta_k)_k \ge 0$ are carefully chosen. Typically $\beta_k \equiv \beta = 0.9$ is a standard setting, but here we show that different sequences of momentum parameters lead to better theoretical and practical performance.

In the deep neural network literature, the SHB method is more commonly written as

$$m_k = \beta_k m_{k-1} + \nabla f_{i_k}(x_k)$$

$$x_{k+1} = x_k - \alpha_k m_k,$$
(3)

where $m_{-1} = 0$ and $\hat{\beta}_k = \frac{\alpha_{k-1}}{\alpha_k} \beta_k$. See Section A in the appendix for a proof of the equivalence between (2) and (3). When written in the form (3) the method is often known as simply the *Momentum method* [35, 32].

1.1 Contributions and Background

An important focus of our work is providing an analysis for SHB which only depends on simple and verifiable assumptions. Our starting point is examining the existing assumptions for the analysis of SGD. Most convergence results on SGD depend on the bounded stochastic gradients or bounded stochastic gradients variance assumptions. If \hat{g}_k is an unbiased estimate of the gradient or a subgradient of the gradient g_k , these assumptions can be written as:

$$\mathbb{E}\left[\left\|\hat{g}_k\right\|^2\right] \le G \qquad \text{(BG)} \qquad \text{and} \qquad \mathbb{E}\left[\left\|\hat{g}_k - g_k\right\|^2\right] \le \sigma^2, \qquad \text{(BV)}$$

where $G, \sigma^2 > 0$ are constants. While using a uniform bound on the subgradients like (BG) seems often necessary to analyze stochastic subgradient descent [21, 27, 34], this bound has been proven in [22] never to hold for a large class of convex functions, namely strongly convex ones. Similarly, it is possible to show that Assumption (BV), used for example in the analysis of an accelerated variant of SGD in [10], does not hold for some convex functions (see Proposition 1 in [15]). Fueled by these observations, a recent line of work [22, 12, 15] has emerged, which aims to avoid Assumptions (BG) and (BV). We follow this line of work. In all of our analysis, we will only assume that f is smooth and convex.

We now present our contributions to the analysis of SHB.

The deterministic Heavy Ball method. The first local convergence of the deterministic Heavy Ball method was given in [25], showing that it converges at an accelerated rate for twice differentiable strongly convex functions. Only recently did [9] show that the deterministic Heavy Ball method converged globally and sublinearly for smooth and convex functions.

Contributions. Our analysis recovers the results of [9] as a special case and extends them to the stochastic setting. Indeed, when specialized to the full batch case, our rates match theirs².

Stochastic Heavy Ball analysis. The SHB has recently been analysed for nonconvex functions and for strongly convex functions in [7]. For strongly convex functions, they prove a $O(1/t^{\beta})$ convergence rate for any $\beta < 1$. An analysis of SHB based on differential equations was given in [23]. There, the authors use a similar Lyapunov function as [9], however, they rely on Assumption (BV). A $O(1/\sqrt{t})$ convergence rate for SHB in the convex setting was given in [39], but again by relying on Assumptions (BG) and (BV). Furthermore, they provide a rate only for the average of the iterates rather than the last iterate of SHB. For the specialized setting of minimizing quadratics, it has

²Up to a small constant factor difference.

been shown that the SHB converges linearly at an accelerated rate, but only in expectation rather than convergence in L2 [19]. By using stronger assumptions on the noise as compared to [16], in [4] the authors show that by using a specific parameter setting, the SHB applied on quadratics converges at an accelerated rate to a neighborhood of a minimizer.

Contributions. We provide the first proof of convergence of SHB in the general convex setting without assuming (BG) nor (BV). Instead, we rely simply on the smoothness of the loss functions. Additionally, for strongly convex functions, we provide new iteration dependent parameters in Section H of the supplementary material that result in sublinear convergence of SHB.

Stochastic Gradient Descent analysis. In the convex setting and without assuming that the gradients are bounded, only *the average of the iterates* of SGD has been shown to converge sublinearly to a neighborhood of the solution, see Theorem 6 in [38]³, which contrasts with what works well in practice, which is using the last iterate of SGD. Motivated by this gap between theory and practice, it was proved very recently in [14] that a $O(1/\sqrt{T})$ convergence rate of the last iterate of SGD can be attained using an elaborate step size scheme, but in a different setting, under Assumption (BG) and the assumption that f is convex and Lipschitz over a closed bounded set⁴.

Contributions. We prove that in contrast with SGD, using a fixed step size, *the last iterate* of SHB converges sublinearly to a neighborhood of the minimum and to the minimum exactly in the interpolation regime, which supports what is done in practice.

Parameter settings. As a rule of thumb, the momentum parameter is often fixed at around 0.9, which often exhibits better empirical performance than SGD [35]. Despite this practical success, there exist simple linear regression problems where SHB is worse than SGD for any choice of a fixed momentum and step size [16].

Contributions. We provide iteration dependent formulae for updating the step size and momentum parameters that result in a fast convergence in theory and in practice. We show through extensive numerical experiments in Figure 1 that our new parameter setting is statistically superior to the standard rule-of-thumb settings on convex problems.

(S)HB is asymptotically faster than (S)GD. The almost sure convergence of the iterates of SGD and SHB is a well-studied question [3, 40, 22, 7]. For SGD, the *almost sure* convergence of the iterates for functions satisfying $\forall (x, x_*) \in \mathbb{R}^d \times \mathcal{X}^*, \langle \nabla f(x), x - x_* \rangle \ge 0$, called *variationally coherent*, was shown in [3] by assuming that the minimizer is unique. Recently in [40], the uniqueness of the minimizer was dropped for variationally coherent functions, but again by assuming (BG). As for SHB, almost sure convergence to a minimizer for nonconvex functions was proven in [7] under Assumption (BV) and an unusual *helliptic condition* which guarantees that SHB escapes any unstable point.

Contributions. Assuming only convexity and smoothness, we prove that the iterates of SHB converge *almost surely* to a minimizer. To the best of our knowledge, this is the first work proving the convergence of the iterates of a stochastic first-order method under these sole assumptions. Moreover, we prove that when the noise at the minimum is 0, which holds when the model is overparametrized (resp. when we use the full gradient at each iteration), SHB (resp. deterministic HB) converges at a rate o(1/k) rather than the known O(1/k) for SGD [38] (resp. GD).

Mini-batching and importance sampling. Our analysis uses arbitrary sampling, which was introduced in [12]. As such, it includes all forms of sampling of the data, such as mini-batching and importance sampling. We are even able to derive an optimal mini-batch size. Such analysis has been done for SGD [12], SVRG [33] and SAGA [8]. There appears to be no prior work analyzing SHB with mini-batching and other samplings.

³They show convergence to the minimum if the gradient noise at the optimum is zero.

⁴Note that the suffix averaging scheme proposed in [21] under Assumption (BG) results in a $O(1/\sqrt{T})$ convergence rate, but when this result is specialized to the extreme case of picking the last iterate, the upper bound on the suboptimality is of the order $O(\sqrt{T})$. This contradicts [13], which claims that for smooth convex functions, the last iterate of SGD was proven to converge in [21] at a $O(1/\sqrt{T})$ rate.

1.2 Assumptions and arbitrary sampling

All of our theory only relies on the following assumption.

Assumption 1.1. For all $i \in [n] \stackrel{def}{=} \{1, \ldots, n\}$, there exists $L_i > 0$ such that for every $x, y \in \mathbb{R}^d$ we have that

$$f_i(y) \ge f_i(x) + \langle \nabla f_i(x), y - x \rangle \tag{4}$$

$$f_i(y) \le f_i(x) + \langle \nabla f_i(x), y - x \rangle + \frac{L_i}{2} ||y - x||^2.$$
 (5)

Let $L_{\max} \stackrel{\text{def}}{=} \max_{i \in [n]} L_i$. Consequently, f(x) is also smooth and we use L > 0 to denote its smoothness constant.

So that we can analyze the SHB method under different forms of mini-batching and non-uniform sampling, we will use an arbitrary sampling vector which was introduced by [8, 12].

Definition 1.2 (Arbitrary sampling). Let $v \in \mathbb{R}^n$ be a random vector drawn from some distribution \mathcal{D} such that $\mathbb{E}_{\mathcal{D}}[v_i] = 1$, for i = 1, ..., n.

We refer to v in the above definition as an arbitrary sampling vector since we can use v to encode any sampling of the f_i functions and their gradients. Indeed, if we define $f_v(x) \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n v_i f_i(x)$, then $f_v(x)$ and $\nabla f_v(x)$ are unbiased estimates of f(x) and $\nabla f(x)$, respectively. This follows from Definition 1.2 since

$$\mathbb{E}_{\mathcal{D}}\left[\nabla f_v(x)\right] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{\mathcal{D}}\left[v_i\right] \nabla f_i(x) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(x) = \nabla f(x),\tag{6}$$

and analogously $\mathbb{E}_{\mathcal{D}}[f_v(x)] = f(x)$. This observation allows us to write an arbitrary sampling version for any stochastic gradient type method. In particular for the SHB method, instead of sampling a single function index i_k at each iteration k, we sample a vector $v_k \sim \mathcal{D}$, and iterate

$$x_{k+1} = x_k - \alpha_k \nabla f_{v_k}(x_k) + \beta_k \left(x_k - x_{k-1} \right).$$
(7)

For all our analysis we will use (7).

The sampling we use also affects how smooth our estimates are in expectation. This change in smoothness is captured by the *Expected Smoothness* constant $\mathcal{L} > 0$ that we introduce in the following lemma.

Lemma 1.3 (Expected smoothness [11]). Let Assumption 1.1 hold and let v be a sampling vector. It follows that there exists $\mathcal{L} > 0$ such that

$$\mathbb{E}_{\mathcal{D}}\left[\left\|\nabla f_{v}(x) - \nabla f_{v}(x^{*})\right\|^{2}\right] \leq 2\mathcal{L}\left(f(x) - f(x^{*})\right).$$
(8)

This expected smoothness (8) also gives us a bound on the gradient noise.

Lemma 1.4. Let σ^2 be the residual gradient noise

$$\sigma^{2} \stackrel{def}{=} \max_{x \in \mathcal{X}^{*}} \mathbb{E}_{\mathcal{D}} \left[\|\nabla f_{v}(x^{*})\|^{2} \right]$$

If Assumption 1.1 holds then

$$\mathbb{E}_{\mathcal{D}}\left[\left\|\nabla f_{v}(x)\right\|^{2}\right] \leq 4\mathcal{L}\left(f(x) - f(x^{*})\right) + 2\sigma^{2}.$$
(9)

Proof. Follows immediately by using (8) with $||a||^2 \leq 2 ||a - b||^2 + 2 ||b||^2$ for $a = \nabla f_v(x)$ and $b = \nabla f_v(x^*)$.

With this bound (9) on the *gradient noise*, we do not need to assume that the stochastic gradients are bounded such as in (BG) or (BV), as is often done when analyzing SGD [21] or SHB [39]. Instead, we simply employ (9) which is a direct consequence of Assumption 1.1. Note that the analysis carried

for SGD and SHB in [21, 39] is more general and applies to the nonsmooth case, for which assuming BG is often necessary. But to our knowledge, there is no existing analysis for SHB without (BG) or (BV) for smooth and convex functions.

Both the expected smoothness constant \mathcal{L} and the residual gradient noise σ^2 will appear in our analysis. Fortunately, we can calculate the expected smoothness constant. The exact expression of the \mathcal{L} constant depends on both the sampling and the smoothness constants of the functions f_i , as we show next. For example, as conjectured in [8] and proven in [12], for mini-batching with size $b \in [n]$ without replacement we have that (9) holds for

$$\mathcal{L} \equiv \mathcal{L}(b) \stackrel{\text{def}}{=} \frac{1}{b} \frac{n-b}{n-1} L_{\max} + \frac{n}{b} \frac{b-1}{n-1} L,$$
(10)

$$\sigma^2 \equiv \sigma^2(b) = \frac{1}{b} \frac{n-b}{n-1} \sigma_1^2,\tag{11}$$

where $\sigma_1^2 \stackrel{\text{def}}{=} \frac{1}{n} \max_{x \in \mathcal{X}^*} \sum_{i=1}^n \|\nabla f_i(x_*)\|^2$. Note that $\sigma^2(n) = 0$ and $\mathcal{L}(n) = L$, as expected, since b = n corresponds to full batch gradients, or equivalently to using the deterministic HB. Similarly, $\mathcal{L}(1) = L_{\max}$, since b = 1 corresponds to sampling one individual f_i function. As for σ^2 when $b \neq n$, there is no easy way to estimate it, excluding for overparametrized models such as deep nets.

overparametrized models. When our models have enough parameters to *interpolate the data* [38] then $\nabla f_i(x^*) = 0$, $\forall i$, and consequently $\sigma^2 = 0$.

Before moving on to our main theoretical results, we first present a lesser known view point of SHB as the iterate-moving-average method. It is this viewpoint that facilitates our forthcoming analysis.

2 An iterative averaging viewpoint of the stochastic heavy ball method

Our forthcoming analysis suggests the following new parametrization of SHB⁵.

Theorem 2.1. Let $\eta_k, \lambda_k \in \mathbb{R}$. Consider the iterate-moving-average (IMA) method:

$$z_{k} = z_{k-1} - \eta_{k} \nabla f_{v_{k}}(x_{k}),$$

$$x_{k+1} = \frac{\lambda_{k+1}}{\lambda_{k+1} + 1} x_{k} + \frac{1}{\lambda_{k+1} + 1} z_{k},$$
(12)

when we set $z_0 = x_0$. If

$$\alpha_k = \frac{\eta_k}{1 + \lambda_{k+1}} \quad and \quad \beta_k = \frac{\lambda_k}{1 + \lambda_{k+1}},\tag{13}$$

then the x_k iterates in (12) are equal to the x_k iterates of the SHB method (7).

The equivalence between this formulation and the original (7) is proven in the supplementary material (Section B).

In all of our theorems, the parameters η_k and λ_k naturally arise in the recurrences and Lyaponuv function. As such, we determine how to set the parameters η_k and λ_k , which in turn gives settings for α_k and β_k through (13).

Having new reformulations often leads to new insights. This is the case for Nesterov's accelerated gradient method, where at least six forms are known [5] and recent research suggests that iterate-averaged reformulations are the easiest to generalize to the combined proximal & variance-reduced case [18].

3 Convex case

Our first theorem provides an upper bound on the suboptimality given any sampling and any sequence of step sizes. Later we develop special cases of this theorem through different choices of the parameters.

⁵This iterate-moving-average method (12) was analyzed in Appendix H of [36]. However, the link with SHB was not established.

Theorem 3.1. Let $x_{-1} = x_0$ and consider the iterates (7). Let $(\eta_k)_k$ be a sequence such that $0 < \eta_k < \frac{1}{2\mathcal{L}}$ for all $k \in \mathbb{N}$. Define

$$\lambda_0 \stackrel{def}{=} 0 \quad and \quad \lambda_k \stackrel{def}{=} \frac{\sum_{t=0}^{k-1} \eta_t \left(1 - 2\eta_t \mathcal{L}\right)}{\eta_k} \text{ for } k \ge 1.$$
(14)

Set

$$\alpha_k = \frac{\eta_k}{1 + \lambda_{k+1}} \text{ and } \beta_k = \frac{\lambda_k}{1 + \lambda_{k+1}}.$$
(15)

Then,

$$\mathbb{E}\left[f(x_k) - f(x_*)\right] \le \frac{\|x_0 - x^*\|^2}{2\sum_{t=0}^k \eta_t \left(1 - 2\eta_t \mathcal{L}\right)} + \sigma^2 \frac{\sum_{t=0}^k \eta_t^2}{\sum_{t=0}^k \eta_t \left(1 - 2\eta_t \mathcal{L}\right)}.$$
(16)

Note that in Theorem 3.1 the only free parameters are the η_k 's which in the iterate-moving-average viewpoint (12) play the role of a learning rate. All our other parameters, including the step sizes α_k and the momentum parameters β_k , are given once we have chosen η_k . We now explore three different settings of the η_k 's in the following subsections.

3.1 Convergence to a neighborhood of the minimum

Using a constant η_k in Theorem 3.1 gives an interesting new sequence of decreasing step sizes $(\alpha_k)_k$ and increasing momentum parameters $(\beta_k)_k$, as we show in the next corollary. **Corollary 3.2.** Let $\eta_k = \eta < 1/2\mathcal{L}$. If we set

$$\alpha_k = \frac{\eta}{1 + (1+k)(1-2\eta\mathcal{L})} \quad and \quad \beta_k = 1 - \frac{2(1-\eta\mathcal{L})}{1 + (k+1)(1-2\eta\mathcal{L})}, \tag{17}$$

we have $\alpha_k = O\left(\frac{1}{k+1}\right)$ and $\beta_k = O\left(\frac{k}{k+1}\right)$. Then the iterates of SHB (7) converge according to

$$\mathbb{E}\left[f(x_k) - f(x_*)\right] \le \frac{\|x_0 - x_*\|^2}{2\eta \left(1 - 2\eta \mathcal{L}\right) \left(k + 1\right)} + \frac{\eta \sigma^2}{1 - 2\eta \mathcal{L}}.$$
(18)

In particular for $\eta = 1/4\mathcal{L}$ we have that $\alpha_k = \frac{1}{2\mathcal{L}} \frac{1}{k+3}$ and $\beta_k = \frac{k}{k+3}$, which gives

$$\mathbb{E}\left[f(x_k) - f(x_*)\right] \le \frac{4\mathcal{L} \|x_0 - x_*\|^2}{(k+1)} + \frac{\sigma^2}{2\mathcal{L}}.$$
(19)

Corollary 3.2 shows how to set the parameters of SHB so that the last iterate converges sublinearly to a neighborhood of the minimum. In particular, for overparametrized models with $\sigma^2 = 0$, the last iterate of SHB converges sublinearly to the minimum. This same result was only known to hold for the average of the iterates of SGD [38]. Moreover, when using the full gradient, which corresponds to sampling all n individual gradients, we have $\mathcal{L} = L$ and $\sigma^2 = 0$, which recovers the rate derived in [9] for the deterministic HB method upto a constant.

We can also translate this and the following convergence results into convenient complexity results, which we defer to the appendix (Section F) due to lack of space. We can also specialize our results to different forms of samplings and derive the mini-batch size which minimizes the total complexity, which we also defer to the appendix (Section G).

3.2 Exact convergence to the minimum

Now we provide parameter settings for α_k 's and β_k 's that guarantee convergence to the minimum. **Corollary 3.3.** Consider the setting in Theorem (3.1). If we set $\eta_k = \frac{\eta}{\sqrt{k+1}}$, where $\eta < \frac{1}{2\mathcal{L}}$ then the SHB method converges according to

$$\mathbb{E}\left[f(x_{k-1}) - f^*\right] \le \frac{\|x^0 - x^*\|_2^2 + 2\sigma^2 \eta^2 \left(\log(k) + 1\right)}{4\eta \left(\sqrt{k} - 1 - \eta \mathcal{L}\left(\log(k) + 1\right)\right)} \sim O\left(\frac{\log(k)}{\sqrt{k}}\right).$$
(20)

For $\eta = \frac{1}{4\mathcal{L}}$ the step size and momentum parameters are given by (15) where

$$\lambda_0 = 0 \quad and \quad \lambda_{k+1} = \frac{\sqrt{k+2}}{\sqrt{k+1}} \left(\lambda_k + \frac{2\sqrt{k+1}-1}{2\sqrt{k+1}} \right)$$

This $O\left(\log(k)/\sqrt{k}\right)$ convergence rate is the same rate that can be derived using *a weighted average* of the iterates of SGD, as is done by [21]. Next we show how to drop the $\log(k)$ factor (21) if we know the stopping time of the algorithm. Note that using the stopping time to drop such $\log(k)$ terms was first introduced in [21] for the analysis of the average of the iterates of SGD.

Corollary 3.4 (Convergence with known stopping time). Suppose Algorithm (7) is run for T iterations. Set $\eta_k = \frac{\eta}{\sqrt{T+1}}$ for all $k \in \{0, ..., T\}$, where $\eta \leq \frac{1}{4\mathcal{L}}$, in Theorem 3.1. Then it follows directly from (18) that

$$\mathbb{E}\left[f(x_T) - f^*\right] \le \frac{\left\|x^0 - x^*\right\|_2^2 + 2\sigma^2 \eta^2}{\eta\sqrt{T+1}}.$$
(21)

4 Faster asymptotic convergence

In this section, we show that SHB is asymptotically faster than SGD when the model is overparametrized, and that the deterministic HB is asymptotically faster than Gradient Descent. Here we use *a.s.* as an abbreviation of *almost surely*, otherwise also known as convergence *with probability one*. Moreover, we prove that the iterates of SHB (2) converge *a.s.* to a minimizer.

Theorem 4.1. Consider the iterates of (2) and the setting of Theorem 3.1. Choose $\forall k \in \mathbb{N}, 0 < \eta_k < 1/4\mathcal{L}$, such that $\sum_k \eta_k^2 \sigma^2 < +\infty$ and $\sum_k \eta_k = \infty$. With $\lambda_k = \sum_{t=0}^{k-1} (1/2 - 2\eta_t \mathcal{L}) \frac{\eta_t}{\eta_k}$ for all $k \in \mathbb{N}^*$ we have a.s. that

- 1. $x_k \xrightarrow[k \to +\infty]{} x_*$ for some $x_* \in \mathcal{X}^*$,
- 2. for any $x_* \in \mathcal{X}^*$, $f(x_k) f(x_*) = o\left(\frac{1}{\sum_{t=0}^{k-1} \eta_t}\right)$.

Note that when specialized to full gradients sampling, *i.e.* when we use the deterministic HB method, our results hold without the need for *almost sure* statements. This is another benefit of our analysis, since it unifies the analysis of both the stochastic and the deterministic versions of the HB method.

To the best of our knowledge, Theorem 4.1 is the first result showing that the iterates of a stochastic first-order method converge to a minimizer assuming only smoothness and convexity. Indeed, existing results on the *a.s.* convergence of the iterates of SGD or SHB all assume either (BG), (BV) or the unicity of the minimizer [3, 40, 22, 7]. For overparametrized models, Theorem 4.1 shows that $f(x_k) - f(x_*)$ converges *faster* than 1/k.

Corollary 4.2. Assume $\sigma^2 = 0$ and let $\eta_k = \eta < 1/4\mathcal{L}$ for all $k \in \mathbb{N}$. By Theorem 4.1 we have

$$\lim_{k \to \infty} k (f(x_k) - f(x_*)) = 0.$$
 a.s

This corollary has fundamental implications in the deterministic and the stochastic case. In the deterministic case, $\sigma^2 = 0$ always holds. Thus Corollary 4.2 shows that the HB method is *asymptotically faster* than gradient descent since gradient descent is only known to converge according to $f(x_k) - f(x_*) = O(1/k)$. In the stochastic and overparametrized regime, this also shows that SHB is *asymptotically faster* than SGD with averaging which is only guaranteed to converge according to $f(\bar{x}_k) - f(x_*) = O(1/k)$, where $\bar{x}_k \stackrel{\text{def}}{=} (1/k) \sum_{t=0}^k x_t$ [38].

It seems that it is our new iteration-dependent momentum coefficients that enable this new fast 'small o' convergence of the objective values. Indeed, in [1] the authors also showed that a version of (deterministic) Nesterov's Accelerated Gradient algorithm with carefully chosen iteration dependent momentum coefficients converges at rate $o(1/k^2)$ rather than the previously known $O(1/k^2)$.

5 Experiments

For our experiments, we selected a diverse set of multi-class classification problems from the LibSVM repository, 25 problems in total. These datasets range from a few classes to a thousand, and they vary from hundreds of data-points to hundreds of thousands. We normalized each dataset by a constant so that the largest data vector had norm 1. We used a multi-class logistic regression loss with no

	SHB	SGD	Momentum 0.9	Momentum 0.99	No best method
Best method for	11	0	0	0	14

Table 1: Count of how many problems each method is statistically significantly superior to the rest on



Figure 1: Average training error convergence plots for 25 LibSVM datasets, with using the best learning rate for each method and problem combination. Averages are over 40 runs. Error bars show a range of +/- 2SE.

regularization so we could test the non-strongly convex convergence properties, and we ran for 50 epochs with no batching.

Here we compare the parameter setting given by our theory against three common alternative parameter settings used throughout the machine learning literature: SGD with fixed momentum $\hat{\beta}$ of 0.9 and 0.99 as well as no momentum, as given in (3). We left the effective step size $\alpha/(1-\beta)$ of these three methods to be determined through a grid search.

We use SHB to denote our method (7) with α_k and β_k set using (15) and left η as a constant to be determined through grid search.

For the gridsearch, we used power-of-2 grid (2^i) , we ran 5 random seeds and chose the learning rate that gave the lowest loss on average for each combination of problem and method. We widened the grid search as necessary for each combination to ensure that the chosen learning-rate was not from the endpoints of our grid search.

Since the α_k and β_k constants in our method depend on the smoothness constant \mathcal{L} , we set these parameters using (15) and the assumption that $\eta = 1/(4\mathcal{L})$, so that $\mathcal{L} = 1/(4\eta)$. Although it is possible to give a closed-form bound for the Lipschitz smoothness constant for our test problems, the above setting is less conservative and has the advantage of being usable without requiring any knowledge about the problem structure.

We then ran 40 different random seeds to produce Figure 1. To determine which method if any was best on each problem, we performed t-tests with Bonferroni correction, and we report how often each method was statistically significantly superior to all of the other three methods in Table 1. The stochastic heavy ball method using our theoretically motivated parameter settings performed better than all other methods on 11 of the 25 problems. On the remaining problems, no other method was statistically significantly better than all of the rest.

Broader Impact

This work develops the theory and a new viewpoint of a commonly used method (the Momentum method) for training supervised machine learning methods. We give new parameter settings that we believe will reduce the training time. Furthermore we develop new iterate-moving-average viewpoints that we believe can also lead to new insights and understanding of all momentum based method. Given that we do not envision any particular application, nor does this work open up any new applications, we see no ethical or immediate societal consequences.

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Supplementary material

In the appendix, we procede to prove the results we derive in the main paper, then we present the optimal minibatch size to use for SHB depending on the problem setting in Section G. In Section H, we extend the theory developed in Section 3 to the strongly convex case, and show that SHB improves over the last iterate convergence result for SGD by a constant.

A Heavy ball and Momentum are the same thing

To see that (2) and (3) are equivalent we first expand (3) so that

$$x_{k+1} = x_k - \alpha_k m_k$$

= $x_k - \alpha_k (\hat{\beta}_k m_{k-1} + \nabla f_{i_k}(x_k))$

Now using that $x_k = x_{k-1} - \alpha_{k-1}m_{k-1}$ which rearranged gives $m_{k-1} = -\frac{x_k - x_{k-1}}{\alpha_{k-1}}$ in the above gives

$$\begin{aligned} x_{k+1} &= x_k + \alpha_k \left(\hat{\beta}_k \left(\frac{x_k - x_{k-1}}{\alpha_{k-1}} \right) - \nabla f_{i_k}(x_k) \right) \\ &= x_k - \alpha_k \nabla f_{i_k}(x_k) + \frac{\alpha_k}{\alpha_{k-1}} \hat{\beta}_k(x_k - x_{k-1}), \end{aligned}$$

which after substituting $\hat{\beta}_k = \frac{\alpha_{k-1}}{\alpha_k} \beta_k$ gives the equivalence.

B Proof of Theorem 2.1

Proof. Consider the iterate-averaging method

$$z_k = z_{k-1} - \eta_k \nabla f_{v_k}(x_k), \qquad (22)$$

$$x_{k+1} = \frac{\lambda_{k+1}}{\lambda_{k+1} + 1} x_k + \frac{1}{\lambda_{k+1} + 1} z_k,$$
(23)

and let

$$\alpha_k = \frac{\eta_k}{\lambda_{k+1} + 1} \quad \text{and} \quad \beta_k = \frac{\lambda_k}{\lambda_{k+1} + 1}.$$
(24)

Substituting (22) into (23) gives

$$x_{k+1} = \frac{\lambda_{k+1}}{\lambda_{k+1} + 1} x_k + \frac{1}{\lambda_{k+1} + 1} \left(z_{k-1} - \eta_k \nabla f_{v_k}(x_k) \right).$$
(25)

Now using (23) at the previous iteration we have that that

$$z_{k-1} = (\lambda_k + 1) \left(x_k - \frac{\lambda_k}{\lambda_k + 1} x_{k-1} \right) = (\lambda_k + 1) x_k - \lambda_k x_{k-1}.$$

Substituting the above into (25) gives

$$\begin{aligned} x_{k+1} &= \frac{\lambda_{k+1}}{\lambda_{k+1}+1} x_k + \frac{1}{\lambda_{k+1}+1} \left((\lambda_k + 1) x_k - \lambda_k x_{k-1} - \eta_k \nabla f_{v_k}(x_k) \right) \\ &= x_k - \frac{\eta_k}{\lambda_{k+1}+1} \nabla f_{v_k}(x_k) + \frac{\lambda_k}{\lambda_{k+1}+1} \left(x_k - x_{k-1} \right). \end{aligned}$$

Consequently by using (24) gives the result.

C Proof of Theorem 3.1

The proof uses the following Lyaponuv function

$$L_{k} = \mathbb{E} \left[A_{k} \right] + 2\eta_{k}\lambda_{k}\mathbb{E} \left[f(x_{k-1}) - f(x_{*}) \right]$$

where

$$A_k \stackrel{\text{def}}{=} \|x_k - x_* + \lambda_k (x_k - x_{k-1})\|^2.$$

Proof. We have

$$\begin{aligned}
A_{k+1} &= \|x_{k+1} - x_* + \lambda_{k+1} (x_{k+1} - x_k)\|^2 \\
\stackrel{(7)}{=} \|x_k - x_* - \alpha_k \nabla f_{v_k}(x_k) + \beta_k (x_k - x_{k-1}) + \lambda_{k+1} (\beta_k (x_k - x_{k-1}) - \alpha_k \nabla f_{v_k}(x_k))\|^2 \\
&= \|x_k - x_* + \lambda_k (x_k - x_{k-1}) - \eta_k \nabla f_{v_k}(x_k)\|^2 \\
&= A_k + \eta_k^2 \|\nabla f_{v_k}(x_k)\|^2 - 2\eta_k \langle \nabla f_{v_k}(x_k), x_k - x_* \rangle \\
&- 2\eta_k \lambda_k \langle \nabla f_{v_k}(x_k), x_k - x_{k-1} \rangle,
\end{aligned}$$
(26)

where we used in (61) that $\lambda_k = \beta_k (1 + \lambda_{k+1})$ and $\alpha_k (1 + \lambda_{k+1}) = \eta_k$. Then taking conditional expectation $\mathbb{E}_k [\cdot] \stackrel{\text{def}}{=} \mathbb{E} [\cdot | x_k]$ we have

$$\mathbb{E}_{k} [A_{k+1}] \stackrel{(6)}{=} A_{k} + \eta_{k}^{2} \mathbb{E}_{k} \left[\|\nabla f_{v_{k}}(x_{k})\|^{2} \right] - 2\eta_{k} \langle \nabla f(x_{k}), x_{k} - x_{*} \rangle
-2\eta_{k} \lambda_{k} \langle \nabla f(x_{k}), x_{k} - x_{k-1} \rangle,
\stackrel{(9)+(4)}{\leq} A_{k} + 4\eta_{k}^{2} \mathcal{L} \left(f(x_{k}) - f(x_{*}) \right) + 2\eta_{k}^{2} \sigma^{2}
-2\eta_{k} \left(f(x_{k}) - f(x_{*}) \right) - 2\eta_{k} \lambda_{k} \left(f(x_{k}) - f(x_{k-1}) \right)
= A_{k} - 2\eta_{k} \left(1 + \lambda_{k} - 2\eta_{k} \mathcal{L} \right) \left(f(x_{k}) - f(x_{*}) \right)
+ 2\eta_{k} \lambda_{k} \left(f(x_{k-1}) - f(x_{*}) \right) + 2\eta_{k}^{2} \sigma^{2}.$$
(27)

Since $\lambda_{k+1} = \frac{\sum_{t=0}^{k} \eta_t (1-2\eta_t \mathcal{L})}{\eta_{k+1}}$ we have that

$$\eta_{k+1}\lambda_{k+1} = \eta_k \left(1 + \lambda_k - 2\eta_k \mathcal{L}\right).$$

Using this in (27) then taking expectation and rearranging gives

 $\mathbb{E}\left[A_{k+1}\right] + 2\eta_{k+1}\lambda_{k+1}\mathbb{E}\left[f(x_k) - f(x_*)\right] \le \mathbb{E}\left[A_k\right] + 2\eta_k\lambda_k\mathbb{E}\left[f(x_{k-1}) - f(x_*)\right] + 2\eta_k^2\sigma^2.$ Summing over t = 0 to k and using a telescopic sum, we have

$$\mathbb{E}[A_{k+1}] + 2\eta_{k+1}\lambda_{k+1}\mathbb{E}[f(x_k) - f(x_*)] \le ||x_0 - x^*||^2 + 2\sigma^2 \sum_{t=0}^k \eta_t^2,$$

where we used that $\lambda_0 = 0$. Thus, writing λ_k explicitly, gives

$$\mathbb{E}\left[f(x_k) - f(x_*)\right] \le \frac{\|x_0 - x^*\|^2}{2\sum_{t=0}^k \eta_t \left(1 - 2\eta_t \mathcal{L}\right)} + \sigma^2 \frac{\sum_{t=0}^k \eta_t^2}{\sum_{t=0}^k \eta_t \left(1 - 2\eta_t \mathcal{L}\right)}.$$

D Proof of Corollary 3.3

Proof. Using the integral bound and plugging in our choice of η_k gives

$$\sum_{t=0}^{k-1} \eta_t^2 = \eta^2 \sum_{t=0}^{k-1} \frac{1}{t+1} \le \eta^2 \left(\log(k) + 1 \right).$$
(28)

Furthermore using the integral bound again we have that

$$\sum_{t=0}^{k-1} \eta_t \geq 2\eta \left(\sqrt{k} - 1\right).$$
⁽²⁹⁾

Now using (28) and (29) we have that

$$\sum_{k=0}^{k-1} \eta_i (1 - 2\eta_i \mathcal{L}) = \sum_{i=0}^{k-1} \eta_i - 2\mathcal{L} \sum_{i=0}^{k-1} \eta_i^2$$

$$\geq 2\eta \left(\sqrt{k} - 1 - \eta \mathcal{L} (\log(k) + 1) \right).$$
(30)

Using (28) and (30) in (16) gives (20).

As for the parameter settings, note that

$$\lambda_{k+1} = \frac{\sum_{t=0}^{k} \eta_t \left(1 - 2\eta_t \mathcal{L}\right)}{\eta_{k+1}}$$
$$= \frac{\eta_k}{\eta_{k+1}} \left(\lambda_k + 1 - 2\eta_k \mathcal{L}\right)$$
$$= \frac{\sqrt{k+2}}{\sqrt{k+1}} \left(\lambda_k + 1 - \frac{2\eta \mathcal{L}}{\sqrt{k+1}}\right)$$

For $\eta = 1/4\mathcal{L}$ the above gives

$$\lambda_{k+1} = \frac{\sqrt{k+2}}{\sqrt{k+1}} \left(\lambda_k + 1 - \frac{1}{2\sqrt{k+1}} \right) \\ = \frac{\sqrt{k+2}}{\sqrt{k+1}} \left(\lambda_k + \frac{2\sqrt{k+1} - 1}{2\sqrt{k+1}} \right).$$

Thus by maintaining and updating λ_k we can compute the step sizes and momentum parameters using (15).

E Proof of Theorem 4.1

A necessary tool to prove Theorem 4.1 is the following Robbins-Siegmund theorem [31].

Lemma E.1 (Simplified Robbins-Sigmund Theorem). Consider a filtration $(\mathcal{F}_k)_k$ and nonnegative sequences of $(\mathcal{F}_k)_k$ –adapted processes $(V_k)_k$, $(U_k)_k$ and $(Z_k)_k$ such that

- $\sum_k Z_k < +\infty$ almost surely.
- $\forall k \in \mathbb{N}$.

$$\mathbb{E}\left[V_{k+1}|\mathcal{F}_k\right] + U_{k+1} \le V_k + Z_k. \tag{31}$$

Then, $(V_k)_k$ converges and $\sum_k U_k < +\infty$ almost surely.

In the remainder of this section, we consider the iterates of (2) and the setting of Theorem 4.1, that is:

$$\lambda_0 = 0, \ \lambda_k = \lambda_k = \frac{\sum_{t=0}^{k-1} \left(\frac{1}{2} - 2\eta_t \mathcal{L}\right) \eta_t}{\eta_k}, \ \alpha_k = \frac{\eta_k}{1 + \lambda_{k+1}} \text{ and } \beta_k = \frac{\lambda_k}{1 + \lambda_{k+1}}, \tag{32}$$

where $0 < \eta_k < 1/4\mathcal{L}$, $\sum_k \eta_k^2 \sigma^2 < \infty$ and $\sum_k \eta_k = \infty$. We also define:

$$z_k = x_k + \lambda_k \left(x_k - x_{k-1} \right) \tag{33}$$

To make the proof more readable, we first state the two following lemmas, for which we give a proof after the proof of the theorem.

Lemma E.2. $\sum_k \eta_k \left(f(x_k) - f(x_*) \right) < +\infty$ almost surely.

Lemma E.3.

$$\sum_{k} \lambda_{k+1} \|x_k - x_{k-1}\|^2 < +\infty,$$
(34)

and thus, $\lim_k \lambda_{k+1} ||x_{k+1} - x_k||^2 = 0$ almost surely.

We can now prove Theorem 4.1.

Proof of the theorem. This proof aims at proving that, *a.s.*

In our road to prove the first point, we will prove the second point as a byproduct.

We will now prove that $\lim_k ||z_k - x_*||^2$ exists a.s..

$$||z_k - x_*||^2 = ||x_k - x_* + \lambda_k (x_k - x_{k-1})||^2$$
(35)

$$= \lambda_k^2 \|x_k - x_{k-1}\|^2 + 2\lambda_k \langle x_k - x_*, x_k - x_{k-1} \rangle + \|x_k - x_*\|^2$$
(36)

$$= (\lambda_k^2 + \lambda_k) \|x_k - x_{k-1}\|^2 + \lambda_k \left(\|x_k - x_*\|^2 - \|x_{k-1} - x_*\|^2 \right) + \|x_k - x_*\|^2$$

Define

$$\delta_k \stackrel{\text{def}}{=} \lambda_k \left(\|x_k - x_*\|^2 - \|x_{k-1} - x_*\|^2 \right) + \|x_k - x_*\|^2.$$
(38)

Then,

$$\|z_{k} - x_{*}\|^{2} = (\lambda_{k}^{2} + \lambda_{k}) \|x_{k} - x_{k-1}\|^{2} + \delta_{k}.$$
(39)

We will first prove that $\lim_k (\lambda_k^2 + \lambda_k) ||x_k - x_{k-1}||^2$ exists *a.s.*, then that $\lim_k \delta_k$ exists *a.s.*.

First, we have from Lemma E.3 that $(\lambda_k ||x_k - x_{k-1}||^2)_k$ converges (to 0) *a.s.*. Hence, it remains to show that $\lim_k \lambda_k^2 ||x_k - x_{k-1}||^2$ exists *a.s.*

From (71), we have that:

$$\lambda_{k+1}^{2} \mathbb{E}_{k} \left[\left\| x_{k+1} - x_{k} \right\|^{2} \right] + 2\eta_{k} \left(\lambda_{k} - 2\eta_{k} \mathcal{L} \right) \left(f(x_{k}) - f(x_{*}) \right)$$

$$(40)$$

$$\leq \lambda_k^2 \|x_k - x_{k-1}\|^2 + 2\eta_k \lambda_k \left(f(x_{k-1}) - f(x_*) \right) + 2\eta_k^2 \sigma^2.$$
(41)

By definition of λ_k , we have $2\eta_k (\lambda_k - 2\eta_k \mathcal{L}) = 2\eta_{k+1}\lambda_{k+1} - \eta_k$. Therefore, noting

$$d_k \stackrel{\text{def}}{=} \|x_k - x_{k-1}\|^2 \text{ and } \theta_k \stackrel{\text{def}}{=} 2\eta_k \left(f(x_{k-1}) - f(x_*) \right),$$
 (42)

we have:

$$\mathbb{E}_k \left[\lambda_{k+1}^2 d_k + \lambda_{k+1} \theta_{k+1} \right] \le \lambda_k^2 d_k + \lambda_k \theta_k + \eta_k \left(f(x_k) - f(x_*) \right) + 2\eta_k^2 \sigma^2.$$
(43)

But from Lemma E.2, we have $\sum_k \eta_k (f(x_k) - f(x_*)) < +\infty$. Moreover, $\sum_k \eta_k^2 \sigma^2 < +\infty$. Hence, we have by Lemma E.1 that $\lim_k \lambda_k^2 d_k + \lambda_k \theta_k$ exists almost surely.

Moreover, by Lemma E.3, $\sum_k \lambda_k d_k < +\infty$, and we have $\sum_k \theta_k < +\infty$ a.s.. Hence, $\sum_k \lambda_k d_k + \theta_k < +\infty$ a.s. Rewriting

$$\lambda_k d_k + \theta_k = \frac{1}{\lambda_k} \left(\lambda_k^2 d_k + \lambda_k \theta_k \right), \tag{44}$$

we have, since $\lim_k \lambda_k^2 d_k + \lambda_k \theta_k$ exists *a.s.*, that is *a.s.*,

$$\lim_{k} \lambda_k^2 d_k + \lambda_k \theta_k = 0, \tag{45}$$

which means that both $\lim_k \lambda_k^2 d_k = 0$ and $\lim_k \lambda_k \theta_k = 0$ a.s. Explicitly written, we have

$$f(x_k) - f(x_*) = o\left(\frac{1}{\sum_{t=1}^{k-1} \eta_t}\right) \ a.s.$$
(46)

This proves the second point of Theorem 4.1.

We have also proved that $\lim_k \lambda_k^2 d_k = 0$ a.s.. It remains to show that $\lim_k \delta_k$ exists a.s.

Note
$$u_k = ||x_k - x_*||^2$$
. We have
 $u_{k+1} = ||x_k - x_* + \beta_k (x_k - x_{k-1})||^2 + \alpha_k^2 ||\nabla f_{v_k}(x_k)||^2 - 2\alpha_k \beta_k \langle \nabla f_{v_k}(x_k), x_k - x_k | (47) - 2\alpha_k \langle \nabla f_{v_k}(x_k), x_k - x_* \rangle$
(48)

Thus,

$$\mathbb{E}_{k} [u_{k+1}] \leq \|x_{k} - x_{*} + \beta_{k} (x_{k} - x_{k-1})\|^{2} - 2\alpha_{k} (1 + \beta_{k} - 2\alpha_{k}\mathcal{L}) (f(x_{k}) - f(x_{*})) (49) + 2\alpha_{k}\beta_{k} (f(x_{k-1}) - f(x_{*})) + 2\alpha_{k}^{2}\sigma^{2}.$$
(50)

And

$$\|x_{k} - x_{*} + \beta_{k} (x_{k} - x_{k-1})\|^{2} = u_{k} + \beta_{k}^{2} d_{k} + 2\beta_{k} \langle x_{k} - x_{*}, x_{k} - x_{k-1} \rangle$$
(51)
$$= u_{k} + \left(\beta_{k}^{2} + \beta_{k}\right) d_{k} + \beta_{k} (u_{k} - u_{k-1})$$
(52)

$$= u_{k} + (\beta_{k}^{2} + \beta_{k}) d_{k} + \beta_{k} (u_{k} - u_{k-1})$$
(52)

Hence, using the fact that $0 \leq \beta_k \leq 1$,

$$\mathbb{E}_{k} [u_{k+1}] \leq u_{k} + 2d_{k} + \beta_{k} (u_{k} - u_{k-1}) - 2\alpha_{k} (1 + \beta_{k} - 2\alpha_{k}\mathcal{L}) (f(x_{k}) - f(x_{*})) (53)
+ 2\alpha_{k}\beta_{k} (f(x_{k-1}) - f(x_{*})) + 2\alpha_{k}^{2}\sigma^{2}.$$
(54)

Multiplying by $(1 + \lambda_{k+1})$:

$$(1+\lambda_{k+1})\mathbb{E}_k \left[u_{k+1} - u_k \right] \leq 2 \left(1 + \lambda_{k+1} \right) d_k + \lambda_k \left(u_k - u_{k-1} \right) - 2\eta_k \left(1 + \beta_k - 2\alpha_k \mathcal{L} \right) \left(f(x_k) - f(x_*) \right) \\ + 2\eta_k \beta_k \left(f(x_{k-1}) - f(x_*) \right) + 2\eta_k^2 \sigma^2.$$

Rewriting this inequality and using the fact that

$$\delta_{k+1} - \delta_k = (1 + \lambda_{k+1}) (u_{k+1} - u_k) - \lambda_k (u_k - u_{k-1}),$$

we have

$$\mathbb{E}_{k}\left[\delta_{k+1} + \left(1 + \beta_{k} - 2\alpha_{k}\mathcal{L}\right)\theta_{k+1}\right] \leq \delta_{k} + \beta_{k}\theta_{k} + 2\left(1 + \lambda_{k+1}\right)d_{k} + 2\frac{\eta_{k}^{2}}{1 + \lambda_{k+1}}\sigma^{2}.$$
(55)

And since,

$$1 + \beta_k - 2\alpha_k \mathcal{L} = 1 + \frac{\lambda_k}{1 + \lambda_{k+1}} - \frac{2\eta \mathcal{L}}{1 + \lambda_{k+1}} = \frac{1}{1 + \lambda_{k+1}} \left(1 + \lambda_{k+1} + \lambda_k - 2\eta \mathcal{L}\right)$$
(56)

$$\geq \quad \frac{\lambda_{k+1}}{1+\lambda_{k+1}} \geq \frac{\lambda_{k+1}}{1+\lambda_{k+2}} = \beta_{k+1}, \quad (57)$$

0

we have

$$\mathbb{E}_{k}\left[\delta_{k+1} + \beta_{k+1}\theta_{k+1}\right] \le \left(\delta_{k} + \beta_{k}\theta_{k}\right) + 2\left(1 + \lambda_{k+1}\right)d_{k} + \frac{2\eta_{k}^{2}}{1 + \lambda_{k+1}}\sigma^{2}.$$
(58)

Since by Lemma E.3 $\sum_{k} 2(1 + \lambda_{k+1}) d_k < +\infty \ a.s.$, and $\sum_{k} \frac{\eta_k^2 \sigma^2}{1 + \lambda_{k+1}} < +\infty$, we have by Lemma E.1 that $\lim_k \delta_k + \beta_k \theta_k$ exists a.s. And since $\lim_k \beta_k \theta_k = 0$ a.s., we deduce that $\lim_k \delta_k$ exists a.s.

Thus we have now shown that $\lim_k ||z_k - x_*||^2$ exists *a.s.* Therefore, since $x_k - x_* = z_k - x_* - \lambda_k (x_k - x_{k-1})$ and

$$|\|x_{k} - x_{*}\| - \|z_{k} - x_{*}\|| \le \lambda_{k} \|x_{k} - x_{k-1}\| \underset{k \to +\infty}{\to} 0 \text{ a.s.},$$
(59)

we have that $\lim_{k} ||x_{k} - x_{*}|| - ||z_{k} - x_{*}||$ exists *a.s.*, and so does $\lim_{k} ||x_{k} - x_{*}||$.

We also have that both $||z_k - x_*||$ and $\lambda_k ||x_k - x_{k-1}||$ are bounded *a.s.*, thus $||x_k - x_*||$ is bounded *a.s.* Hence, $(x_k)_k$ is bounded *a.s.*, thus *a.s.* sequentially compact.

Let $(x_{n_k})_k$ be a subsequence of $(x_n)_n$ which converges to some $x \in \mathbb{R}^d$ a.s. Since $f(x_n) \to_n f(x^*)$ a.s. for all $x^* \in \operatorname{argmin} f$, we have $x \in \operatorname{argmin} f$ a.s. Finally, applying Lemma 2.39 in [2] (restricted to our finite dimensional setting, where weak convergence and strong convergence are equivalent), there exists $x_* \in \operatorname{argmin} f$ such that

$$\begin{array}{c} x_k \xrightarrow[k \to +\infty]{} x_* \ a.s. \end{array}$$
(60)

This proves the first point of Theorem 4.1.

We now turn to prove Lemma E.2.

Proof of Lemma E.2. We have

$$\begin{aligned} \|z_{k+1} - x_*\|^2 &= \|x_{k+1} - x_* + \lambda_{k+1} (x_{k+1} - x_k)\|^2 \\ \stackrel{(7)}{=} \|x_k - x_* - \alpha_k \nabla f_{v_k}(x_k) + \beta_k (x_k - x_{k-1}) + \lambda_{k+1} (\beta_k (x_k - x_{k-1}) - \alpha_k \nabla f_{v_k}(x_k))\|^2 \\ &= \|x_k - x_* + \lambda_k (x_k - x_{k-1}) - \eta_k \nabla f_{v_k}(x_k)\|^2 \\ &= \|z_k - x_*\|^2 + \eta_k^2 \|\nabla f_{v_k}(x_k)\|^2 - 2\eta_k \langle \nabla f_{v_k}(x_k), x_k - x_* \rangle \\ &- 2\eta_k \lambda_k \langle \nabla f_{v_k}(x_k), x_k - x_{k-1} \rangle, \end{aligned}$$
(61)

where we used in (61) that $\lambda_k = \beta_k (1 + \lambda_{k+1})$ and $\alpha_k (1 + \lambda_{k+1}) = \eta_k$. Then taking conditional expectation $\mathbb{E}_k [\cdot] \stackrel{\text{def}}{=} \mathbb{E} [\cdot | x_k]$ we have

$$\mathbb{E}_{k} \left[\|z_{k+1} - x_{*}\|^{2} \right] = \|z_{k} - x_{*}\|^{2} + \eta_{k}^{2} \mathbb{E}_{k} \left[\|\nabla f_{v_{k}}(x_{k})\|^{2} \right] - 2\eta_{k} \langle \nabla f(x_{k}), x_{k} - x_{*} \rangle
-2\eta_{k} \lambda_{k} \langle \nabla f(x_{k}), x_{k} - x_{k-1} \rangle,$$

$$\stackrel{(4)+(9)}{\leq} \|z_{k} - x_{*}\|^{2} + 4\eta_{k}^{2} \mathcal{L} \left(f(x_{k}) - f(x_{*}) \right) + 2\eta_{k}^{2} \sigma^{2}
-2\eta_{k} \left(f(x_{k}) - f(x_{*}) \right) - 2\eta_{k} \lambda_{k} \left(f(x_{k}) - f(x_{k-1}) \right)
= \|z_{k} - x_{*}\|^{2} - 2\eta_{k} \left(1 + \lambda_{k} - 2\eta_{k} \mathcal{L} \right) \left(f(x_{k}) - f(x_{*}) \right)
+2\eta_{k} \lambda_{k} \left(f(x_{k-1}) - f(x_{*}) \right) + 2\eta_{k}^{2} \sigma^{2}.$$
(62)

Rearranging,

$$\mathbb{E}_{k}\left[\left\|z_{k+1}-x_{*}\right\|^{2}\right]+2\eta_{k}\left(1-2\eta_{k}\mathcal{L}+\lambda_{k}\right)\left(f(x_{k})-f(x_{*})\right)$$
(63)

$$\leq ||z_k - x_*||^2 + 2\eta_k \lambda_k \left(f(x_{k-1}) - f(x_*) \right) + 2\eta_k^2 \sigma^2.$$
(64)

Let
$$\lambda_k = \frac{\sum_{t=0}^{k-1} \eta_t \left(\frac{1}{2} - 2\eta_t \mathcal{L}\right)}{\eta_k}$$
 and $\lambda_0 = 0$. Then, it is clear that:

$$\mathbb{E}_k \left[\|z_{k+1} - x_*\|^2 + 2\eta_{k+1}\lambda_{k+1} \left(f(x_k) - f(x_*)\right) \right] + \eta_k \left(f(x_k) - f(x_*)\right) \qquad (65)$$

$$\leq \|z_k - x_*\|^2 + 2\eta_k \lambda_k \left(f(x_{k-1}) - f(x_*)\right) + 2\eta_k^2 \sigma^2. \qquad (66)$$

Hence, applying Lemma E.1, we have

$$\sum_{k} \eta_k \left(f(x_k) - f(x_*) \right) < +\infty \ a.s.$$

(69)

We now turn to prove Lemma E.3.

Proof of Lemma E.3. We have,

$$\mathbb{E}_{k} \left[\|x_{k+1} - x_{k}\|^{2} \right] = \beta_{k}^{2} \|x_{k} - x_{k-1}\|^{2} + \alpha_{k}^{2} \|\nabla f_{v_{k}}(x_{k})\|^{2} - 2\alpha_{k}\beta_{k} \langle \nabla f(x_{k}), x_{k} - x_{k-4} \langle \mathbf{0} \rangle^{7}$$
Thus, multiplying by $(1 + \lambda_{k+1})^{2}$ and using the fact that $\beta_{k} = \frac{\lambda_{k}}{1 + \lambda_{k+1}}$ and $\alpha_{k} = \frac{\eta_{k}}{1 + \lambda_{k+1}}$, we have:
 $(1 + \lambda_{k+1})^{2} \mathbb{E}_{k} \left[\|x_{k+1} - x_{k}\|^{2} \right] = \lambda_{k}^{2} \|x_{k} - x_{k-1}\|^{2} + \eta_{k}^{2} \|\nabla f_{v_{k}}(x_{k})\|^{2} - 2\eta_{k}\lambda_{k} \langle \nabla f(x_{k}), x_{k} - x_{k-1} \rangle$
Thus using the convexity of f and $\mathbb{E}_{k} \left[\|\nabla f_{v_{k}}(x_{k})\|^{2} \right] \leq 4\mathcal{L} \left(f(x_{k}) - f(x_{*}) \right) + 2\sigma^{2}$, we have:
 $(1 + \lambda_{k+1})^{2} \mathbb{E}_{k} \left[\|x_{k+1} - x_{k}\|^{2} \right] \leq \lambda_{k}^{2} \|x_{k} - x_{k-1}\|^{2} - 2\eta_{k} \left(\lambda_{k} - 2\eta_{k}\mathcal{L}\right) \left(f(x_{k}) - f(x_{*}) \right) \delta^{8} + 2\eta_{k}\lambda_{k} \left(f(x_{k-1}) - f(x_{*}) \right) + 2\eta_{k}^{2}\sigma^{2}.$
(69)

Hence,

$$(1 + \lambda_{k+1})^2 \mathbb{E}_k \left[\|x_{k+1} - x_k\|^2 \right] + 2\eta_k \left(\lambda_k - 2\eta_k \mathcal{L}\right) \left(f(x_k) - f(x_*) \right)$$
(70)

$$\leq \lambda_k^2 \|x_k - x_{k-1}\|^2 + 2\eta_k \lambda_k \left(f(x_{k-1}) - f(x_*)\right) + 2\eta_k^2 \sigma^2.$$
Plugging back this equation into (64):
$$(71)$$

 $\mathbb{E}_{k}\left[\left\|z_{k+1}-x_{*}\right\|^{2}\right]+4\eta_{k}\left(\frac{1}{2}-2\eta_{k}\mathcal{L}+\lambda_{k}\right)\left(f(x_{k})-f(x_{*})\right)+\left(1+\lambda_{k+1}\right)^{2}\mathbb{E}_{k}\left[\left\|x_{k+1}-x_{k}\right\|^{2}\right]$ $\leq ||z_k - x_*||^2 + 4\eta_k \lambda_k \left(f(x_{k-1}) - f(x_*) \right) + \lambda_k^2 ||x_k - x_{k-1}||^2 + 4\eta_k^2 \sigma^2.$

Hence,

$$||z_{k+1} - x_*||^2 + 4\eta_{k+1}\lambda_{k+1}(f(x_k) - f(x_*)) + (1 + \lambda_{k+1})^2 ||x_{k+1} - x_k||^2$$
(72)

$$\leq \|z_k - x_*\|^2 + 4\eta_k \lambda_k \left(f(x_{k-1}) - f(x_*) \right) + \lambda_k^2 \|x_k - x_{k-1}\|^2 + 4\eta_k^2 \sigma^2.$$
(73)

Hence, noting $\mathcal{E}_{k} \stackrel{\text{def}}{=} ||z_{k} - x_{*}||^{2} + 4\eta_{k}\lambda_{k} (f(x_{k-1}) - f(x_{*})) + \lambda_{k}^{2} ||x_{k} - x_{k-1}||^{2}$, we have $\mathbb{E}_{k}\left[\mathcal{E}_{k+1}\right] + \left(2\lambda_{k+1} + 1\right) \|x_{k} - x_{k-1}\|^{2} \le \mathcal{E}_{k} + 4\eta_{k}^{2}\sigma^{2}.$ (74)

Hence, since $\sum_k \eta_k^2 \sigma^2 < +\infty$, applying lemma E.1, we have

$$\sum_{k} \lambda_{k+1} \|x_k - x_{k-1}\|^2 < +\infty \ a.s., \text{ thus } \lim_{k} \lambda_{k+1} \|x_{k+1} - x_k\|^2 = 0 \ a.s. \tag{75}$$

F **Complexity results**

F.1 Complexity result for Corollary 3.2

We can translate the convergence result of Corollary 3.2 into a convenient complexity result. **Corollary F.1.** *Consider the setting in Corollary 3.2. For any* $\epsilon > 0$ *, if we choose*

$$\eta = \frac{\epsilon}{4\left(\sigma^2 + \epsilon\mathcal{L}\right)} \tag{76}$$

and

$$k \ge 8 \frac{\|x_0 - x_*\|^2}{\epsilon} \left(\frac{\sigma^2}{\epsilon} + \mathcal{L}\right),\tag{77}$$

then we have $\mathbb{E}\left[f(x_{k-1}) - f(x_*)\right] \leq \epsilon$.

Proof. With $\eta = \frac{\epsilon}{4(\sigma^2 + \epsilon \mathcal{L})} \leq \frac{1}{4\mathcal{L}}$ we have that the second term in (18) is bounded with $\frac{\eta \sigma^2}{1 - 2\eta \mathcal{L}} < \frac{\epsilon}{2}$. Furthermore, since $\eta \leq \frac{1}{4\mathcal{L}}$ we have that $\frac{\|x_0 - x_*\|^2}{2\eta(1 - 2\eta\mathcal{L})} \leq \frac{\|x_0 - x_*\|^2}{\eta}$. Consequently we can bound the first term in (18) by $\sqrt{21}$ first term in (18) by $\epsilon/2$ by enforcing

$$\frac{\|x_0 - x_*\|^2}{2\eta \left(1 - 2\eta \mathcal{L}\right)} \frac{1}{k} \le \frac{\|x_0 - x_*\|^2}{\eta} \frac{1}{k} \le \frac{\epsilon}{2} \quad \Leftrightarrow \quad k \ge \frac{2\|x_0 - x_*\|^2}{\epsilon \eta} = 8 \frac{\|x_0 - x_*\|^2}{\epsilon} \left(\frac{\sigma^2}{\epsilon} + \mathcal{L}\right).$$
Using these two bounds in (18) gives the result.

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F.2 Complexity result for Corollary 3.4

Corollary F.2. If we choose

$$\eta = \min\left\{\frac{1}{4\mathcal{L}}, \frac{\|x_0 - x_*\|}{\sqrt{2\sigma^2}}\right\}$$
(78)

and

$$T \ge \left(\max\left\{ 4\mathcal{L} \|x_0 - x_*\|^2, \sqrt{2\sigma^2} \|x_0 - x_*\| \right\} + \min\left\{ \frac{\sigma^2}{2\mathcal{L}}, \sqrt{2\sigma^2} \|x_0 - x_*\| \right\} \right)^2 \frac{1}{\epsilon^2},$$
(79)

we have $\mathbb{E}\left[f(x_{T-1}) - f(x_*)\right] < \epsilon$.

G Optimal mini-batch size

In this section, we present specializations of our complexity results to the case of *b*-minibatch sampling, and determine what is the optimal mini-batch to use for SHB depending on the parameter settings.

First, we formally define *b*-minibatch sampling

Definition G.1 (*b*-mini-batch sampling). Let $b \in [n]$. The random vector defined by

$$\operatorname{Prob}\left(v = \frac{n}{b} \sum_{i \in B} e_i\right) = \frac{1}{\binom{n}{b}}, \quad \forall B \subset [n], \ |B| = b,$$
(80)

is a sampling vector. We refer to v as the b-mini batch sampling.

Since Corollary F.1 holds for any sampling vector, we now have a precise expression for the complexity of SHB when using *b*-mini-batching (Definition G.1). In particular, we can even determine the mini-batch size *b* that minimizes the *total computational cost* of SHB. We define the total computational cost as the total number of individual gradients ∇f_i computed to reach a certain precision ϵ . That is, the total computational cost of SHB with the setting of Corollary F.1 is the iteration complexity (77) times the mini-batch size

$$C(b) \stackrel{\text{def}}{=} 8b\left(\frac{\sigma^2(b)}{\epsilon} + \mathcal{L}(b)\right) \frac{\|x_0 - x_*\|^2}{\epsilon},\tag{81}$$

where $\mathcal{L}(b)$ and $\sigma^2(b)$ are defined in (10) and (11).

This total cost is straightforward to minimize in *b*, as we see next. **Corollary G.2.** *We have that the mini-batch size which minimizes the total complexity* (81) *is given*

by:

$$b^* \stackrel{def}{=} \begin{cases} 1 & \text{if } \sigma_1^2 \le \epsilon (nL - L_{\max}) \\ n & \text{otherwise.} \end{cases}$$
(82)

Curiously, and unlike SGD in the strongly convex setting (see Eq. 38 in [12]), the optimal mini-batch size is either 1 or the full gradient. If we used a different model of computational cost, for instance where stochastic gradients can be computed in parallel, then we would arrive at a different optimal mini-batch size.

H Strongly convex case

In this section, we assume that f is strongly convex: there exists $\mu > 0$ such that for all $x, y \in \mathbb{R}^d$

$$f(x) \ge f(y) + \langle \nabla f(y), x - y \rangle + \frac{\mu}{2} ||x - y||^2.$$
(83)

Note that (83) implies that there is a unique x^* solution.

Following the same layout to Section 3, we first present a general theorem that depends on a sequence of auxiliary parameters η_k .

Theorem H.1. Consider the iterates of Algorithm 7. Let $(\eta_k)_k$ be a decreasing sequence such that $\eta_0 = \eta$ with $0 < \eta < \frac{1}{2\ell}$. Define

$$\lambda_k \stackrel{\text{def}}{=} \frac{1 - 2\eta \mathcal{L}}{\eta \mu} \left(1 - (1 - \eta \mu)^k \right)$$
$$A_k \stackrel{\text{def}}{=} \|x_k - x_* + \lambda_k \left(x_k - x_{k-1} \right) \|^2 , \qquad (84)$$

$$\mathcal{E}_k \stackrel{\text{def}}{=} A_k + 2\eta_k \lambda_k \left(f(x_{k-1}) - f(x_*) \right). \tag{85}$$

By setting the parameters of SHB as

$$\alpha_k = \frac{\eta_k}{1 + \lambda_{k+1}} \quad and \quad \beta_k = \lambda_k \frac{1 - \eta_k \mu}{1 + \lambda_{k+1}},\tag{86}$$

we have that

$$\mathbb{E}\left[\mathcal{E}_{k+1}\right] \le \left(1 - \eta_k \mu\right) \mathbb{E}\left[\mathcal{E}_k\right] + 2\eta_k^2 \sigma^2.$$
(87)

Next we consider specializations of Theorem H.1 in two following corollaries.

H.1 Convergence to a neighborhood of the minimizer

Corollary H.2. Consider the setting of Theorem H.1. Let $\eta_k = \eta$ for all $k \in \mathbb{N}$, with $0 < \eta \leq \frac{1}{2\mathcal{L}}$ and $\lambda_k = \frac{1-2\eta\mathcal{L}}{\eta\mu} \left(1 - (1 - \eta\mu)^k\right)$. If we set the parameters of the SHB method (7) according to

$$\alpha_k = \frac{\eta}{1 + \lambda_{k+1}} \quad and \quad \beta_k = \lambda_k \frac{1 - \eta \mu}{1 + \lambda_{k+1}},\tag{88}$$

then the iterates converge according to

$$\mathbb{E}\left[\mathcal{E}_{k}\right] \le \left(1 - \eta\mu\right)^{k} \|x_{0} - x^{*}\|^{2} + \frac{2\eta\sigma^{2}}{\mu}.$$
(89)

In particular, (89) shows that for $\eta < 1/2\mathcal{L}$ the suboptimality gap converges globally according to

$$\mathbb{E}\left[f(x_k) - f(x^*)\right] \le \frac{\mu \left(1 - \eta \mu\right)^{k+1} \|x_0 - x^*\|^2 + 2\eta \sigma^2}{2\left(1 - (1 - \eta \mu)^{k+1}\right) (1 - 2\eta \mathcal{L})}$$
(90)

If we choose $\eta = 1/2\mathcal{L}$ then $\lambda_k = \beta_k = 0$, thus the SHB method (7) becomes the SGD method and (89) becomes

$$\mathbb{E}\left[\left\|x_{k}-x_{*}\right\|^{2}\right] \leq \left(1-\eta\mu\right)^{k}\left\|x_{0}-x^{*}\right\|^{2}+\frac{2\eta\sigma^{2}}{\mu},$$
(91)

which recovers the best known convergence rate for SGD in this setting given recently in Theorem 3.1 in [12].

The suboptimality convergence in (90) is also faster than that of SGD given in [12]. Indeed, looking at the proof of Theorem 3.1 in [12], we can see that the x_k iterates of SGD (that is (7) with $\beta_k = 0$ and $\alpha_k = \eta$) converge according to

$$\mathbb{E}\left[f(x_k) - f(x_*)\right] \le \frac{\mu \left(1 - \eta \mu\right)^k \|x_0 - x_*\|^2 + 2\eta \sigma^2}{2\eta \mu \left(1 - 2\eta \mathcal{L}\right)},\tag{92}$$

where $\eta \leq 1/2\mathcal{L}$. Thus the rate of convergence in (90) is faster than the rate of SGD in (92) by a factor of

$$\frac{1 - (1 - \eta\mu)^k}{\eta\mu} \ge 1, \quad \forall k \in \mathbb{N}.$$

Consequently, Corollary H.2 not only recovers the best known convergence of the iterates of SGD as a special case, but also shows that we achieve a (slightly) tighter upper bound at the last iterate for SHB under the same assumptions.

H.2 Optimal mini-batching and non-uniform sampling

From (89), we can see that for any $\epsilon > 0$, we have $\mathbb{E}\left[\|x_k + \lambda_k (x_k - x_{k-1}) - x_*\|^2\right] \le \epsilon$ if $\eta = \min\left\{\frac{1}{2\mathcal{L}}, \frac{\epsilon\mu}{4\sigma^2}\right\}$ and

$$k \ge \max\left\{\frac{2\mathcal{L}}{\mu}, \frac{4\sigma^2}{\epsilon\mu^2}\right\} \log\left(\frac{2\|x_0 - x_*\|^2}{\epsilon}\right).$$
(93)

Under this choice of η , the iteration complexity for the convergence of the iterates (93) and that obtained in Theorem 3.1 in [12] are identical. Therefore, the total complexities are also identical. Consequently, all the results on optimal mini-batch sizes and optimal non-uniform probabilities established in [12] apply to the SHB method verbatim in this setting.

H.3 Switching η_k and global convergence

Much like what has been done in [12], we can show that by keeping η_k constant for a number of iterations, and then switching to a decreasing sequence, we can prove the convergence of SHB to the minimizer.

Corollary H.3. Consider the setting of Theorem H.1. Let $\mathcal{K} = \frac{1}{2\eta\mu}$, $\lambda_k = \frac{1-2\eta\mathcal{L}}{\eta\mu} \left(1 - (1-\eta\mu)^k\right)$ and

$$\eta_k = \begin{cases} \eta & \text{if } k \le 4 \lceil \mathcal{K} \rceil \\ \frac{2k+1}{(k+1)^2 \mu} & \text{if } k > 4 \lceil \mathcal{K} \rceil. \end{cases}$$
(94)

If we set the parameters α_k and β_k of the SHB method (7) as in Theorem H.1 with η_k in place of η , then for $k \ge 4 \lceil \mathcal{K} \rceil$ we have that

$$\mathbb{E}\left[\mathcal{E}_{k}\right] \leq \frac{\sigma^{2}}{\mu^{2}} \frac{8}{k} + \frac{16\left[\mathcal{K}\right]^{2}}{e^{2}k^{2}} \|x_{0} - x^{*}\|^{2}.$$
(95)

In particular, if we choose $\eta = 1/2\mathcal{L}$ then $\lambda_k = \beta_k = 0$, thus the resulting method is the SGD method and Corollary H.3 recovers the exact same result as Theorem 3.2 in [12].